Circuit Simulation of All-Spin Logic

Thesis by
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In Partial Fulfillment of the Requirements
For the Degree of
Master of Science

King Abdullah University of Science and Technology
Thuwal, Kingdom of Saudi Arabia

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ABSTRACT

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Meshal Alawein

With the aggressive scaling of complementary metal-oxide semiconductor (CMOS) nearing an inevitable physical limit and its well-known power crisis, the quest for an alternative/augmenting technology that surpasses the current semiconductor electronics is needed for further technological progress. Spintronic devices emerge as prime candidates for Beyond CMOS era by utilizing the electron spin as an extra degree of freedom to decrease the power consumption and overcome the velocity limit connected with the charge. By using the nonvolatility nature of magnetization along with its direction to represent a bit of information and then manipulating it by spin-polarized currents, routes are opened for combined memory and logic. This would not have been possible without the recent discoveries in the physics of nanomagnetism such as spin-transfer torque (STT) whereby a spin-polarized current can excite magnetization dynamics through the transfer of spin angular momentum. STT have expanded the available means of switching the magnetization of magnetic layers beyond old classical techniques, promising to fulfill the need for a new generation of dense, fast, and non-volatile logic and storage devices.

All-spin logic (ASL) is among the most promising spintronic logic switches due to its low power consumption, logic-in-memory structure, and operation on pure spin currents. The device is based on a lateral nonlocal spin valve and STT switching. It utilizes two nanomagnets (whereby information is stored) that communicate with pure spin currents through a spin-coherent nonmagnetic channel. By using the well-known spin physics and the recently proposed four-component spin circuit formalism, ASL devices can be thoroughly studied and simulated. Previous attempts to model ASL in the linear and diffusive regime either neglect the dynamic characteristics of transport or do not provide a scalable and robust platform for full micromagnetic simulations and inclusion of other effects like spin Hall effect and spin-orbit torque. In this thesis, we propose an improved stochastic magnetization dynamics/time-dependent spin transport model based on a finite-difference scheme of both the temporal and spatial derivatives to capture the key features of ASL. The approach yields new finite-difference conductance matrices, which, in addition to recovering the steady-state results, captures the dynamic behavior. The new conductance matrices are general in that the discretization framework can be readily applied and extended to other spintronic devices. Also, we provide a stable algorithm that can be used to simulate a generic ASL switch using the developed model.
ACKNOWLEDGEMENT

I would like to express my gratitude to everyone I met during my journey, especially my advisor, Dr. Hossein Fariborzi, for whom I would like to express my deepest appreciation and thanks for his advice, patience, continuous support, and insightful comments.
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<tr>
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<tbody>
<tr>
<td>AFM</td>
<td>Antiferromagnet</td>
</tr>
<tr>
<td>AMR</td>
<td>Anisotropic Magnetoresistance</td>
</tr>
<tr>
<td>AP</td>
<td>Antiparallel</td>
</tr>
<tr>
<td>ASL</td>
<td>All-Spin Logic</td>
</tr>
<tr>
<td>BE</td>
<td>Backward Euler</td>
</tr>
<tr>
<td>BisFET</td>
<td>Bilayer Pseudo-Spin Field-Effect Transistor</td>
</tr>
<tr>
<td>BMR</td>
<td>Ballistic Magnetoresistance</td>
</tr>
<tr>
<td>CAD</td>
<td>Computer-Aided Design</td>
</tr>
<tr>
<td>CIP</td>
<td>Current-in-Plane</td>
</tr>
<tr>
<td>CLT</td>
<td>Central Limit Theorem</td>
</tr>
<tr>
<td>CMOS</td>
<td>Complementary Metal-Oxide Semiconductor</td>
</tr>
<tr>
<td>CNTFET</td>
<td>Carbon Nanotubes Field-Effect Transistor</td>
</tr>
<tr>
<td>CPP</td>
<td>Current-Perpendicular-to-Plane</td>
</tr>
<tr>
<td>CPU</td>
<td>Central Processing Unit</td>
</tr>
<tr>
<td>DOS</td>
<td>Density of States</td>
</tr>
<tr>
<td>DSA</td>
<td>Directed Self-Assembly</td>
</tr>
<tr>
<td>DW</td>
<td>Domain Wall</td>
</tr>
<tr>
<td>EUV</td>
<td>Extreme Ultraviolet</td>
</tr>
<tr>
<td>ExFET</td>
<td>Exciton Field-Effect Transistor</td>
</tr>
<tr>
<td>FD-SOI</td>
<td>Fully-Depleted Silicon-on-Insulator</td>
</tr>
<tr>
<td>FET</td>
<td>Field-Effect Transistor</td>
</tr>
<tr>
<td>FinFET</td>
<td>Fin Field-Effect Transistor</td>
</tr>
<tr>
<td>FM</td>
<td>Ferromagnet</td>
</tr>
<tr>
<td>GAA</td>
<td>Gate-All-Around</td>
</tr>
<tr>
<td>GMR</td>
<td>Giant Magnetoresistance</td>
</tr>
<tr>
<td>Acronym</td>
<td>Definition</td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
</tr>
<tr>
<td>IC</td>
<td>Integrated Circuit</td>
</tr>
<tr>
<td>IMOS</td>
<td>Ionization Metal-Oxide Semiconductor</td>
</tr>
<tr>
<td>ITRS</td>
<td>International Technology Roadmap for Semiconductors</td>
</tr>
<tr>
<td>KCL</td>
<td>Kirchoff’s Current Law</td>
</tr>
<tr>
<td>KVL</td>
<td>Kirchoff’s Voltage Law</td>
</tr>
<tr>
<td>LL</td>
<td>Landau-Lifshitz</td>
</tr>
<tr>
<td>LLG</td>
<td>Landau-Lifshitz-Gilbert</td>
</tr>
<tr>
<td>LLGS</td>
<td>Landau-Lifshitz-Gilbert-Slonczewski</td>
</tr>
<tr>
<td>LLSV</td>
<td>Lateral Local Spin Valve</td>
</tr>
<tr>
<td>LNLSV</td>
<td>Lateral Nonlocal Spin Valve</td>
</tr>
<tr>
<td>LSDA</td>
<td>Local Spin Density Approximation</td>
</tr>
<tr>
<td>LSV</td>
<td>Lateral Spin Valve</td>
</tr>
<tr>
<td>MEMS</td>
<td>Microelectromechanical Systems</td>
</tr>
<tr>
<td>MNA</td>
<td>Modified Nodal Analysis</td>
</tr>
<tr>
<td>MR</td>
<td>Magnetoresistance</td>
</tr>
<tr>
<td>MTJ</td>
<td>Magnetic Tunnel Junction</td>
</tr>
<tr>
<td>NEGF</td>
<td>Nonequilibrium Green’s Function</td>
</tr>
<tr>
<td>NEMS</td>
<td>Nanoelectromechanical Systems</td>
</tr>
<tr>
<td>NIL</td>
<td>Nanoinprint Lithography</td>
</tr>
<tr>
<td>NM</td>
<td>Nonmagnet</td>
</tr>
<tr>
<td>NML</td>
<td>Nanomagnet Logic</td>
</tr>
<tr>
<td>P</td>
<td>Parallel</td>
</tr>
<tr>
<td>RKKY</td>
<td>Ruderman-Kittel-Kasuya-Yosida</td>
</tr>
<tr>
<td>RMS</td>
<td>Root-Mean-Square</td>
</tr>
<tr>
<td>RTD</td>
<td>Resonant Tunneling Diode</td>
</tr>
<tr>
<td>SD</td>
<td>Source-Drain</td>
</tr>
<tr>
<td>SDDE</td>
<td>Spin Drift-Diffusion Equation</td>
</tr>
<tr>
<td>SET</td>
<td>Single Electron Transistor</td>
</tr>
<tr>
<td>SHE</td>
<td>Spin Hall Effect</td>
</tr>
<tr>
<td>sLLG</td>
<td>Stochastic Landau-Lifshitz-Gilbert</td>
</tr>
<tr>
<td>sLLGS</td>
<td>Stochastic Landau-Lifshitz-Gilbert-Slonczewski</td>
</tr>
<tr>
<td>SO</td>
<td>Spin-Orbit</td>
</tr>
<tr>
<td>SOI</td>
<td>Spin-Orbit Interaction</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>-----------------------------------</td>
</tr>
<tr>
<td>SOT</td>
<td>Spin-Orbit Torque</td>
</tr>
<tr>
<td>spinFET</td>
<td>Spin Field-Effect Transistor</td>
</tr>
<tr>
<td>SS</td>
<td>Subthreshold Slope</td>
</tr>
<tr>
<td>STT</td>
<td>Spin-Transfer Torque</td>
</tr>
<tr>
<td>SV</td>
<td>Spin Valve</td>
</tr>
<tr>
<td>SW</td>
<td>Stoner-Wohlfarth</td>
</tr>
<tr>
<td>TFET</td>
<td>Tunneling Field-Effect Transistor</td>
</tr>
<tr>
<td>TMR</td>
<td>Tunnel Magnetoresistance</td>
</tr>
<tr>
<td>TR</td>
<td>Trapezoidal Rule</td>
</tr>
</tbody>
</table>
LIST OF SYMBOLS

A  Magnetic Vector Potential  \( V \cdot s \cdot m^{-1} \)
B  Magnetic Flux Density  \( \text{Wb} \cdot m^{-2} \)
C  Electrostatic Capacitance  \( F \)
\( C_q \)  Quantum Capacitance  \( F \cdot m^{-3} \)
\( \chi_c \)  Charge Compressibility Factor  \( J^{-1} \cdot m^{-3} \)
D  Electric Flux Density  \( C \cdot m^{-2} \)
\( D \)  Diffusion Coefficient  \( m^2 \cdot s^{-1} \)
E  Electric Field Intensity  \( V \cdot m^{-1} \)
\( E_F, \mu \)  Fermi Energy  \( J \)
\( f_F \)  Fermi-Dirac Distribution  \( - \)
g  Density of States  \( J^{-1} \cdot m^{-3} \)
\( G_L \)  Landau-Gibbs Free Energy  \( J \)
\( G_\sigma \)  Spin-Dependent Conductance  \( S \)
\( G_{\sigma,-\sigma} \)  Spin-Mixing Conductance  \( S \)
H  Magnetic Field Intensity  \( A \cdot m^{-1} \)
I  Electric/Total Current  \( A \)
\( I_m \)  Magnetic Current  \( V \)
\( I_C \)  Charge Current  \( A \)
\( I_S \)  Spin Current  \( A \)
J  Electric/Total Current Density  \( A \cdot m^{-2} \)
\( J_m \)  Magnetic Current Density  \( V \cdot m^{-2} \)
\( J_C \)  Charge Current Density  \( A \cdot m^{-2} \)
\( J_S \)  Spin Current Density  \( A \cdot m^{-2} \)
\( K_n \)  Knudsen Number  \( - \)
\( K_{eff} \)  Effective Anisotropy Constant  \( J \cdot m^{-3} \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tbody>
<tr>
<td>$l_{sf}$</td>
<td>Spin-Diffusion Length</td>
<td>m</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Mean-Free Path</td>
<td>m</td>
</tr>
<tr>
<td>$\lambda_{sf}$</td>
<td>Spin-Flip Mean-Free Path</td>
<td>m</td>
</tr>
<tr>
<td>$\lambda_t$</td>
<td>Total Mean-Free Path</td>
<td>m</td>
</tr>
<tr>
<td>$\lambda_F$</td>
<td>Fermi Wavelength</td>
<td>m</td>
</tr>
<tr>
<td>$m$</td>
<td>Magnetic Moment</td>
<td>A · m²</td>
</tr>
<tr>
<td>$M$</td>
<td>Magnetization</td>
<td>A · m⁻¹</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Mobility</td>
<td>m² · V⁻¹ · s⁻¹</td>
</tr>
<tr>
<td>$\bar{\mu}$</td>
<td>Electrochemical Potential</td>
<td>J</td>
</tr>
<tr>
<td>$n$</td>
<td>Particle Concentration</td>
<td>m⁻³</td>
</tr>
<tr>
<td>$N$</td>
<td>Total Number of Particles</td>
<td>–</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Resistivity</td>
<td>Ω · m</td>
</tr>
<tr>
<td>$\rho_v$</td>
<td>Volume Electric Charge Density</td>
<td>C · m⁻³</td>
</tr>
<tr>
<td>$\rho_{mv}$</td>
<td>Volume Magnetic Charge Density</td>
<td>Wb · m⁻³</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Electric Flux</td>
<td>C</td>
</tr>
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<td>$\psi_m$</td>
<td>Magnetic Flux</td>
<td>Wb</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Conductivity</td>
<td>S · m⁻¹</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Mean-Free Time</td>
<td>s</td>
</tr>
<tr>
<td>$\tau_{sf}$</td>
<td>Spin-Diffusion Time</td>
<td>s</td>
</tr>
<tr>
<td>$\tau_t$</td>
<td>Transit Time by Diffusion</td>
<td>s</td>
</tr>
<tr>
<td>$\tau_{sw}$</td>
<td>Switching Time</td>
<td>s</td>
</tr>
<tr>
<td>$\tau_d$</td>
<td>Dielectric Relaxation Time</td>
<td>s</td>
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<tr>
<td>$\tau_m$</td>
<td>Magnetic Torque</td>
<td>N · m</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>K</td>
</tr>
<tr>
<td>$T_F$</td>
<td>Fermi Temperature</td>
<td>K</td>
</tr>
<tr>
<td>$V$</td>
<td>Electric/Total Voltage</td>
<td>V</td>
</tr>
<tr>
<td>$V_m$</td>
<td>Magnetic Voltage</td>
<td>A</td>
</tr>
<tr>
<td>$V_C$</td>
<td>Charge Voltage</td>
<td>V</td>
</tr>
<tr>
<td>$V_S$</td>
<td>Spin Voltage</td>
<td>V</td>
</tr>
<tr>
<td>$v$</td>
<td>Velocity</td>
<td>m · s⁻¹</td>
</tr>
<tr>
<td>$v_F$</td>
<td>Fermi Velocity</td>
<td>m · s⁻¹</td>
</tr>
<tr>
<td>$W$</td>
<td>Electric Work</td>
<td>J</td>
</tr>
<tr>
<td>$W_m$</td>
<td>Magnetic Work</td>
<td>J</td>
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</table>
# LIST OF PHYSICAL CONSTANTS

<table>
<thead>
<tr>
<th>Physical Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed of Light</td>
<td>( c = 2.997 \times 10^8 \text{ m/s} )</td>
</tr>
<tr>
<td>Permeability of Vacuum</td>
<td>( \mu_0 = 1.256 \times 10^{-6} \text{ N/A}^2 )</td>
</tr>
<tr>
<td>Permittivity of Vacuum</td>
<td>( \varepsilon_0 \equiv \frac{1}{\mu_0 c^2} = 8.854 \times 10^{-12} \text{ F/m} )</td>
</tr>
<tr>
<td>Planck Constant</td>
<td>( h = 6.626 \times 10^{-34} \text{ J/s} )</td>
</tr>
<tr>
<td>Reduced Planck Constant</td>
<td>( \hbar = h/2\pi = 1.054 \times 10^{-34} \text{ J/s} )</td>
</tr>
<tr>
<td>Boltzmann Constant</td>
<td>( k_B = 1.380 \times 10^{-23} \text{ J/K} )</td>
</tr>
<tr>
<td>Electron Charge Magnitude</td>
<td>( e = 1.602 \times 10^{-19} \text{ C} )</td>
</tr>
<tr>
<td>Electron Mass</td>
<td>( m_e = 9.109 \times 10^{-31} \text{ kg} )</td>
</tr>
<tr>
<td>Proton Mass</td>
<td>( m_p = 1.167 \times 10^{-27} \text{ kg} )</td>
</tr>
<tr>
<td>Bohr Magneton</td>
<td>( \mu_B \equiv \frac{e}{2m_e} = 9.274 \times 10^{-24} \text{ J/T} )</td>
</tr>
<tr>
<td>Nuclear Magneton</td>
<td>( \mu_N \equiv \frac{e}{2m_p} = 5.050 \times 10^{-27} \text{ J/T} )</td>
</tr>
<tr>
<td>Orbital Gyromagnetic Ratio</td>
<td>( \gamma_L \equiv -g_L\mu_B/h = -8.794 \times 10^{10} \text{ rad/s/T} )</td>
</tr>
<tr>
<td>Spin Gyromagnetic Ratio</td>
<td>( \gamma_S \equiv -g_S\mu_B/h \approx -1.758 \times 10^{11} \text{ rad/s/T} )</td>
</tr>
<tr>
<td>Fine-Structure Constant</td>
<td>( \alpha \equiv \frac{e^2}{4\pi\varepsilon_0 hc} = 7.297 \times 10^{-3} )</td>
</tr>
<tr>
<td>Conductance Quantum</td>
<td>( G_0 \equiv 2e^2/h = 7.748 \times 10^{-5} \text{ S} )</td>
</tr>
<tr>
<td>Magnetic Flux Quantum</td>
<td>( \phi_0 \equiv \hbar/2e = 2.067 \times 10^{-15} \text{ Wb} )</td>
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Chapter 1

Introduction

1.1 Motivation

1.1.1 Post-CMOS Era

The successful scaling of planar complementary metal-oxide semiconductor (CMOS) over the last five decades at an exponential pace in what is commonly known as Moore’s law [1] is astonishing. Driven by the power of human invention and high demand of the market, the scaling sustained and has spanned more than two orders of magnitude in both feature size and speed and has made CMOS the technology of choice for memory and logic. With the ever-increasing volume of information, the shrinking continues in the deep nanometer regime and has now reached the 14 nm node [2].

Although Moore’s law has a habit of defying the skeptics, the law is undoubtedly experiencing asperities and is running out of steam as CMOS is approaching an inevitable physical (atomistic) limit. In fact, even if we can push the physics further, other serious challenges accompany scaled transistors. For example, we expect scaled transistors to provide us with higher performance, lower power, and lower cost per function, but the benefits of scaling have been decreasing for some time whereas the cost has been rising [4, 5]. In fact, the clock frequencies of high-end chips have plateaued around 2005. CMOS, in general, is confronted by the intractable physics of thermionic emission and resulting source-drain (SD) subthreshold leakage that limits the scaling of the supply voltage. The steady increase in power density in recent years lowered the energy-efficiency and heat-dissipation capabilities of the integrated circuit (IC) chips.

\footnote{The number of people predicting the death of Moore’s law doubles every two years”, jokes Peter Lee, a vice-president at Microsoft Research.}
Moore’s Law Defined

Figure 1.1: Moore’s law, which states that computer power doubles every two years at the same cost. The figure represents the number of transistors in a central processing unit (CPU) manufactured by Intel [3].

As a result, CMOS is facing a “power crisis”, a fact believed to be the main roadblock for further downscaling. These and other issues such as material/performance-related (gate stack reliability, interconnects delay, channel mobility degradation), economical (high cost of production and testing), and fabrication (lithography, device variability) might limit the miniaturization and scalability of next generations of CMOS devices, as identified by the International Technology Roadmap for Semiconductors (ITRS) [6].

Although novel transistor structures (FD-SOI, FinFET, GAA), dopant and material engineering (SiGe, III-V), and lithography techniques (EUV, multi-patterning) can extend CMOS for a longer period in what is known as “Extending CMOS” [2], there is no guarantee that Moore’s law will not hit a brick wall. It is apparent that we also need new frontier devices that are, preferably, compatible with the current semiconductor chips. Novel “Beyond CMOS” device proposals targeted toward revolutionizing the current semiconductor technology have been extensively addressed recently, and there are serious attempts to reinvent the transistor [4]. In fact, “Beyond CMOS” have been added by the ITRS committee to the list of seven focus topics announced in 2014. The list consists of both charge- and noncharge-based devices. Some of these devices are shown in Fig. 1.2.

For example, chip manufacturers have plans for a new 10 nm process (likely to be realized by multiple patterning) and also 7 nm (that may require 3D packaging). In fact, Intel [3] claims that it can sustain Moore’s law for another ten years, aiming to reach 5 nm, a size that is about the thickness of a cell membrane.
A radical approach to tackle the intractable physics of CMOS is to replace the entire charge-based architecture with one based on a noncharge state variable. Spintronics (or spin-based electronics) [8–11] are one of the most promising candidates for Beyond CMOS technologies to sustain the advancements of Moore’s law. Those are devices that enable the control of a noncharge computational state variable, namely the intrinsic electron spin. The extra degree of freedom in electron, just like the charge, is of binary nature (e.g., “1” = spin up, “0” = spin down, see Fig. 1.3) and thus can carry and process magnetic information in a digital manner and hence function for logic and memory with the extra advantage of being nonvolatile. In addition, using spin, one can overcome the limitations of the velocity of charge and also reduce the energy consumption [8, 12]. In fact, it has been shown that at room temperature one can switch the spins in a nanomagnet with an energy as low as $40k_BT \approx 0.17 \text{ aJ}$, where $k_B$ is Boltzmann constant [13]. Thus, in addition to providing zero stand-by power (due to nonvolatility), spintronic devices also consume low switching energies. Such properties have greater and farther-reaching implications as it coincides with the current trend of normally-off and instant-on computing for hopefully a greener world. Moreover, spintronic devices contribute toward long-term prospects in applications to quantum information processing and quantum cryptography [12, 14, 15]. Hence, by exploiting the esoteric quantum features of electrons, spintronics offers an unprecedented opportunity for further technological progress.
Figure 1.3: In spintronics, information is stored in the alignment of spins. The quantum mechanically “digitized” angular momentum allows the spin to be viewed as a binary entity. For example, if (a) up-spin electron can be considered “1”, then (b) down-spin electron is considered “0”.

1.1.2 Novel Switching Mechanisms

The concept of magnetic devices for information processing and storage is widely used, with the latter typically done through the use of the material anisotropy (e.g., magnetocrystalline anisotropy) for data retention. The method by which the magnetization direction of a magnetic layer is reversed has been through the use of applied fields, e.g. by passing dc currents through (usually mutually perpendicular) small coils or wires to generate Oersted fields that will reorient the magnetization through a torque $\tau_m = m \times B$, driving the magnetic potential energy into its lowest configuration [16]. Though simple, this concept is still (though decreasingly) being used in some of today’s applications such as in the read-write heads used in hard drives, in addition to some of the conventional nonvolatile magnetic random access memories (MRAMs) which are known for their high speed, low power consumption, immunity to radiation, and nearly infinite endurance [17–21]. In such memories, the switching (writing) mechanism, “0” and “1” separation, and unselected bits disturbance are all key considerations in the design [23]. The first is of prominent importance as problems arises with shrinking of technology. The stray fields that surround wires decay slowly in space, and hence can limit storage density and result in magnetic-bits-coupling problems in which a magnetic bit experiences magnetic fields from neighboring wires [15, 24]. Moreover, the stray fields depend on the geometrical shape of the cell [25], and the current used in these wires increases as the demagnetizing field increases, and the latter is inversely proportional to the bit size (magnetic device volume), which implies that higher currents are needed for smaller bits, and this brings about write-energy and scalability problems [15, 16, 18, 23, 25, 26]. This is also true when considering the magnetic element coercivity that must be increased as the cell shrinks to

\[3\] The first prototype of a magnetic memory using such a switching mechanism used a cross-point architecture and achieved speeds of few nanoseconds where, interestingly, the limitations were due to the CMOS itself [22].
prevent erroneous thermal reversal, which consequently result in higher currents [15, 16]. All of these issues have been major hurdles in the commercialization of MRAMs and brings questions about its potential to function as a future universal memory.

Given the issues of switching with applied fields, and in conjunction with the recent interest of the magnetoelectronic community in current-induced switching of magnetic elements by local application of electric currents [12, 26–29], recent discoveries in the physics of nanomagnetism, such as spin-transfer torque (STT) [30, 31], have expanded the known methods of switching the magnetization of magnetic layers beyond the old classical techniques. It has been found that in multilayer thin films a spin-polarized current injected from a nonmagnet (NM) into a ferromagnet (FM) can interact with the local magnetization in the FM and induce magnetization precession, which, for large enough currents, can overcome the intrinsic layer damping and induce a total magnetization reversal [21, 30–32]. STT can fulfill the need for new generations of dense, fast, and nonvolatile information processing/storage devices, and is more power efficient than classical switching methods [17, 21]. In fact, since it has been found that switching currents merely depends on the energy barrier between “1” and “0” states, once a threshold current density meets the criteria at one feature size, the required switching current will scale down with smaller nodes [16]. Also, with STT one can make devices with no moving mechanical parts as opposed to hard-disk drives [16]. Furthermore, devices based on STT can be CMOS compatible, especially those based on tunnel junctions since they can be impedance-matched and thus easily integrated and augmented with the current IC chips, permitting the ultimate miniaturization of MRAMs and logic devices [16, 21]. In fact, the applications of STT are not limited to only logic and memory but extend even to designing oscillators, detectors, mixers, and phase shifters [21, 29] as STT can excite long-term oscillations of a nanomagnet [33–35]. The research in this field is ongoing, and recent demonstrations clearly show the potential of STT to deliver a new generation of switching devices.

### 1.2 All-Spin Logic (ASL)

The success of planar CMOS has naturally triggered extensive research on spintronic structures that resembles the field-effect transistor (FET). Namely, lateral structures made up of conducting channels and at least two terminals that act as the source and drain of carriers. Fig. 1.4 shows two examples of such devices. Fig. 1.4a shows a lateral local spin valve (LLSV) that switches due to the locally injected spin currents, whereas Fig. 1.4b shows a lateral nonlocal spin valve (LNLSV) that switches due to the nonlocally injected spin currents [36–42]. Although both devices work on the principles
of STT switching, the nonlocal device is rather preferred. This is because the LNLSV decouples charge from spin, generating pure spin currents. This is advantageous because it eliminates the spurious effects accompanying spin-polarized (and pure charge) currents [37, 43].

![Figure 1.4](image1.png)

**Figure 1.4:** Schematics showing the difference between local and nonlocal spin-transfer torque (STT) in a lateral spin valve (LSV). (a) Local STT. (b) Nonlocal STT.

Among the most promising spintronic logic switches is a device called all-spin logic (ASL) [44–46] that is based on a LNLSV structure with isolations between the input and output sides (Fig. 1.5). The device has recently attracted increasing interest due to its low power operation and logic-in-memory structure. In addition, the device utilizes pure spin currents throughout every stage of its operation, eliminating the need for repeated spin-to-charge conversion and thus any extra hardware [44, 46]. This is in contrast to most spintronic logic switches which uses spins internally but have logic gates with charge-based terminals [44]. The latter property has also the extra advantage of eliminating the spurious effects accompanying charge currents.

![Figure 1.5](image2.png)

**Figure 1.5:** A generic all-spin logic (ASL) switch is made up of two ferromagnets (FM), a nonmagnetic (NM) channel, contacts, and two spacers.

---

4Less voltage operation also means less parasitic capacitance and stray charge [47]. Moreover, non-volatility ideally implies zero stand-by power.
1.3 Contribution of This Work

To assess the feasibility of ASL as a new generation switch, equivalent circuit modeling is important for rapid computer-aided design (CAD) and verification. Previous successful attempts have been made to model ASL with circuit components, and most fall into one of two categories:

1. Self-consistently solving the magnetization dynamics (governed by the Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation) and the spin transport model (governed by the steady-state spin drift-diffusion equation (SDDE) represented in the four-component spin circuit formalism), as in [45, 47–57].

2. Simulations solely based on circuit models of the LLGS and the time-dependent SDDE for implementation in SPICE and similar software as performed in [58].

As pointed out in [47, 52], the framework of simultaneously solving the magnetization dynamics and the steady-state spin transport (Fig. 1.6) is accurate as long as the transit time of carrier diffusion in the transport section is much shorter than the dynamics of the nanomagnets, i.e. for \( \tau_t \ll \tau_{sw} \), where the transit time by diffusion can be estimated as \( \tau_t = L^2/2D \), with \( L \) being the section length and \( D \) the diffusion coefficient. Although this condition holds sufficiently well for metals of a few 100’s of nm [59], these times might become comparable as we advance in technology where magnetization switching becomes faster and/or in the case of moderately long channel devices. In fact, we are not restricted to all-metallic structures and might use semiconducting channels, which, in addition to modifying the diffusion coefficient, brings up the advantage of longer spin-diffusion lengths. Moreover, parasitics can be present in the transport section due to different reasons, and the effects of energy storing elements have to be taken into account. In any of the previous scenarios, a dynamical description of carrier transport is necessary. Although the second model provides the necessary tools to capture the dynamics in the transport section, it lacks the freedom provided by the first model and the ability to program in common languages as it was meant for SPICE implementation. In addition, it assumes a macrospin magnet, and thus neglects any spatial variations in magnetization. It might also be difficult to augment or modify to include other interesting phenomena like spin Hall effect (SHE) and spin-orbit torque (SOT). These considerations suggest an extension of the currently available models.

Starting from the theory introduced throughout the thesis, and based on the four-component spin circuit formalism, we present our improved stochastic magnetization
dynamics/time-dependent spin transport model based on new finite-difference conductance matrices which can capture both the dissipative and dynamic behavior of spins in the channel of spintronic devices in general, and ASL in particular.

In short, our contribution in this thesis is two fold:

- We propose an enhanced magnetization dynamics/spin transport model that can capture any introduced dynamics in the transport section, and present new finite-difference conductance matrices.

- Provide a simple, stable, and robust algorithm to obtain the magnetization trajectories from the stochastically perturbed dynamic equations that are coupled to the spin circuit model.

Our work follows in the spirit of [47, 48, 60], but using our model and algorithm. Throughout the thesis, we describe the principles in details and present the full derivations for most of the results (with some twists, modifications, and additions) in the hopes that it will be a useful startup material for newcomers and a reference for researchers.
1.4 Outline of the Thesis

Below, we give a brief outline of the thesis and its organization:

Chapter 2 provides a minimal theoretical background for understanding the operation of spintronics devices. Moreover, in this chapter we describe the statics and dynamics of nanomagnets in some detail. We also analyze the stochastic effects and present a simple numerical scheme to obtain the magnetization trajectories from the stochastically perturbed dynamic equations in the presence of spin-polarized currents.

Chapter 3 introduces the recently proposed four-component spin circuit theory used in analyzing spintronic devices. In particular, we introduce the basics of magnetoelectronics, charge and spin transport, and the extension of circuit theory and its various techniques (e.g. modified nodal analysis) to spin space.

Chapter 4 presents ASL, our finite-difference scheme-based spin circuit model, the algorithm developed, and the numerical simulations. This chapter is based heavily on the stochastic magnetization dynamic equations (from Chapter 2) and spin circuit theory (from Chapter 3).

Chapter 5 gives a brief summary and outlook on future work.
Chapter 2

Nanomagnetism and Spintronics

In this chapter, we heuristically introduce the basic concepts of spintronics and follow that with a more detailed and rigor treatment of nanomagnetism. In particular, after introducing spintronics, we review magnetostatics, and talk about domains, domain walls, and present the typical length scales involved in the description of magnetic behavior. We then delve into the description of the static character of a ferromagnet by formally presenting the definitions and postulates of micromagnetism along with the boundary conditions and energy terms involved. We then describe the deterministic dynamics of magnetization starting from the Landau-Lifshitz (LL) equation, and present the mathematically equivalent Landau-Lifshitz-Gilbert equation (LLG) equation, which is usually the preferred form for large damping. Following that, we include the spin-transfer torque (STT) term in the dynamics, which is of utmost importance in our modeling of ASL and current-induced switching in general. The introduction of STT leads to a generalization of the LLG equation to the so-called Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation. We conclude this chapter with a brief discussion about the stochastic LLG (sLLG) and stochastic LLGS (sLLGS) equations and present a simple and stable numerical scheme to solve such equations.
2.1 Concepts in Spintronics

Below we give a heuristic introduction to the essential concepts of spintronics. We try to be qualitative for the most part and leave the quantitative treatment for the (more relevant) description of magnetization dynamics later.

2.1.1 Ferromagnets and Spin Polarization

In contrast to mainstream electronics which exploit charge only, spintronic devices utilize both charge and spin [8, 9]. Spin, being a fundamental property of electrons (in addition to mass and charge), is defined as the intrinsic angular momentum [15]. It is intimately related to magnetism, and therefore, magnetism is inherently quantum mechanical in nature. In conventional electronic circuits, an electric current is unpolarized and consists of an equal number of up- and down-spin electrons, and thus spin has been ignored in these circuits [21, 63]. However, when ferromagnets (FMs) are incorporated, spins can polarize along a certain direction, allowing information to be stored in the system and for magnetism to affect electrical transport (and vice versa) [21, 64, 65]. Typically, FMs such as the itinerant “delocalized” electron systems: Fe, Co, and Ni are usually what we mean when we talk about the magnetic behavior (Fig. 2.1). FMs in general are characterized by a spontaneous magnetization and a very strong attraction to magnetic fields, in contrast to paramagnets (weak attraction) and diamagnets (weak repulsion) [66, 67].

Figure 2.1: The periodic table of chemical elements. The elements in red are the 3d transition metal ferromagnets (FMs).

1: “Electron spin” is in fact a misnomer. Although it could be useful to think of an electron as a spinning sphere, this classical picture bears no resemblance to reality [61] (see [62] for an interesting argument).
The magnetism of FMs originates almost always from the spin angular momentum of electrons.² The ferromagnetic order arises from the electron-electron interaction. In particular, from the interplay between exchange interaction (which favors parallel spins) and Pauli exclusion principle (which states that no identical fermions may occupy the same quantum state simultaneously) [14, 15, 21, 61, 69–71]. When metal atoms condense to form a bulk metal, the electronic energy levels from atoms combine to form bands of finite energy width [61, 72]. The result is that, the electronic distribution, called density of states (DOS), changes. Exchange interaction [73], which is a purely quantum effect, will force all uncompensated spins to align parallel to lower the system energy. However, since the kinetic energy cost (which increases with the principal and orbital quantum numbers) to maintain the atomic magnetic moment with spins aligned on each atom increases,³ at some point the spin angular momentum will be traded for kinetic energy [21]. According to the free-electron Stoner model of itinerant ferromagnetism, electron bands can be spontaneously split into up and down spins if the relative gain in exchange interaction is larger than the loss in kinetic energy (Fig. 2.2) [14, 69, 74]. The model is typically formulated in terms of the spin-dependent dispersion relations [75]

\[ E_{\uparrow}(k) = E(k) - I \frac{n_{\uparrow}}{n_{\uparrow} + n_{\downarrow}} \]  

\[ E_{\downarrow}(k) = E(k) + I \frac{n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}} \]  

where \( E(k) \) is the dispersion relation of spinless electrons without exchange interaction, \( E_{\uparrow,\downarrow}(k) \) the spin-dependent dispersion relation, and \( n_{\uparrow,\downarrow} \) the spin-dependent electron occupation. The second term in both equations accounts for exchange energy through the Stoner parameter \( I \). When the formulas above are summed over the whole \( k \)-space, the Stoner criterion results, viz. [75, 76]

\[ \bar{g}(E_F) I > 1 \]  

where \( \bar{g}(E_F) \) is the density of states at the Fermi level per atom per spin [75]. This criterion has to be fulfilled for the ferromagnetic order to arise in a solid.⁴

²The orbital angular momentum of electrons of course also contributes to the magnetic moment (as will be shown later in 2.2.1) [15, 21]. However, the orbital momenta for transition metals are usually “quenched” (≈ 0.1\( \mu_B \)) by the large hybridization of the \( d \) electrons which might also include the effect of the crystal electric field due to charge environment (where the crystal field energy \( \approx 10^8 \text{ cm}^{-1} \gg \) spin-orbit coupling \( \approx 10^6 \text{ cm}^{-1} \)) and thus neglected [14, 15, 21, 68]. This is usually not the case for rare earths (lanthanides) in which spin-orbit interaction is stronger (≈ 10³ cm⁻¹) than the crystal field energy (≈ 10² cm⁻¹), a fact usually attributed to the deep-buried 4f shell which result in a shielding of the crystal field by the filled 5p and partially-filled 5d and 6s outer orbitals [68].

³Keeping many electrons with the same spin (but different states) implies that they must have different principal and orbital quantum numbers to satisfy Pauli’s principle, resulting in an increase in the kinetic energy.

⁴The Stoner model essentially states that a FM order arises from the spontaneously spin-split bands caused by exchange interaction. Although this simplified model has been verified for transition metal
In general, and depending on the FM material, a mismatch in population between minority and majority spins occur where one type is excess in number. In this case, \( n_\uparrow \neq n_\downarrow \), and a net spin polarization results, i.e. a nonzero \( P = (n_\uparrow - n_\downarrow) / (n_\uparrow + n_\downarrow) \) \([65, 69]\). Within the framework introduced above, the magnetization can be computed as \([77]\)

\[
M = \mu_B \int_0^\infty [g_\downarrow (E) - g_\uparrow (E)] f_F (E) \, dE
\]

(2.4)

where \( \mu_B \) is Bohr’s magneton and \( f_F (E) \) is the Fermi-Dirac distribution.

### 2.1.2 Spin Current

As mentioned above, electrons possess spin (intrinsic angular momentum) in addition to mass and charge. In analogy to the charge current, we formally define the spin current as the flow of angular momentum \([15, 16]\). In particular, if \( J_\uparrow \) and \( J_\downarrow \) are the current densities of up- and down-spin electrons,\(^5\) then the charge and spin current densities are

\(^5\)Up and down with respect to a specific spin quantization axis \([15, 62]\).
defined as\textsuperscript{6,7} [71, 78, 79]

\[ J_C = J_T + J_\parallel \] \quad (2.7)
\[ J_S = J_T - J_\parallel \] \quad (2.8)

Given the above equations, three types of currents can result:

- **Pure Charge Current**: \( J_C \neq 0 \) and \( J_S = 0 \).
- **Pure Spin Current**: \( J_C = 0 \) and \( J_S \neq 0 \).
- **Spin-Polarized Current**: \( J_C \neq 0 \) and \( J_S \neq 0 \).

The first two are illustrated in Fig. 2.3.

Interestingly, and in contrast to charge currents, spin currents behave in some unusual (and counter intuitive) ways. For example, a current will pass more easily if electron spins line up with, rather than opposite to, the magnetization of a FM. This is what happens in a process called *spin filtering* at a NM/FM interface, whereby a FM transmits electrons of different spin orientations at different rates (roughly shown in Fig. 2.4) [15, 21, 75, 80]. This occurs because near a NM/FM interface, the potential experienced by the electrons changes and becomes spin dependent and inside the FM the spin-split DOS causes a spin-dependent transmission and reflection [21, 75]. This process is ultimately governed by the \( s\text{-}d\text{ exchange interaction between the magnetic moments of the magnetization and the conduction electrons} [80]. The electrons that passes easily are usually called “majority”, and the electrons that scatter are called “minority”.\textsuperscript{8}

Conduction in FMs therefore depends on the magnetization orientation in addition to the bulk properties [71].

\textsuperscript{6}In this section we neglect any noncollinear components in spins/magnetizations and assume spins to be collinear to magnetization (except for the discussion regarding spin-transfer torque). The general formalism will be given in Chapter 3.

\textsuperscript{7}In general, for a single electron, the charge current density is the vector given by \( J_C = q \frac{\hbar}{m} \text{Im} (\psi^\dagger \nabla \psi) \) [77], which has to satisfy the following conservation law

\[ \oint \oint J_C \cdot dS = - \iiint_{\Omega} \frac{\partial \rho}{\partial t} dV \] \quad (2.5)

where \( \rho = q \psi^\dagger \psi \) is the charge density. The spin current density, on the other hand, is a tensor (in particular, a second-order pseudo-tensor); a quantity with both a direction of charge flow and a direction of spin polarization [71]. The spin current density is given by the outer product \( J_S = v \otimes s = \frac{\hbar}{2m} \text{Im} (\psi^\dagger \mathbf{\sigma} \otimes \nabla \psi) \) [21, 77], where \( v \) is the average electron velocity, \( s = \frac{\hbar}{2m} \mathbf{\sigma} \), and \( \mathbf{\sigma} \) the Pauli spin vector. An element \( J_{ij} \) refers to the component of the spin current flowing in the \( i \)-th direction with a spin polarization along the \( j \)-th direction. If no torques are applied, the spin current satisfies the conservation equation [77]

\[ \oint \oint J_S \cdot dS = - \iiint_{\Omega} \frac{\partial S}{\partial t} dV \] \quad (2.6)

where \( S = \frac{\hbar}{2} \psi^\dagger \mathbf{\sigma} \psi \) is the spin density.

\textsuperscript{8}Some authors [79] define the majority spin as the spin species of the larger electronic density, and the one with the smaller electronic density as the minority spin.
Figure 2.3: Illustration of pure charge and spin currents. (a) Charge and spin as two degrees of freedom. (b) Up- and down-spin electrons of equal amount cancel in spin when moving in the same direction, effectively creating a pure charge current. (c) Up- and down-spin electrons of equal amount cancel in charge when moving in opposite directions, effectively creating a pure spin current.

NM metals, on the other hand, have an equal number of electrons with up and down spins and their conduction is thus merely determined by the bulk properties (with a resistance possibly disordered on a microscopic scale) [65]. Moreover, because of spin relaxation processes, spin currents cannot transmit for long distances\(^9\) (whether in FMs or NMs) as opposed to charge currents [15, 64]. This essentially means that spin is not a conserved quantity (again, in contrast to charge) [15, 65, 84]. Despite these disadvantages, spin have the advantages over charge in that it requires less energy to process and is faster to manipulate. In addition, not only can a spin exist in the classical “0” and “1” states, it can also be in a coherent superposition of both, forming the so-called quantum bit (qubit) [62]. This allows for combinatorial calculations, something that cannot be performed with normal computers. A rough comparison between charge and spin is shown in Table 2.1.

Spin currents can be generated from nonequilibrium spin states, i.e., spin accumulation and spin dynamics. For example, by temperature gradient (spin Seebeck effect) [85], sound waves (acoustic spin pumping) [86–88], optical orientation [89], mechanical

\(^9\)Longer than the spin-flip mean-free path \(\lambda_{sf}\), which is the mean distance between spin-flipping collisions [65, 81]. However, due to scattering events, the length over which an electron travels with fixed spin orientation is typically smaller than \(\lambda_{sf}\), and one usually uses a different length scale. The alternative length scale is the spin-diffusion length \(l_{sf}\), defined as the length over which an electron “diffuses” before losing its spin memory due to spin-flipping collisions [14, 21, 64, 65, 71, 82]. If one defines the mean-free path \(\lambda = v_F \tau\) and the spin-flip mean-free path \(\lambda_{sf} = v_F \tau_{sf}\), then the spin-diffusion length is given by the the geometric mean \(l_{sf} = \sqrt{\lambda \lambda_{sf}}\) [76, 83]. If, instead of \(\lambda\) (related to momentum exchange), we used the total mean-free path \(\lambda_t = v_F \tau_t\) (related to collision of all kinds whether spin conserving or not), then \(l_{sf} = \sqrt{(1/3) \lambda_t \lambda_{sf}}\) [81]. In general, \(l_{sf}\) follows a diffusion equation, can be written in terms of the diffusion constant \(D_{sf}\), and obeys (most of the time) the inequality \(\lambda_F < \lambda_t < l_{sf} < \lambda_{sf}\) [65, 81].
Table 2.1: Comparison between charge and spin.

<table>
<thead>
<tr>
<th></th>
<th>Charge</th>
<th>Spin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conserved</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Transmission Distance</td>
<td>Long</td>
<td>Short</td>
</tr>
<tr>
<td>Power Dissipation</td>
<td>High</td>
<td>Low or None (debatable)</td>
</tr>
<tr>
<td>Processing Speed</td>
<td>Fast</td>
<td>Faster</td>
</tr>
<tr>
<td>Processing Energy</td>
<td>Low</td>
<td>Lower</td>
</tr>
</tbody>
</table>

motion [90–93], spin Hall effect (SHE) [94, 95],\(^{10}\) or by spin injection through a FM/NM interface [36, 37, 43, 99–102]; the latter being the mostly used method [15, 64].

Figure 2.4: Nearly-perfect spin filtering process at a FM/NM interface. Here, most up-spin electrons are scattered (minority), whereas most down-spin electrons pass easily (majority). Ideally, a perfect spin-filter would pass all spins that are parallel to the magnetization and reflect all spins that are antiparallel [80]. Figure adapted by the author from [15].

We note that, for the spin-polarization to be well defined so that we can think of a current as being polarized in $\uparrow$ or $\downarrow$ direction, we must have $\lambda \ll l_{sf}$ [65, 76].\(^{11}\) Usually $\lambda$, which characterizes the scattering processes that relaxes the momentum (determining the resistivity), is usually very small, implying frequent collisions. This, however, does not mean that frequent collisions causes the electron to lose its spin memory, since spin-flipping can only occur through exchange interaction or spin-orbit coupling with impurities and defects [10, 69].

\(^{10}\)Whether extrinsic (due to spin-orbit scattering by impurities or the host lattice) [96, 97] or intrinsic (due to the direct spin-orbit coupling on the underlying band structure—i.e. can appear even for “clean” systems where impurities are absent—) [98].

\(^{11}\)This is because in a mean distance $\lambda$, we would like the spin to be conserved in a time $\tau$. See footnote 9 for some definitions of the characteristic lengths.
2.1.3 Spin-Dependent Transport: The Two-Current Model

The simplest formula for the electrical conductivity is given by Drude’s formula [14, 61, 65]

\[ \sigma = \frac{e^2 n \tau}{m_e^*} \]  

(2.9)

where \( e \) is the electron charge, \( n \) the electron number density, \( \tau \) the elastic scattering time, and \( m_e^* \) the effective mass of the band. Within the framework of Drude’s transport theory, the concept of the Fermi surface plays a central role. Due to exchange splitting between the up- and down-spin bands in FMs, the nature of up- and down-spin electronic states at the Fermi surface and their coupling to scattering potentials will be different [14, 15, 65]. Consequently, in FMs the DOSs and Fermi velocities for the majority and minority spins are different. This transcends to \( n, \tau \) and \( m_e^* \) being different (i.e., spin-dependent) [71, 79]. Therefore one will require an extension of Drude’s model to FMs.

In the mid-1930s, N. F. Mott [103] proposed that at sufficiently low temperatures (where electron-magnon scattering can be neglected [104]), up- and down-spin electrons in FM metals carry current independently, corresponding to two current channels connected in parallel (Fig. 2.5) [78]. That is, the total resistivity is given by the parallel combination

\[ \rho = \frac{\rho_\sigma \rho_{-\sigma}}{\rho_\sigma + \rho_{-\sigma}} \]  

(2.10)

where \( \rho_\sigma \) is the spin-dependent resistivity and \( \sigma = \uparrow, \downarrow \).\(^{12}\) Mott’s model can be thought as the first understanding of spin-polarized transport.

\[ \rho_\uparrow \]

\[ \rho_\downarrow \]

\[ \rho \]

Figure 2.5: Mott’s two-current model.

In this model, the conduction is mainly contributed by \( s \) electrons.\(^{13}\) Moreover, due to the large density of states of 3d bands at \( E_F \) [75], \( s-d \) scattering via \( s-d \) mixing is assumed

\(^{12}\)Here \( \sigma \) is not the conductivity, but rather the spin index.

\(^{13}\)In FMs, both of \( s \) and \( d \) bands electrons participate in conduction [65]. However, the \( s \) bands are wide, whereas the \( d \) bands are narrow (Fig. 2.2b). Thus electrons in the \( d \) bands have a large effective mass (and thus low mobility), in contrast to the ones in \( s \) bands; this is evident from the relations \( m^* = \hbar^2 (\partial^2 E/\partial k^2)^{-1}_{E_F} \) and \( \bar{\mu} = e\tau/m^* \) [61, 69, 74].
to occur much more frequently than $s$-$s$ scattering [12]. This model [105] assumes that the resistivity is merely determined by interband scattering from $4s$ to $3d$ bands (and vice versa). The probability of scattering is thus proportional to the DOS at the Fermi level in $3d$ bands [12, 14, 74]

$$\rho_\sigma \propto g_\sigma (E_F)$$  \hspace{1cm} (2.11)$$

Given the picture above, Mott’s model implies that spins have different distribution functions $f_\sigma$ and relaxation times $\tau_\sigma$ [14, 69]. Implicit in the “independence” condition of current channels is the main assumption that spin-flip events are rare (or negligible) so that one can disregard any transition (or mixing) between the channels. This means that the spin-angular momentum along the spin quantization axis is conserved by the single-particle Hamiltonian [14]. This is true in general for $3d$ transition metals where the probability of spin-flip scattering is small compared to the conserving scattering events (e.g., electron-phonon scattering) and where spin-orbit interaction (which mixes spin and orbital angular momenta) is small [14, 59]. If one includes spin-flip scattering processes (e.g., the non-conserving electron-magnon scattering at temperatures close to the Curie point, fluctuating magnetic field, lose spins due to magnetic impurities, or hyperfine coupling with nuclei), a relaxation time $\tau_{\uparrow\downarrow}$ appears [14, 15, 59, 62, 69, 71, 106]. In this case, and within the free-electron model, Boltzmann’s equation has an extra spin-relaxation term due to spin-flip scattering (in addition to the usual momentum-relaxation term due to lattice defects and vibrations) [59]. Namely, the coupled equations [69, 76]

$$eE \cdot \mathbf{v} \frac{\partial f_0}{\partial E} = -\frac{f_\sigma - f_0}{\tau_\sigma} - \frac{f_\sigma - f_{-\sigma}}{\tau_{\sigma,-\sigma}}$$  \hspace{1cm} (2.12)$$

where $f_0$ is the equilibrium distribution function, $f_\sigma$ the spin-dependent distribution function, $E$ the applied electric field, $\mathbf{v}$ the velocity, $\tau_\sigma$ the spin-dependent transport relaxation time, and $\tau_{\sigma,-\sigma}$ ($\tau_{\sigma,-\sigma}$) the spin-flip relaxation time from $\sigma$ to $-\sigma$ ($-\sigma$ to $\sigma$). Since $\tau_\sigma \ll \tau_{\sigma,-\sigma}$, momentum relaxation occurs first, followed by slow spin-relaxation.

In late-1960s, I. A. Campbell and A. Fert [107, 108] investigated the two-current model. They solved (2.12) and obtained the total resistivity [76]

$$\rho = \frac{\rho_\sigma \rho_{-\sigma} + \rho_{\sigma,-\sigma} (\rho_\sigma + \rho_{-\sigma})}{\rho_\sigma + \rho_{-\sigma} + 4 \rho_{\sigma,-\sigma}}$$  \hspace{1cm} (2.13)$$
where, in the nondegenerate limit

$$\rho_\sigma = \frac{m^*}{n_\sigma e^2 \tau_\sigma} \quad (2.14)$$

$$\rho_{\sigma,-\sigma} = \frac{m^*}{ne^2 \tau_{\sigma,-\sigma}} \quad (2.15)$$

When spin-flip scattering is neglected, (2.13) reduces to the two-current model (2.10). We note that the two-current model generally holds if \( \lambda \ll l_{sf} \), whether \( L > l_{sf} \) or \( L < l_{sf} \) [43, 65]. However, some FMs (e.g., Py) have short \( l_{sf} \) that can in fact be comparable to \( \lambda \) [110–112]. In the latter case, one has to include spin-mixing effects.

### 2.1.4 Spin Injection and Spin Accumulation

From thermodynamics, the chemical potential \( \mu \) is defined as the variation of the thermodynamic potential of the system when one particle is added at constant entropy and constant volume [61, 78, 84].\(^{15,16}\) For particles obeying the Fermi-Dirac statistics and in the framework of the free-electron model, the chemical potential is given by the Sommerfeld expansion (assuming \( k_B T \ll E_F \)) [61, 109]

\[
\mu = E_F \left[ 1 - \frac{\pi^2}{12} \left( \frac{k_B T}{E_F} \right)^2 + \ldots \right] \quad (2.17)
\]

where \( E_F \) is the Fermi energy and \( k_B \) is Boltzmann’s constant. From this equation, it is apparent that at \( T = 0 \) K, one has \( \mu = E_F \). For a metal, \( \mu \) is constant.\(^{18}\) If a voltage is applied the electrochemical potential \( \bar{\mu} = \mu - eV_C \) varies along the conductor and as a result, a charge current density flows according to Ohm’s law [61, 78, 84]

\[
J_C = \sigma e \nabla \bar{\mu} \quad (2.18)
\]

At an interface between two conductors, \( \bar{\mu} \) varies in such a way that it presents no discontinuity at the interface [61, 78].

---

\(^{14}\)In the degenerate limit, one has \( \rho_\sigma = 1/n_\sigma E_F e^2 g_\sigma [109] \).

\(^{15}\)This follows from the differential form of the combined 1st and 2nd laws (sometimes called Gibbs fundamental form) [84]

\[
du = TdS - PdV + \mu dn \quad (2.16)
\]

\(^{16}\)For charged particles (in the absence of magnetic fields), one speaks of an electrochemical potential \( \bar{\mu} = \mu + qV_C \), defined as the work done against chemical composition plus internal and/or external potential when adding a particle, opposed to the chemical potential \( \mu \) which is concerned only with the work done against chemical interaction when adding a particle. The two coincide for uncharged species.\(^{17}\) Since the Fermi temperature is given by \( T_F = E_F/k_B \), the condition can be restated as \( T \ll T_F \).

Thus it is obvious that this holds for most metals. For example, for a metal with \( E_F = 5 \) eV, one has \( T \approx 58000 \) K, which is 10 times higher than the temperature of the Sun.

\(^{18}\)Because the density \( n \) is almost fixed. However, for semiconductors \( n \) varies considerably in space and thus \( \mu \) has to be taken as a function of position [84].
In the same way, one may define an electrochemical potential for each spin carrying particle so that electrons with different spins have different electrochemical potentials. In this way, the out of equilibrium spin electrochemical potential $\bar{\mu}_s$ is defined as the half-difference between the electrochemical potentials of up- and down-spin electrons, viz. \( [71, 78, 104] \)

$$\bar{\mu}_s = \frac{1}{2} (\bar{\mu}_\uparrow - \bar{\mu}_\downarrow)$$  \hspace{1cm} (2.19)

and is sometimes referred to as the spin accumulation.\(^{19}\) The spin accumulation is related to the out of equilibrium spin density $\delta s = \delta n_\uparrow - \delta n_\downarrow$ through

$$\bar{\mu}_s = \frac{1}{2e} \frac{g_\uparrow (E_F) + g_\downarrow (E_F)}{g_\uparrow (E_F) g_\downarrow (E_F)} \delta s$$  \hspace{1cm} (2.20)

and thus sometimes one might also refer to $\delta s$ as the spin accumulation. Unlike $\bar{\mu}$, the spin accumulation undergoes a discontinuity at the FM/NM interface by an amount given by $\bar{\mu}_{FM}^{NM}$.\(^{20}\) In fact, the drop at the interface is $eV_S$, where $V_S$ is known as the spin accumulation voltage (or just spin voltage) \([61]\). This quantity arises whenever there is a discontinuity in conductance between the two spin channels.

\[\text{Figure 2.6: Schematic showing the spin accumulation at a FM/NM interface. The dashed lines enclose the zone of spin accumulation. In the figure, electrons are assumed to be injected from the NM to the FM (i.e., current is flowing from FM to NM). (a) Spatial variation of the spin-dependent electrochemical potentials. (b) At each point in the multilayer, a difference in the electrochemical potentials determines a spin current. Figure adapted by the author from [113].}\]

\[\text{In 1976, Aronov [99] theoretically predicted the possibility of injecting a spin-polarized current from a FM to a NM metal attached to it, effectively establishing a nonequilibrium magnetization in the NM region (i.e., magnetizing the NM region) within a spin-coherent}\]

\[\text{\hspace{1cm} A semiclassical quantity [71].}\]

\[\text{\hspace{1cm} In particular, the average spin accumulation is discontinuous at the interface. The individual chemical potentials for the two spin channels is continuous at the FM/NM interface (if one neglects interface conductance) [61, 104].}\]
distance phenomenologically determined by the spin-diffusion length \( \ell_{sd} \). The nonequilibrium magnetization is equivalent to a nonequilibrium spin-accumulation in the NM region \([71, 78]\); in other words, the build-up of spin polarization at the FM/NM interface when there is a current flowing across the interface \([61]\). This prediction was proved later in 1985 by the pioneering studies of Johnson and Silsbee \([36, 101, 102]\) in a structure similar to that in Fig. 2.7a. This structure is called a nonlocal spin valve (NLSV), since a current injected in one electrode can be nonlocally detected as a voltage difference in the other electrode (i.e., without passing the current directly from one end to the other as in Fig. 2.7b). The nonlocal voltage detected is attributed to the nonequilibrium magnetization (spin accumulation) established in the NM region after injecting the spin-polarized current \([71, 106]\). For this reason, the two electrodes are appropriately named injector and detector. The main advantage of using a NLSV is the generation of a pure spin current, in contrast to the LSV in which the pure spin current is associated with a charge current \([21]\).

The spin transport and spin injection across FM/NM junctions have then been extensively studied, for example in \([37, 43]\). It is worth noting that in contrast to NMs (which can have spin-diffusion lengths in the micron range), FMs have very small spin-diffusion lengths and thus spin-accumulation is mainly an interface property in these materials (although a spin-current persist in the bulk, recall Fig. 2.6) \([71]\).

![Figure 2.7](image.png)

**Figure 2.7:** Illustration of nonlocal spin valve (NLSV) and local spin valve (LSV). The nonequilibrium magnetization of the spin accumulation injected from FM\(_1\) to NM decays over the spin-diffusion length \( \ell_{sd}^{FM} \). The spin accumulation in FM\(_1\) has been ignored since it is localized at the interface because \( \ell_{sd}^{FM} \ll \ell_{sd}^{NM} \) \([71]\). (a) NLSV. (b) LSV.

\(^{21}\)Aronov and Pikus also suggested a similar procedure to be carried in a NM semiconductor \([100]\).
2.1.5 Magnetoresistance (MR)

The term magnetoresistance (MR) refers to the dependency of electrical resistance of a FM/NM multilayer on the relative magnetization orientation of the adjacent FMs [14]. The MR is typically given as the ratio [65, 82]

\[
MR = \frac{R_{AP} - R_P}{R_P} \times 100\%
\]  

(2.21)

where \(R_P\) and \(R_{AP}\) are the resistances in the parallel and antiparallel states, respectively.\(^{22}\) Magnetoresistive structures can be made of several layers of different materials like FM, AFM, and NM (whether metal, insulator, semiconductor, or even organic) [15, 114].\(^{23}\) In its simplest form, an MR device is made up of two FMs sandwiching an NM spacer (usually a metal or an insulator). As shown in Fig. 2.8, one of the FM layers is called “free”, “switching”, “sensing”, or “soft”, in that its magnetization is free to rotate in the plane of the layer. The other layer is “fixed” or “hard” by either being naturally hard, or by virtue of being thicker\(^{24}\) or by exchange bias coupling [115] (i.e., by “pinning” it to an AFM “pinning layer” such that the hysteresis loop is shifted); the latter implies that the hard layer is usually comprised of two or more layers\(^{25}\) [15, 21, 26, 61, 114]. The hard layer is also sometimes called a “polarizer” or a “reference” layer, especially in the context of current-induced switching and spin-filtering processes (Fig. 2.4). To obtain high MR ratios, the multilayer is chosen/engineered in a way that the FMs are highly spin-polarized and the spin scattering of electrons in the NM is low.

Typically, MR structures come in two flavors: either as a current-in-plane (CIP) or a current-perpendicular-to-plane (CPP) (Fig. 2.9), with the latter being most widely used nowadays [21, 119].

\(^{22}\)Some authors define the MR as

\[
MR = \frac{R_{AP} - R_P}{R_{AP}} \times 100\%
\]

(2.22)

and typically call it the “pessimistic” definition (in contrast to the “optimistic” one we used), due to the lower MRs since most of the time \(R_{AP} > R_P\) [65].

\(^{23}\)Usually the FMs used are the transition FM materials (Fe, Co, Ni) and their alloys (Py, CoFe, CoFeB, FePt, SmCo, NdFeB). The conducting NMs are usually transition metals (Cr or Ru) or noble metals (Cu, Ag, and Au). The insulating NMs are usually oxides (Al\(_2\)O\(_3\), MgO). AFMs, on the other hand, are usually Mn-based alloys (PtMn, PdMn, IrMn, RhMn, FeMn, NiMn, CrMn) and oxides (CoO, NiO).

\(^{24}\)This also breaks the “inversion” symmetry of the stack [16].

\(^{25}\)More layers are generally needed for different purposes like increasing spin polarization, minimization of stray fields, etc. [26]. In fact, simply pinning a soft FM by depositing it on top of an AFM and making use of the exchange coupling at the interface will not prevent erroneous events that may occur in some structures due to the stray fields surrounding the FMs. That is, the FMs can couple via the stray fields, which prefers an antiparallel alignment of the free FM to the reference FM, causing a shift in the switching curve of the free FM, precluding information storage [114]. To avoid this effect, one can cancel the unwanted stray fields [116] by using the so-called artificial or synthetic AFM structures. These are made by two FMs sandwiching a thin NM such as Cu or Ru, and it makes use of the oscillatory behavior
Figure 2.8: Simple FM/NM multilayer.

Figure 2.9: Illustration of CIP-MR and CPP-MR. (a) CIP-MR. (b) CPP-MR.

Below we discuss the most widely used MR structures, namely the GMR and TMR.

2.1.5.1 Giant Magnetoresistance (GMR)

In 1988 and influenced by the discovery of the antiferromagnetic Heisenberg (or bilinear) exchange coupling [120] between ultrathin films came the groundbreaking discovery of giant magnetoresistance (GMR) from the pioneering work of both Fert’s [121] and Grünberg’s [122] groups. On the same line, and after the striking GMR measurements, Parkin and collaborators [117, 118] have observed an oscillatory (or alternating) AFM-FM behavior of the exchange coupling in metallic multilayers as a function of the NM spacer (Fig. 2.10) [21]. The GMR discovery marked the beginning of a new era in data storage technology, an impact that was later recognized by Fert and Grünberg sharing of exchange coupling [117, 118] so that one can select an optimal NM thickness to make them oppositely magnetized (Fig. 2.10), canceling their stray fields. The origin of this behavior has been accounted to the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mediated by a spin-polarized cloud of electrons [78, 82, 123].
the 2007 Nobel Prize in Physics. It is not an exaggeration to say that GMR kicked off the start of spintronics as a new scientific field.

Figure 2.10: Exchange coupling in NM metals.

GMR is an effect that manifests itself in metallic structures whereby the MR of an ultra-thin multilayer experiences a giant change when the magnetization direction changes [21].\(^\text{27}\) The effect is based on spin-dependent scattering of electrons traveling across metallic thin films [15, 65, 80, 82, 124]. As one injects an electric current, the spins parallel to the magnetization of the FM will pass through quite easily while those antiparallel will scatter. Thus, the device acts as a spin filter (or a “spin valve”), letting more electrons with certain spins; hence the name. Figs. 2.11a and 2.11b illustrate the scattering picture. The scattering process can also be understood in the Stoner picture (Fig. 2.2) of FMs as follows. For P alignment, majority-spin electrons are located within the \(s-p\) band and their conduction is similar to those in the NM. For minority-spin electrons, on the other hand, the \(s-p\) bands are hybridized and \(E_F\) lies within the \(d\) band. Because of the higher DOS of the hybridized band, minority spins scatter more than the majority, implying shorter mean-free path for minority-spin electrons. For AP alignment, the former argument applies to either spin in at least one layer.

When both magnetizations are parallel (P), spins of one orientation passes easily, and the resistance is low. When they are antiparallel (AP), both spins are scattered in at least one layer, and the multilayer presents a high resistance. The measure of change of

\(^{27}\)Although ordinary MR effect had been known for more than 100 years ago by William Thomson—better known as Lord Kelvin—the MR measured was typically low [61, 65, 82, 123].
resistances is given by the GMR ratio

\[ GMR = \frac{R_{AP} - R_P}{R_P} \times 100\% \]  

(2.23)

\[ R_P = 2 \frac{R_{\uparrow} R_{\downarrow}}{R_{\uparrow} + R_{\downarrow}} \]  

(2.24)

\[ R_{AP} = \frac{1}{2} (R_{\uparrow} + R_{\downarrow}) \]  

(2.25)

from which we write the GMR as [78]

\[ GMR = \frac{1}{4} \frac{(R_{\uparrow} - R_{\downarrow})^2}{R_{\uparrow} R_{\downarrow}} \]  

(2.26)

As mentioned previously, the CPP geometry is nowadays preferred. This is usually because of the higher symmetry, the greater MR ratios, and its importance for spin-transfer torque applications (although CIP geometry is experimentally simpler to implement) [21, 65, 78, 82, 119]. In addition to the geometry used, there are certain factors that control the value of GMR. Some of these factors are the spin-dependent random potential at FM/NM interfaces and band matching/mismatching between the
FM and NM layers [65]. The GMR effect technically occurs when $t$ (the layer thickness of magnetic multilayers) satisfies $t \leq \lambda [10, 65]$. 

In many cases, spin-relaxation effects cannot be disregarded and one has to resort to more accurate formalisms. The theory of CPP-GMR structures is known as the Valet-Fert theory, in honor of Valet and Fert who extensively analyzed this structure in 1993. Their analysis is based on the diffusive spin-dependent Boltzmann equations. The quantum formalism of CPP-GMR has been applied by using the quantum Kubo formula [125, 126]. The results of both Boltzmann and Kubo description turned out to be equivalent since the band structure was assumed to be parabolic. The more realistic band structure have been employed in [127–129] using models based on both pictures.\(^{28}\)

2.1.5.2 Tunneling Magnetoresistance (TMR)

Tunneling magnetoresistance (TMR) in its simplest form is observed in trilayers made up of two FMs sandwiching an insulating NM spacer, a structure called a magnetic tunnel junction (MTJ). The idea is that, for sufficiently thin insulating spacers ($\approx 1–2$ nm), electrons can tunnel through [14, 16]. The measure of resistance change in MTJs is given by the TMR ratio

$$TMR = \frac{R_{AP} - R_P}{R_{AP}} \times 100\%$$

(2.27)

where we have swapped the roles of $R_P$ and $R_{AP}$ in the denominator, adopting the convention used in most TMR experiments [65].

Although TMR was well-known [132, 133] before the discovery of GMR, the observed MRs were rather small. However, the discovery of GMR (and the advances of thin film techniques) has triggered extensive research on tunnel junctions again, first in (the heavily disordered [21]) Al$_2$O$_3$ tunnel barriers [134–136] and later in (the potentially well-ordered [21]) MgO barriers [137, 138]. TMR is typically far larger than the GMR, and this explains the shift in attention from GMRs to TMRs, especially in the implementation of memory cells and commercial recording heads [16, 65]. High TMRs can generally be obtained by choosing materials with different symmetries of the wavefunction for both electrons spins so that the resistance (which depends on the overlap) is high in the AP state [16]. The TMR ratio, in general, depends on many factors like the shape of the Fermi surface of the electrodes, electron scattering at the FM/NM interface, symmetry of the wave functions, and spin-slip tunneling [65]. Additionally, it varies with temperature and also with the barrier’s height, width, and impurities [15, 65].

\(^{28}\)For CIP-GMR, see [130] for classical and [131] quantum formalisms.
TMR is a consequence of spin-dependent tunneling, and it can be understood in terms of Jullièrè’s model proposed in 1975 [132]. This model is based on the assumption that spin is conserved in the tunneling process so that up- and down-spin electrons tunnel independently. With reference to Fig. 2.12, the assumption implies that electrons from one spin state in the first FM will be accepted by unfilled states of the same spin in the second FM. If the FMs are in P alignment, down-spin electrons tunnel to the down-spin states and up-spin electrons tunnel to the up-spin states, which implies a large flow of electrons and hence a low resistance. For AP alignment, up-spin electrons tunnel to the down-spin states and down-spin electrons tunnel to the up-spin states, implying a small flow of electrons and hence a high resistance.

In Jullière’s model, it is also assumed that the rate of tunneling is proportional to the product of the DOSs at that particular energy on each side of the barrier [15, 78]. If one denotes the polarization of two FMs by $P_1$ and $P_2$, then the TMR can be expressed by the so-called Jullière’s formula [78, 82]

$$TMR = \frac{2P_1 P_2}{1 - P_1 P_2}$$

(2.28)

where the polarization of electrons can be given as [78, 82]

$$P = \frac{g_+ (E_F) - g_- (E_F)}{g_+ (E_F) + g_- (E_F)}$$

(2.29)

which is assumed to be constant in the framework of his model.

### 2.1.6 Spin-Transfer Torque (STT)

Spin-transfer torque (STT) is a recently discovered phenomenon whereby magnetization dynamics can be excited by the transfer of spin angular momentum from spin-polarized electrons [16, 21, 26]. The effect has been predicted theoretically (and independently) in 1996 by Slonczewski and Berger [30, 31] and later experimentally verified in 1998 by Tsoi et al. and Myers et al. [139, 140]. STT can be thought of as the converse of GMR (or TMR) [29, 80]. It manifests itself in trilayer FM$_1$/NM/FM$_2$ structures composed of two thin FM layers (fixed and free) with noncollinear magnetizations [26, 80] sandwiching an ultra-thin NM spacer [21]. The effect is most easily understood in the ideal case of perpendicular incidence of electrons and perfect spin-filtering at the interface. By injecting a current through FM$_1$ (polarizer), the spin filtering process polarizes the current upon transmission through (or reflection from) this layer, Figs. 2.13a and 2.14a) [15, 21]. Under certain conditions (e.g., ultra thin spacers)\(^{29}\) the current can maintain most of

\(^{29}\)Such that the NM thickness is less than the spin-diffusion length $\ell_s^{NM}$. 
Figure 2.12: Spin-dependent tunneling in a magnetic tunnel junction (MTJ). (a) P alignment. (b) AP alignment. (c) Large flow of electrons results for P alignment. (d) Small flow of electrons results for AP alignment.

its polarization. Once this current reaches the NM/FM$_2$ interface, the spin filtering process implies that FM$_2$ will polarize the current and thus spins will align themselves along its magnetization direction, or equivalently, that the transverse component of the incoming electrons will be filtered out (leaving the longitudinal component unchanged, (Figs. 2.13b and 2.14b) [80]. This lost in spin implies an angular momentum transfer [15]. The conservation of angular momentum dictates that a torque has to be applied on the magnetization of FM$_2$.\footnote{The magnetization exerts a torque on the incident noncollinear electron spins, changing their angular momentum, and the electrons exert an equal and opposite torque on the magnetization [21].} If this current is large enough, the torque can overcome the layer intrinsic damping and drive its magnetization into high-frequency oscillations around its equilibrium point [33–35] or totally reverse it [139–144] into another stable state.

STT can also be understood as follows. Electron spins that are not collinear to the magnetization are not eigenstates of the FM [29]. Their states can be, however, described by a (normalized) wavefunction written as a coherent linear superposition of up and down spinor components having amplitudes $\cos \theta/2$ and $\sin \theta/2$, where $\theta$ is the angle with respect to the magnetization (Fig. 2.13b) [21, 29, 75, 80, 106]. In particular, if the noncollinear spins are moving in the $x$-direction and the magnetization is titled\footnote{Something like $\psi = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$, where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the spin eigenstates of $\sigma_z$ and $\alpha$ and $\beta$ are the (generally complex) amplitudes [61, 62].}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure212.png}
\caption{Spin-dependent tunneling in a magnetic tunnel junction (MTJ). (a) P alignment. (b) AP alignment. (c) Large flow of electrons results for P alignment. (d) Small flow of electrons results for AP alignment.}
\end{figure}
from $z$-axis by an angle $\theta$ (and thus spins are polarized in the $xz$-plane), then we have incident spinors of the form [21]

$$
\psi_i = \left( \cos \frac{\theta}{2} \uparrow + \sin \frac{\theta}{2} \downarrow \right) e^{ikx} = \begin{bmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{bmatrix} e^{ikx} \quad (2.30)
$$

We can write the reflected and transmitted spinors as

$$
\psi_r = \left( r_\uparrow \cos \frac{\theta}{2} \uparrow + r_\downarrow \sin \frac{\theta}{2} \downarrow \right) e^{-ikx} = \begin{bmatrix} r_\uparrow \cos \frac{\theta}{2} \\ r_\downarrow \sin \frac{\theta}{2} \end{bmatrix} e^{-ikx} \quad (2.31)
$$

$$
\psi_t = \left( t_\uparrow \cos \frac{\theta}{2} \uparrow + t_\downarrow \sin \frac{\theta}{2} \downarrow \right) e^{ikx} = \begin{bmatrix} t_\uparrow \cos \frac{\theta}{2} \\ t_\downarrow \sin \frac{\theta}{2} \end{bmatrix} e^{ikx} \quad (2.32)
$$
where \( r_\sigma \) and \( t_\sigma \) are the reflection and transmission coefficients of a \( \sigma \)-spin electron (\( \sigma = \uparrow, \downarrow \)). For the case of a perfect spin filter\(^\text{32}\)

\[
\psi_r = \left( \sin \frac{\theta}{2} |\downarrow\rangle \right) e^{-ikx} = \begin{bmatrix} 0 \\ \sin \frac{\theta}{2} \end{bmatrix} e^{-ikx} \tag{2.33}
\]

\[
\psi_t = \left( \cos \frac{\theta}{2} |\uparrow\rangle \right) e^{ikx} = \begin{bmatrix} \cos \frac{\theta}{2} \\ 0 \end{bmatrix} e^{ikx} \tag{2.34}
\]

and thus, there is a discontinuity in the transverse spin current at the interface. In fact, the expectation values of the spin angular momentum are given by

\[
\langle S_z \rangle = \langle \psi_\uparrow | S_z | \psi_\downarrow \rangle = \frac{\hbar}{2} \left[ \begin{array}{c} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{array} \right] \left[ \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right] \left[ \begin{array}{c} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{array} \right] = \frac{\hbar}{2} \cos \theta \tag{2.35}
\]

\[
\langle S_x \rangle = \langle \psi_\uparrow | S_x | \psi_\downarrow \rangle = \frac{\hbar}{2} \left[ \begin{array}{c} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{array} \right] \left[ \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right] \left[ \begin{array}{c} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{array} \right] = \frac{\hbar}{2} \sin \theta \tag{2.36}
\]

This can be understood in the Stoner picture where exchange splitting inside the FM causes the states in the minority-spin band to shift higher in energy than the majority-spin band \(^{21}\). Because of the different kinetic energies of the two spin components (due to the difference in exchange energy), we have \( k_\uparrow \neq k_\downarrow \)^\ref{footnote31}. In transition metal FMs, a large number of states (wave vectors) are available around \( E_F \)^\ref{footnote29}. Once the states reach the NM/FM interface, the transverse states will precess in the exchange field of the magnet as a function of position \(^{16, 21, 29}\). Therefore, an injected (transverse) spin current will generate a large number of wave functions oscillating about \( z \)-direction with different wave length on a period of precession \( 2\pi/k_\uparrow - k_\downarrow \)^\ref{footnote33}, leading to decoherence of the spin angular momentum \(^{21, 29}\). For distances larger that the magnetic (spin) coherence length \( \lambda_c = \pi/k_\uparrow - k_\downarrow \) (\( \approx 1 - 2 \) nm),\(^{34}\) the transverse spin current will be destructed \(^{29, 71, 145}\).

The torque applied on the free FM layer can be decomposed into two components: \textit{adiabatic} (also known as \textit{in-plane}, \textit{Slonczewski}) torque that is related to the conduction electrons following the local magnetization direction, and a \textit{non-adiabatic} (also known as \textit{perpendicular} or \textit{field-like}) torque that occurs with a rapid change of magnetization \(^{16, 26, 146}\). Although the adiabatic component is well understood, the origins of the non-adiabatic component is still under debate, and different explanations have been put to describe it as such as spin mistracking, spin-flip scattering, and momentum transfer \(^{146, 147}\). The relative importance of these components depends on the device structure.

\(^{32}\)Recall the discussion in 2.1.2.

\(^{33}\)Very short for transition metal FMs \(^{21}\).

\(^{34}\)The length over which the magnetic order decays, which in transition metal FMs is larger than the Fermi wavelength \( \lambda_F \); the latter typically on the order of 0.1 nm for metals \(^{71, 75, 78}\).
geometry, and material [16]. Both components determine important design parameters like threshold currents for switching and the oscillation frequency. In general, for metallic structures, the non-adiabatic torque is assumed to be weaker than the adiabatic [148–150].

STT is important in most magnetic materials, including dilute and oxide semiconductors, transition-metal/rare-earth and oxide ferromagnets. Its importance also stems from the fact that it is a local effect in that it occurs only where spin currents flow and thus can be directed for applications [16]. Moreover, it is in interface effect, and it occurs in structures of lateral dimensions of about < 250 nm so that STT dominates over the Oersted fields produced by the passing current [21, 151].

2.2 Basics of Magnetism

2.2.1 Atomic Origin of Magnetism

Magnetism arises from the properties and arrangements of electrons in materials [15, 61, 68, 70]. In accordance with Hund’s rule, all isolated atoms (ions) with odd number of electrons and unfilled orbital shells (e.g., 3d, 4f, or 5f) will always possess magnetic moments [15, 21, 61, 68, 152, 153]. That is, a necessary condition for the appearance of a nonzero magnetic moment is the existence of partially filled shells (i.e. unpaired electrons) [70]. In condensed matter systems, a magnetic moment generally originates from both the spin and orbital angular momenta that are coupled by spin-orbit interaction [61].

In the language of quantum mechanics, the orbital and spin magnetic moment operators \( \hat{m}_L \) and \( \hat{m}_S \) (corresponding to the observables \( m_L \) and \( m_S \)) are given in terms of the orbital and spin operators \( \hat{L} \) and \( \hat{S} \) as [21, 61, 70, 155, 156]

\[
\hat{m}_L = -g_L \frac{\mu_B}{\hbar} \hat{L} \quad \text{(2.37)}
\]

\[
\hat{m}_S = -g_S \frac{\mu_B}{\hbar} \hat{S} \quad \text{(2.38)}
\]

\[35\] A magnetic moment also arises from nucleons (the constituents of the atomic nucleus), and its interaction with the electron magnetic moment results in the so-called hyperfine interaction [152, 153]. However, the nuclear magnetic moment is three orders of magnitude smaller than the electron magnetic moment (see Physical Constants) and thus usually neglected, except for special applications (e.g., NMR) [61, 154].
where $\mu_B = e\hbar/2m_e$ is the Bohr magneton, $\hbar = h/2\pi$ the reduced Planck constant, $g_L = 1$ the orbital g-factor, and $g_S \approx 2$ the spin g-factor.\(^{36}\) The minus sign arises from the negative charge of the electron and it indicates that the orbital (spin) magnetic moment is opposite to the orbital (spin) angular momentum. Moreover, the operator relations implies that the magnetic moment is quantized the same way angular momentum is quantized. One cannot measure neither the magnetic moment nor the angular momentum directly, but rather along a specific axis \(^{62,70}\). In fact, since the sizes and $z$-components of the angular momenta are given by \(^{62,68}\)

\[
\begin{align*}
|L| &= \sqrt{\ell (\ell + 1)} \hbar, \quad \ell = 0, 1, 2, \ldots \\
L_z &= m_\ell \hbar, \quad m_\ell = -\ell, -\ell + 1, \ldots, 0, \ldots, \ell - 1, \ell \\
|S| &= \sqrt{s(s+1)} \hbar, \quad s = \frac{1}{2} \\
S_z &= m_s \hbar, \quad m_s = -\frac{1}{2}, \frac{1}{2}
\end{align*}
\]

the corresponding quantities for the magnetic moments are given by \(^{68}\)

\[
\begin{align*}
|m_L| &= \sqrt{\ell(\ell + 1)\mu_B}, \quad \ell = 0, 1, 2, \ldots \\
m_{L,z} &= -m_\ell \mu_B, \quad m_\ell = -\ell, -\ell + 1, \ldots, 0, \ldots, \ell - 1, \ell \\
|m_S| &\approx 2\sqrt{s(s+1)} \mu_B, \quad s = \frac{1}{2} \\
m_{S,z} &\approx -2m_s \mu_B, \quad m_s = -\frac{1}{2}, \frac{1}{2}
\end{align*}
\]

For many low electron atoms (typically in periods 1-4 \(^{159}\)) and as long as external fields are weak (in comparison to the system’s internal field), Russell-Saunders (LS) coupling holds where inter-electronic repulsion is much greater than spin-orbit interaction,\(^{37}\) in which the latter is treated as a perturbation \(^{159}\). In this case, the electron orbital and spins momenta interact independently so one can write \(\hat{S} = \sum_i \hat{s}_i, \quad \hat{L} = \sum_i \hat{\ell}_i\) and couple the two momenta together, forming a total angular momentum \(\hat{J} = \hat{L} + \hat{S}\) \(^{61}\). The total angular momentum will give rise to a total magnetic moment

\[
\hat{m}_J = -g_J \frac{\mu_B}{\hbar} \hat{J}
\]

\(^{36}\)The g-factor for a free electron can only be explained in the framework of the relativistic Dirac equation. For solids, this factor might slightly (or largely) vary around this value as it depends on the material and is strongly affected by spin-orbit interaction due to the lattice ions (and thus one might expect dramatic changes in semiconductors) \(^{62,79,157}\). The value 2 is just an approximation; the quantum field theory correction to the spin g-factor is given by \(g_S = 2(1 + \alpha/2\pi + \cdots) = 2.0023192\ldots\) where \(\alpha = e^2/4\pi\varepsilon_0\hbar c\) is the fine-structure constant \(^{61,79,158}\).

\(^{37}\)For heavier atoms (atoms of the 5th and 6th periods like actinides \(^{61,159}\)), spin-orbit interaction is larger than the electronic repulsion \(^{159}\) and another scheme of coupling, called jj coupling, applies. In this case, each \(\hat{\ell}_i\) combines first with \(\hat{s}_i\) to give \(\hat{j}_i\), and then the total angular momentum is written as \(\hat{J} = \sum_i \hat{j}_i\).
where \( g_J \), the \( g \)-factor of total angular momentum, is typically called the Landé \( g \)-factor and is given by \([15, 61, 76]\)

\[
g_J = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}
\]

(2.48)

which only depends on \( L \), \( S \), and \( J \). For a given configuration, \( J \) and \( g_J \) follow Hund’s rules \([61]\). Similar to the arguments above, one can write \([68]\)

\[
|J| = \sqrt{j(j+1)}\hbar, \quad j = \ell - \frac{1}{2}, \ell + \frac{1}{2}
\]

(2.49)

\[
J_z = -m_J\hbar, \quad j = \ell - \frac{1}{2}, \ell + \frac{1}{2}
\]

(2.50)

from which we write the corresponding quantities for the magnetic moment \([68]\)

\[
|m_J| = g_J\sqrt{j(j+1)}\mu_B, \quad j = \ell - \frac{1}{2}, \ell + \frac{1}{2}
\]

(2.51)

\[
m_{Jz} = -g_Jm_J\mu_B, \quad j = \ell - \frac{1}{2}, \ell + \frac{1}{2}
\]

(2.52)

2.2.2 Brief Review of Magnetostatics

In this section, we briefly review the classical theory of magnetism on the bases of Maxwell’s equations. Some of the results below will be used throughout the chapter.

2.2.2.1 Breakthroughs in the History of Magnetism

Magnetism were known since antiquity. Its history dates back to few millennia when the attractive properties of mineral lodestone—a naturally occurring form of magnetite\(^{38}\)—were discovered by Ancient Greeks and Chinese between 500 and 1200 B.C. \([160–163]\). Though the phenomenon has been known for too long (for example magnets were used in compasses since early days by Chinese \([162, 164]\)) and systematic experiments and theoretical investigations of both magnetism and electricity have been made by many scientists such as Petrus Peregrinus \([160, 162]\), William Gilbert \([165]\), Carl Gauss \([162]\), John Michell and Charles-Augustin Coulomb \([162]\), the deep understanding of magnetism and its connection to electricity did not begin until a revolutionary experiment in the 19th century \([166]\). In Denmark in 1820, Hans Oersted linked magnetism to electricity by showing that a current-carrying wire caused a deflection of a nearby compass needle, suggesting the association of a magnetic field with the electric current \([66, 39]\). This was remarkable because it linked electricity to magnetism and hence unified the two

\(^{38}\)A mineral with chemical formula \( \text{Fe}_3\text{O}_4 \) \([160]\).

\(^{39}\)Believed by some people to be a mere 'chance' event or an accident \([164]\).
sciences into what is now known as *electromagnetism* [67]. Shortly thereafter in 1820, and influenced by Oersted’s discovery, scientists over all Europe started investigating the astonishing result of his experiment and tried to reproduce it [164]. In particular, Andre-Marie Ampere experimentally verified his conjecture that just as a wire exerts a kind of 'force at a distance' on a compass needle, two current-carrying wires should interact in a similar manner [161]. He showed that the two wires attract each other when the currents flow in the same direction and repel each other when the currents flow in opposite directions [161, 164]. He formulated the relation between the electric currents and forces between the wires mathematically and this has led to his *force law*, which some consider the first theory in electrodynamics. More importantly, Ampere also hypothesized that a small current loop acts as a tiny magnet, and a macroscopic specimen is dynamically alive and is composed of such microscopic currents, leading him to coin the term *electrodynamics* [161]. He also observed that the magnetic field generated by a current loop depends on both the shape of the loop and the amount of current being carried, and this has led to his famous *circuit law* [161, 164]. In fact, Ampere correctly hypothesized that all magnetic phenomena are due to moving electric charges [166]. At the same time in France, Jean-Baptise Biot and Felix Savart [66] derived another relationship between electric current and the magnetic field it produces in a law now called *Biot-Savart’s law*. Another fundamental law has also been attributed to Carl Gauss and now famously referred to as *Gauss’s law of magnetism*, which is more of a conservation law and implicitly states that there can be no isolated magnetic charges (monopoles) as opposed to electric charges [66]. The ingenious results made by scientists (particularly Ampere) has laid the theoretical foundations for electromagnetism and furnished the way for new theories in electromagnetics such as Faraday’s law of electromagnetic induction in 1831 [161], the latter who also speculated that light is electrical in nature [166].

All of the previous work on magnetism has finally put the theory of electromagnetics on solid ground, and investigations on both electric and magnetic phenomena continued until 1961, when the Scottish scientist James Maxwell—with his keen mathematical skills—reduced all of the current knowledge at his time to 20 simultaneous differential equations in 20 variables [66, 161, 164, 167]. Maxwell also rederived Ampere’s law using a different approach and from this came his major contribution: the addition of displacement current which made the propagation of electromagnetic waves possible (later verified by Heinrich Hertz in 1888) [66, 164]. Maxwell’s equations were later reformulated in a more convenient (and compact) vector form. The 4 celebrated Maxwell equations are given in differential and integral forms as\(^\text{40}\) [66, 166, 168]

\(^{40}\)Usually one carries the differential form around since it is more mathematically convenient. The integral form, however, is better in describing the underlying physical law. The latter can be obtained
where $D$ and $B$ are the electric and magnetic flux densities, $E$ and $H$ the electric and magnetic field intensities, $\rho$ and $\rho_{mv}$ are the electric and magnetic volume charge densities, and $J$ and $J_m$ are electric and magnetic current densities.\(^{41}\)

### 2.2.2.2 Maxwell’s Equations for Magnetostatics

From Maxwell’s equation (2.53d), it is apparent that magnetic fields are produced by two means: Either by a time-varying electric field or by a DC current. Under stationary conditions (when time-varying fields vanish), magnetic fields are also stationary and are thus solely produced by charges moving with constant velocity $^{66, 166}$. If this is the case, Maxwell’s equations for stationary magnetic fields becomes

\[
\nabla \cdot B = 0 \quad \text{(2.54a)}
\]

\[
\nabla \times H = J \quad \text{(2.54b)}
\]

where we ignored the fictitious magnetic sources for the time being. Since now the current density satisfies $\nabla \cdot J = 0$, Maxwell’s equations are decoupled.\(^{42}\) The decoupling of Maxwell’s equations under static conditions is the reason why magnetostatic phenomena can be studied separately from electrostatics $^{160}$.

from the former by invoking two important theorems from vector calculus: Stokes’ (A.138) and Gauss’ (A.139) theorems.

\(^{41}\)The fictitious magnetic sources have been introduced to make Maxwell’s equations symmetric. Moreover, those concepts facilitate certain mathematical computations, especially when solving electromagnetic boundary-value problems applying field equivalence principles $^{168}$.

\(^{42}\)Maxwell’s equation are generally not independent and are in fact coupled through the continuity equation for electric and magnetic current densities $^{168}$

\[
\nabla \cdot J = -\frac{\partial \rho}{\partial t} \quad \text{(2.55)}
\]

\[
\nabla \cdot J_m = -\frac{\partial \rho_{mv}}{\partial t} \quad \text{(2.56)}
\]
2.2.2.3 Biot-Savart’s Law, Flux, and Flux Density

Biot-Savart’s law is the general law of magnetostatics (analogous to Coulomb’s law for electrostatics) and is given as the vector integral

\[ \mathbf{H} = \int_L \frac{I \mathbf{d} \times \mathbf{a}_R}{4\pi R^2} \]  

where \( I \mathbf{d} \) is the current element and \( \mathbf{a}_R \) is a unit vector in the direction of the separation vector \( \mathbf{R} = \mathbf{r} - \mathbf{r}' \). One can formulate this law for other current distributions by using the equivalence relation of the differential line, surface, and volume current elements (analogous to the line, surface, and volume charge configurations in electrostatics) \[ 66, 166 \]

\[ I \mathbf{d} \equiv \mathbf{K} d\mathbf{S} \equiv J dV \]  

(2.58)

which yields the three relations

\[ \mathbf{H} = \int_L \frac{I \mathbf{d} \times \mathbf{a}_R}{4\pi R^2} \]  

(2.59a)

\[ \mathbf{H} = \int\int_{\Sigma} \frac{\mathbf{K} d\mathbf{S} \times \mathbf{a}_R}{4\pi R^2} \]  

(2.59b)

\[ \mathbf{H} = \int\int\int_{\Omega} \frac{J dV \times \mathbf{a}_R}{4\pi R^2} \]  

(2.59c)

Having found the magnetic field \( \mathbf{H} \) by either (2.54b) or (2.59), we define the magnetic flux density \( \mathbf{B} \) in free space by

\[ \mathbf{B} = \mu_0 \mathbf{H} \]  

(2.60)

where \( \mu_0 \) is the permeability of free space. The magnetic flux density is sometimes known as the magnetic induction, since it quantifies the response of the material to the application of \( \mathbf{H} \) \[ 67 \]. The magnetic flux through a surface \( \Sigma \) is given by

\[ \psi_m = \int_C \mathbf{B} \cdot d\mathbf{S} \]  

(2.61)

2.2.2.4 Magnetic Scalar Potential

For a current-free region, \( \mathbf{J} = 0 \), and Ampere’s law (2.54b) becomes

\[ \nabla \times \mathbf{H} = 0 \]  

(2.62)

One can then write the magnetic field \( \mathbf{H} \) using (A.142) in terms of a magnetic scalar potential \( V_m \) as

\[ \mathbf{H} = -\nabla V_m \]  

(2.63)
By plugging in the last relation into (2.54a) after using (2.60) and the vector identity (A.156), the scalar potential can be written as

$$\nabla^2 V_m = 0$$  \hspace{1cm} (2.64)

which is Laplace’s equation. The equation holds only in a current-free region.

### 2.2.2.5 Magnetic Vector Potential

Following an approach similar to that made for the scalar potential, we start from Gauss’ law for magnetostatics (2.54a) and use (A.143) to write the magnetic flux density $\mathbf{B}$ in terms of a magnetic vector potential $\mathbf{A}$ as

$$\mathbf{B} = \nabla \times \mathbf{A}$$  \hspace{1cm} (2.65)

To find $\mathbf{A}$, we follow a similar approach to that made in [66, 166, 169]. We start from Biot-Savart’s law

$$\mathbf{B} = \frac{\mu_0}{4\pi} \int_L \frac{I d\ell' \times \mathbf{R}}{R^3}$$  \hspace{1cm} (2.66)

where the prime denotes source coordinates and $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ is the separation vector. We would like to introduce the del operator inside the integral so that we can use an appropriate vector identity to represent the whole thing as a curl, in particular, a form similar to (2.65). If we use the definition of gradient (A.103)

$$\nabla (R^n) = \frac{\partial}{\partial x} R^n a_x + \frac{\partial}{\partial y} R^n a_y + \frac{\partial}{\partial z} R^n a_z = n x R^{n-2} a_x + n y R^{n-2} a_y + n z R^{n-2} a_z = n R^{n-2} \mathbf{R}$$

we find, for $n = -1$

$$\nabla \left( \frac{1}{R} \right) = - \frac{\mathbf{R}}{R^3}$$  \hspace{1cm} (2.67)

which yields the following form of Biot-Savart’s law

$$\mathbf{B} = -\frac{\mu_0}{4\pi} \int_L I d\ell' \times \nabla \left( \frac{1}{R} \right)$$  \hspace{1cm} (2.68)

Now, using the vector identity (A.160) by taking $V = 1/R$, $\mathbf{A} = d\ell'$, we obtain

$$\nabla \times \left( \frac{d\ell'}{R} \right) = \frac{1}{R} \nabla \times d\ell'^0 + \left( \frac{\nabla}{R} \right) \times d\ell'$$
where the term $\nabla \times d\mathbf{\ell}'$ vanishes since $\nabla$ operates with respect to the unprimed coordinates $(x, y, z)$ while $d\mathbf{\ell}'$ is a function of $(x', y', z')$. Thus

$$\nabla \times \left( \frac{d\mathbf{\ell}'}{R} \right) = -d\mathbf{\ell}' \times \left( \frac{\nabla 1}{R} \right)$$

(2.69)

And (2.68) becomes

$$\mathbf{B} = \nabla \times \int_{L} \frac{\mu_0 I d\mathbf{\ell}'}{4\pi R}$$

(2.70)

which when compared with (2.65) yields

$$\mathbf{A} = \int_{L} \frac{\mu_0 I d\mathbf{\ell}'}{4\pi R}$$

(2.71)

or more generally (using (2.58))

$$\mathbf{A} = \int_{L} \frac{\mu_0 I d\mathbf{\ell}'}{4\pi R}$$

(2.72a)

$$\mathbf{A} = \int_{\Sigma} \frac{\mu_0 \mathbf{K} dS'}{4\pi R}$$

(2.72b)

$$\mathbf{A} = \int_{\Omega} \frac{\mu_0 \mathbf{J} dV'}{4\pi R}$$

(2.72c)

If fields go to zero at infinity, then Helmholtz’s theorem guarantees that every vector field is uniquely specified if both its divergence and curl are given at each point [66, 166, 169]. We already know the curl, but we have to specify the divergence. This process (i.e., specifying the divergence) is known as choosing a gauge. A proper choice for the magnetostatic problem is the so-called Coulomb gauge [66, 166]

$$\nabla \cdot \mathbf{A} = 0$$

(2.73)

Now, since we are in free space, we use (2.60) in (2.54b) along with (2.65) to obtain

$$\nabla \times (\nabla \times \mathbf{A}) = \mu_0 \mathbf{J}$$

where we can invoke the vector identity (A.162) and the Coulomb gauge (2.73) to obtain

$$\nabla^2 \mathbf{A} = -\mu_0 \mathbf{J}$$

(2.74)

which is the vector Poisson equation which has the same solution (2.72a) under appropriate boundary conditions [169]. Moreover, by invoking Stokes’ theorem (A.138) in (2.61) and using the result (2.65), one obtains a relation between the magnetic vector potential and the magnetic flux

$$\psi_m = \oint_{L} \mathbf{A} \cdot d\mathbf{\ell}$$

(2.75)
2.2.2.6 Magnetic Forces and Torques

A magnetic force is generally experienced by three means:-

- **On a Charged Particle**: A moving charge in the presence of a magnetic field experiences a force given by Lorentz’s force law [66, 166]

\[
F_m = Q (v \times B)
\]

where \(Q\) is the electric charge and \(v\) is the velocity. Note that since \(F_m\) and \(v\) are vectors, \(B\) is actually a *pseudovector* [166]. One feature of magnetic forces is that they do no work, i.e. they cannot speed up or slow down a moving particle but can only alter its direction [66, 166]. This is evident from

\[
dW_m = F_m \cdot d\ell = Q (v \times B) \cdot v dt = 0
\]

- **On a Current Element**: From the fact that the convection current \(J = \rho v\) is related to the current element \(Id\ell\) by (2.58), we write

\[
Id\ell = \rho v dV = (\rho dv) v = dQ v
\]

and use the differential charge \(dQ\) in (2.76) to obtain \(dF_m = dQ v \times B\). Then by replacing \(dQ v\) with \(Id\ell\), we can write general relations for the force experienced by integrating the differential force for any of the current elements (2.58) to obtain [66, 166]

\[
F_m = \int_L Id\ell \times B
\]

\[
F_m = \int \int K dS \times B
\]

\[
F_m = \int \int \int J dV \times B
\]

- **Between Two Current Elements**: A current element can feel the magnetic field of another current element and thus experience a force. Hence, if we have two current elements, according to Biot-Savart’s law (2.57), each element will produce its own magnetic field, and each of these magnetic fields will interact with the other element (but not with the element producing it.) If we take the differential

---

\[\text{Alternatively, we may use the definition of electric current}\]

\[
Id\ell = \frac{dQ}{dt} d\ell = dQ \frac{d\ell}{dt} = dQ v
\]
of (2.78a) twice, we obtain \( d (dF_m) = Id\ell \times dB \). Then upon using the differential of (2.66) in the last relation, we obtain, for example, the force \( F_1 \) on current loop 1 due to current loop 2 as the double integral

\[
F_1 = \frac{\mu_0 I_1 I_2}{4\pi} \oint_{L_1} \oint_{L_2} \frac{d\ell_1 \times (d\ell_2 \times a_{R_{21}})}{R_{21}^2}
\]

(2.79)

Now that we considered the forces, we can define the magnetic torque classically as the cross product

\[
\tau_m = r \times F_m
\]

(2.80)

where \( r \) is the moment arm.

### 2.2.2.7 Magnetic Dipoles

The concept of magnetic moment (or dipole) is central to the study of magnetostatics. This is because in the absence of magnetic monopoles (see footnote 52), the most fundamental source and building block of magnetism is the magnetic dipole [160]. In brief, the magnetic dipole moment is defined through a torque relation, and we typically model it classically\(^{44}\) as either an infinitesimal current loop (the physicist’s way) or as a pair of oppositely charged magnetic poles in juxtaposition (the engineer’s way) [67]. The two models are shown in Fig. 2.15 below.

\(\text{Figure 2.15: Classical representations of a magnetic dipole. For the current loop, the direction of the magnetic moment is determined by the right-hand rule. For the piece of magnet, the magnetic moment points from S to N. (a) Current loop model. (b) Magnetic poles model.}\)

**Current Loop:** Referring to Fig. B.2, we define the magnetic dipole moment in terms of a planar current-carrying loop as

\[
\mathbf{m} = J\mathbf{S}
\]

(2.81)

\(^{44}\)We say classically because magnetism is a purely quantum mechanical phenomenon.
where $I$ is the current and $\mathbf{S}$ is an areal vector which points in the normal direction in accordance with the right-hand rule. In the limit as $|\mathbf{S}| \to 0$ while $I \to \infty$, $|\mathbf{m}|$ is finite and the result is an ideal point dipole. The magnetic field produced by this dipole\textsuperscript{45}

$$
\mathbf{B} = \frac{\mu_0}{4\pi} \left[ \frac{3 (\hat{\mathbf{r}} \cdot \mathbf{m}) \hat{\mathbf{r}} - \mathbf{m}}{r^3} + \frac{8\pi}{3} \mathbf{m} \delta (r) \right] 
$$

(2.82)

When the magnetic field is non-uniform, there will be a force given by \textsuperscript{[61]}

$$
\mathbf{F}_m = \nabla (\mathbf{m} \cdot \mathbf{B})
$$

(2.83)

\textbf{Magnetic Poles:} Referring to Fig. B.3, we define the magnetic dipole moment in terms of two opposite Gilbertian charges as

$$
\mathbf{m} = Q_m \ell
$$

(2.84)

where $Q_m$ is the magnetic charge strength and $\ell$ the distance vector which points from $S$ to $N$. The field lines originate from the positive magnetic charge (source) and terminate at the negative magnetic charge (sink). This is analogous to the definition of the electric dipole in electrostatics.\textsuperscript{46} In the limit as $|\ell| \to 0$ while $Q_m \to \infty$, $|\mathbf{m}|$ is finite and the result is an ideal point dipole. The magnetic field produced by this dipole is

$$
\mathbf{B} = \frac{\mu_0}{4\pi} \left[ \frac{3 (\hat{\mathbf{r}} \cdot \mathbf{m}) \hat{\mathbf{r}} - \mathbf{m}}{r^3} - \frac{4\pi}{3} \mathbf{m} \delta (r) \right] 
$$

(2.85)

When the magnetic field is non-uniform, there will be a force given by

$$
\mathbf{F}_m = (\nabla \cdot \mathbf{m}) \mathbf{B}
$$

(2.86)

Looking at the force relations above, one can immediately notice that the force between the two models are related by \textsuperscript{[61]}

$$
\mathbf{m} \times (\nabla \times \mathbf{B}) = \nabla (\mathbf{m} \cdot \mathbf{B}) - (\nabla \cdot \mathbf{m}) \mathbf{B}
$$

(2.87)

which implies that the forces in both models are identical when there are no free currents ($\mathbf{J} = 0$) or time varying electric fields ($\partial \mathbf{D} / \partial t = 0$), see (2.53d).

\textsuperscript{45}Readers who are interested in the derivations of both models are referred to Appendix B.

\textsuperscript{46}One should not take this analogy too far since magnetic dipoles are fundamentally different and are related to angular momentum.
According to (B.15), a magnetic moment aligned with a uniform magnetic field experiences no net torque. If there is a misalignment by an angle $\theta$, the torque is nonzero and work has to be done by the field. Integrating the potential energy $dE_m = |\tau_m| d\theta$, one finds

$$E_m = \int |\mathbf{m}| |\mathbf{B}| \sin \theta d\theta = - |\mathbf{m}| |\mathbf{B}| \cos \theta + C$$

where $C$ is a constant of integration. For simplicity, one can take $C = 0$ and write the potential energy of a magnetic dipole as

$$E_m = - \mathbf{m} \cdot \mathbf{B}$$

which is usually called the Zeeman energy.

### 2.2.3 Magnetism in Condensed Matter

#### 2.2.3.1 Magnetization

Macroscopically, all substances are magnetic to some extent, and every material acquires a magnetization when placed in a magnetic field, which is a measure of the net alignment of magnetic moments [66, 152, 166, 170]. We define the magnetization as the net magnetic moment per unit volume. For $N$ magnetic moments in an infinitesimal volume $\Delta V$, the magnetization is given by [61, 66, 78, 152, 169]

$$\mathbf{M} = \lim_{\Delta V \rightarrow 0} \sum_{i=1}^{N} \frac{\mathbf{m}_i}{\Delta V}$$

The value of $\mathbf{M}$ is a property of the material itself and generally depends on the individual magnetic moments of the ions, atoms, or molecules and how these moments interact with one other [66, 67]. In a condensed matter, the magnetic flux density will be [66, 169]

$$\mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M})$$

The above relation holds for all materials (whether linear or nonlinear, isotropic or anisotropic) [66]. For linear and isotropic materials, the magnetization is proportional to the magnetic field [66, 169]

$$\mathbf{M} = \chi_m \mathbf{H}$$

where $\chi_m$ is a dimensionless number called the magnetic susceptibility of the material. Using (2.91) in (2.90), one can write [66, 169]

$$\mathbf{B} = (1 + \chi_m) \mu_0 \mathbf{H} = \mu_r \mu_0 \mathbf{H} = \mu \mathbf{H}$$
where $\mu$ is the **magnetic permeability** and $\mu_r$ the **relative permeability** of the material. For anisotropic media (e.g., crystals), the vector fields are not parallel, and we speak of susceptibility and permeability tensors\(^{47}\)

\[
\chi_m = \begin{bmatrix}
\chi_{m11} & \chi_{m12} & \chi_{m13} \\
\chi_{m21} & \chi_{m22} & \chi_{m23} \\
\chi_{m31} & \chi_{m32} & \chi_{m33}
\end{bmatrix}
\] (2.93)

\[
\mu = \begin{bmatrix}
\mu_{11} & \mu_{12} & \mu_{13} \\
\mu_{21} & \mu_{22} & \mu_{23} \\
\mu_{31} & \mu_{32} & \mu_{33}
\end{bmatrix}
\] (2.94)

where each component of the vector now obeys the relations

\[
M_i = \chi_{mj}^i H_j
\] (2.95)

\[
B_i = \mu_{ij}^i H_j
\] (2.96)

If we wish to define a magnetic scalar potential $V_m$ inside a material, we can still follow the approach in 2.2.2.4. However, the divergence equation (2.54a) is now modified. In particular, if we use (2.90) in Maxwell’s equations for magnetostatics (2.54) while still assuming a current-free region ($J = 0$), we obtain

\[
\nabla \cdot \mathbf{H} = -\nabla \cdot \mathbf{M}
\] (2.97a)

\[
\nabla \times \mathbf{H} = 0
\] (2.97b)

where we have eliminated $\mu_0$ since it is a scalar. Then from (2.97b), we can use (A.142), to write $\mathbf{H} = -\nabla V_m$ so that (2.97a) becomes $\nabla \cdot (\nabla V_m) = \nabla \cdot \mathbf{M}$. Thus we obtain

\[
\nabla^2 V_m (\mathbf{r}) = \begin{cases}
\nabla \cdot \mathbf{M}, & \mathbf{r} \in \Omega \\
0, & \mathbf{r} \in \mathbb{R}^3 \setminus \Omega
\end{cases}
\] (2.98)

Together with the jump conditions

\[
\left. \frac{\partial V_m}{\partial n} \right|_{in} - \left. \frac{\partial V_m}{\partial n} \right|_{out} = \mathbf{M} \cdot \mathbf{a}_n
\] (2.100)

The equation has the well-known solution \([61, 163, 169]\)

\[
V_m = \frac{1}{4\pi} \left[ -\iiint_{\Omega} \frac{\nabla' \cdot \mathbf{M} (\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' + \iint_{\Sigma} \frac{\mathbf{M} (\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dS' \right]
\] (2.101)

\(^{47}\)See A.1.2.2 for a brief overview of tensors.
where the integrands, in fact, play the role of source volume and surface magnetic charges

\[ \rho_{mv} = -\nabla \cdot M(r') \]  
\[ \rho_{mS} = M(r') \cdot a_n \]  

(2.102)  
(2.103)

Using a similar approach but for the vector potential \( A \) (which can be the natural approach when source currents are present), one can show that the general solution of the vector Poisson equation (2.74) is given by \([66, 169]\)

\[ A = \frac{\mu_0}{4\pi} \left[ \iiint_{\Omega} \frac{\nabla' \times M(r')}{|r - r'|} dV' + \int_{\Sigma} \frac{M(r') \times a_n}{|r - r'|} dS' \right] \]  

(2.104)

where the integrands now play the role of volume and surface magnetization currents

\[ J_m = \nabla' \times M(r') \]  
\[ K_m = M(r') \times a_n \]  

(2.105)  
(2.106)

### 2.2.3.2 Classes of Magnetic Materials

The magnetic behavior depends not only on the type of atom (ion) and unpaired spins but also on the lattice symmetry and cell size. This essentially means that every material responds to a magnetic field differently \([153]\). Phenomenologically, a magnetic material can be characterized by a magnetic susceptibility \([15, 78]\). Some materials show a non-cooperative magnetic behavior; examples are diamagnetic and paramagnetic materials (Fig. 2.16) \([61, 78]\). In diamagnetic materials, \( \chi_m \) is reversible, small, and negative, and as a result \( M \) is slightly repelled by \( H \) \([153, 171]\). Diamagnetism is a fundamental property of all materials (although often masked by stronger effects) and is temperature independent \([15, 66, 67]\). It is essentially observed in materials with filled orbital shells, i.e. atoms with no unpaired electrons \([15, 66, 67, 153]\). In paramagnetic materials, \( \chi_m \) is reversible, small, and positive, and \( M \) is thus slightly attracted by \( H \) \([66, 67]\). Unlike diamagnetism, paramagnetism results from unpaired spins which align with the application of a magnetic field and reorient randomly once the field is removed due to the thermal disorder and is thus temperature dependent \([67, 78, 171]\).

Because of electron-electron interaction, another class of materials show a cooperative (or collective) magnetic behavior (i.e. magnetic order) below certain ordering temperatures, even in the absence of magnetic fields; e.g. ferromagnetism, antiferromagnetism, and ferrimagnetism (Fig. 2.17) \([61, 68, 70, 78, 153, 171]\). In contrast to paramagnets, in which individual spins of atoms or ions respond independently to an external field, electron spins of the atoms constituting a ferromagnet are more coupled \([67]\).
The local magnetic moments in these materials align along a certain direction, showing a very large and positive $\chi_m$, causing $\mathbf{M}$ to be highly attracted by $\mathbf{H}$ [66, 70]. This is manifested by the lattice geometry and spacing which allows for direct exchange interaction between neighboring electrons, forcing a mutual alignment of their spins [67, 172]. The ferromagnetic order can only exist below an ordering temperature called the Curie temperature $T_C$, above which ferromagnetic order vanishes and paramagnetism results [67, 78, 153, 173]. Some crystal structures, on the other hand, permit an indirect exchange interaction, conferring magnetic behaviors that are similar to ferromagnetism, e.g. antiferromagnetism and ferrimagnetism [15, 75, 171]. Antiferromagnetic materials have adjacent sublattices with equal and opposite magnetic moments, showing a net zero moment and hence no spontaneous magnetization [61, 68, 171]. The antiferromagnetic order breaks down at a temperature known as the Néel temperature $T_N$ [61, 67]. Ferrimagnetic materials, on other hand, have opposite but unequal magnetic moments of sublattices, resulting in a nonzero net moment and a spontaneous magnetization. Like ferromagnetism, the ferrimagnetic order breaks down at the Curie point $T_C$ [68, 171].

2.2.4 Magnetic Domains

In his two papers, and based on earlier work of Ampere, Weber, and Ewing, Weiss proposed [174, 175] a hypothesis trying to explain why a virgin ferromagnetic sample has no net magnetic moment (i.e., demagnetized or in null state) and came up with what is now known as the domain theory of ferromagnetism (sometimes linked to the molecular or mean field theory) [61, 82, 169, 173]. Weiss postulated the existence of an
**internal molecular field**\textsuperscript{48} below a critical temperature (the Curie temperature, \(T_C\)) that causes the magnetic dipoles to align parallel and set up a spontaneous magnetization, and that a macroscopic ferromagnetic specimen is generally composed of domains\textsuperscript{49} (regions of uniform magnetization) that are separated by domain walls (narrow transition region between magnetic domains) \[78, 172\]. His theory, though too simple and incomplete, was probably the first and most important advancement in understanding ferromagnetism \[173\]. Weiss did not try to explain the origin of that molecular field, the hysteresis behavior (Fig. 2.18), or why those domains form in the first place \[173\]. It was not until 1928, when Heisenberg \[73\], based on Pauli’s exclusion principle, showed that the molecular field is \textit{electrostatic} in nature, being caused by \textit{exchange interaction} between electrons \[61\]. Few years later, Bitter \[178, 179\] confirmed the existence of domains using a fine magnetic powder and Bloch \[180\] provided a theoretical analysis of domain walls. Later in 1935, L. D. Landau and E. M. Lifshitz \[158\] explained the subdivision of a large sample into several magnetic domains to be a consequence of energy minimization. The model proposed by Landau and Lifshitz was too simple, and further improvements and refinements were needed to explain actual observations. The currently accepted form can be found in \[181, 182\].

\textsuperscript{48}In an analogy with van der Waals theory of 'internal pressure' \[176\]. Although no such field exists in reality, the concept served as an approximation to the interatomic Coulomb interaction in quantum mechanics (which Heisenberg later explained) \[61\].

\textsuperscript{49}The term 'domain' did not appear until 1926 \[177\].
2.2.4.1 Formation of Domains: Energy Considerations

In general, magnetic domains form due to different interactions present in the material such as exchange interaction (favoring parallel alignment of spins), anisotropy\(^{50}\) (favoring the alignment of spins along certain preferential axes), dipolar (favoring antiparallel alignment of spins), and Zeeman (favoring alignment of spins with the external field)\(^{51}\) [15, 78, 82, 169, 183]. The formation of domains does not seem to have a common origin as it could arise from the necessity to reduce stray fields or the adoption of some anisotropy (determined by the crystal structure, shape, and material parameters) [176]. However, it is intuitive to explain the phenomenon using arguments concerning energy minimization.

Consider the scenario in Fig. 2.19a, which shows a large, uniformly magnetized (initially single domain) ferromagnet with no applied magnetic fields in the space surrounding it. It is useful to associate the magnet with \textit{pseudo}-surface magnetic monopoles that are 'smeared' around each end of the sample (Fig. 2.19b).\(^{52}\) In an analogy with electric charges, magnetic charges act like sources and sinks. That is, magnetic flux lines (whether inside or outside the sample) will originate from the positive magnetic charge (radially outward) and terminate on the negative magnetic charge (radially inward). Hence, the poles at the surface contribute by producing a stray magnetic field that extends into the space outside the sample (Fig. 2.19c) [82]. Moreover, \textit{inside} the sample, the poles themselves produce another field that is opposite in direction to the field \textit{outside}. This field is called the \textit{demagnetizing field}, since it reflects the tendency of that field to reduce

\(^{50}\)Anisotropy generally refers to the dependence of magnetization/magnetic properties on direction. A good anisotropy is a prerequisite for hard magnets, whereas near-zero anisotropy is a prerequisite for soft ones [61].

\(^{51}\)The energy terms will be discussed in detail later.

\(^{52}\)We said 'pseudo' because there are no known magnetic charges; they are fictitious elements. In contrast to electric charges, isolated magnetic charge do not exist [66, 67]. This follows from Gauss' law of magnetostatics (2.54a). However, one can think of \textit{dipoles} or equivalently, \textit{two oppositely charged monopoles} (see 2.2.2.7). For example, inside the material the flux density is given by \(\mathbf{B} = \mu_0 (\mathbf{H}_m + \mathbf{M})\). From (2.97) and the boundary conditions, one can associate the magnetic field \(\mathbf{H}_m\) with volume and surface magnetic charge densities \(\rho_{mv} = -\nabla \cdot \mathbf{M}\) and \(\rho_{mS} = \mathbf{M} \cdot \mathbf{a}_n\).
the total magnetic moment and hence 'demagnetize' the specimen. The dipolar field will require a lot of internal magnetostatic energy to be stored in the material, an energy equivalent to the total interaction energy of all the magnetic dipoles in the material.

![Demagnetizing Field](image)

**Figure 2.19:** The demagnetizing field of a uniformly magnetized ferromagnet. (a) Magnetized magnet. (b) Pseudo-charge formation. (c) Demagnetizing field.

Given the picture above, one can immediately see how even in the absence of external fields, the configuration corresponding to a single domain is not the most favorable (or stable). In fact, since all spins are aligned together, along the anisotropy axis, the exchange and anisotropy energies are both zero, and the dipolar energy is maximized \([82]\). In order to minimize the potential energy associated with the single domain specimen, the material has to break into several uniformly magnetized regions (domains) with different orientations of magnetization (Fig. 2.20) \([15, 71, 78]\). For example, the dipolar energy can be approximately halved if the single domain splits into two domains with oppositely directed magnetizations. It reduces since the spatial extent of the stray field has decreased when the (+) and (-) surface charge are brought closer. The energy can be further halved by another split. The division continues until the energy of the whole sample is minimized (or equivalently, until all oppositely charged monopoles are brought closer) \([176, 184, 185]\). A closure configuration can bring the magnetostatic energy to almost zero (or equivalently, oppositely charged monopoles canceling one another). This is usually related to the **pole-avoidance principle**, which simply reflects the fact that the magnetization will tend to reduce the magnetic poles as much as possible \([78, 169]\).

### 2.2.4.2 Domain Walls

According to the arguments given about domain formation, the subdivision of an arbitrarily shaped magnet might continue indefinitely, which is physically impossible. The subdivision will stop at some point because of the energy needed to produce domain walls (and maintain them) \([15, 78, 169]\). Domain walls are transition regions of finite
widths where the magnetization of a magnetic body change direction from that in one domain to that in the other. The energy associated with the formation of a domain wall is merely determined by exchange interaction and anisotropy [21, 78, 82, 169]. The more gradual the rotation in a domain wall, the less the cost in exchange energy. The thinner the domain wall, the less cost in anisotropy energy. Such variations give rise to different types of domain walls. The three main types are the Bloch (magnetization rotates in the plane of the wall), Néel (magnetization rotates in the plane of the film), and cross-tie walls [61, 78, 82, 169].

2.2.5 Characteristic Length Scales—The Big Picture

Modern spintronic devices utilize magnets with dimensions in the nanoscopic (1–100 nm) and mesoscopic (100–1 μm) scales [12, 78]. At such reduced dimensions, material properties change dramatically and differ from their bulk counterparts. Some of the size-specific properties observed in nanodevices are random anisotropy, superparamagnetism, Coulomb blockade, oscillatory exchange interaction, magnetic moment enhancement, high saturation field, current-induced switching, GMR, TMR, and BMR [15, 21, 61, 65, 68, 78, 82]. The emergence of nanomagnetism phenomena in spintronics lies essentially in the fact that at least one the device dimensions is comparable to the

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53When we say 'magnet', we usually mean a ferromagnet. The distinction is important since domain walls also exist in other magnetically ordered materials but exhibit different forms and properties [172].
so-called characteristic lengths\textsuperscript{54} of the sample, below which interesting phenomena are observed \textsuperscript{68}. By transcending these length scales, the observed magnetic (and electric) properties can either be enhanced or suppressed. Moreover, these length scales will determine the ultimate limits on the performance of the device \textsuperscript{82}.

Many of the defining length scales in magnetism are determined from considerations regarding energy minimization \textsuperscript{82, 184}.\textsuperscript{55, 56} In particular, by a competition between different energy terms \textsuperscript{68}. The length scales will determine the “most appropriate description” of the magnetic sample. For example, consider a large macroscopic magnet. The stray (or dipolar) fields will cause splitting of the sample into many domains that are separated by domain walls. The macroscopic average magnetization (determined by the alignment of domains) adequately describe the character of the magnet as a function of the applied magnetic field (top of Fig. 2.22). As the size reduces, one has to include other forms of energy (e.g. exchange and magnetocrystalline anisotropy) and describe the structure of domains and domain walls \textsuperscript{15}. There exist two models for that matter: the domain theory, which deals with the microstructure of discrete domains and domain walls, while assuming vanishing walls widths and thus discontinuous magnetization at the boundaries; and micromagnetism, which invokes a continuum hypothesis and assumes continuous magnetic moments distribution \textsuperscript{183}. As we reduce the size even further, atomic description is necessary and one has to deal with the structure of spins and their arrangement in the crystal lattice \textsuperscript{183}.

Some of the typical length scales are the exchange length $l_{ex}$, domain wall width parameter $d_{DW}$, and critical single domain diameter $d_{sd}$, respectively given by \textsuperscript{21, 61, 68, 78, 169}

\begin{align*}
l_{ex} &= \sqrt{\frac{2A}{\mu_0 M_s^2}} \\
d_{DW} &= \sqrt{\frac{A}{K_1}} \\
d_{sd} &= 72\frac{\sqrt{AK_1}}{\mu_0 M_s^2}
\end{align*}

where $A$ is the exchange coefficient within a grain and $K_1$ is the bulk anisotropy constant. The exchange length separates the zone where exchange interaction dominates ($L < l_{ex}$.

\textsuperscript{54}Plus broken translational symmetry, and the fact that nanoscopic objects contain higher proportion of surface/interfacial atoms and low coordination numbers \textsuperscript{61, 68, 78}.

\textsuperscript{55}See the discussion in 2.2.4.1 and 2.2.4.2.

\textsuperscript{56}Other length scales like the spin-diffusion length $\ell_{sf}$ and the spin-precession length $\ell_{sp}$ could result from the diffusion processes of energy, momentum or magnetization \textsuperscript{61, 82}. 
Magnetic Hysteresis (> 0.1 mm)
Describes the average magnetization vector of a sample as a function of the applied field

Domain Theory (1 – 1000 μm)
Describes the magnetic microstructure of a sample with details about the domains and domain boundaries

Micromagnetic Analysis (1 – 1000 nm)
Describes the internal structure and substructure of domain walls using a continuum theory

Atomic Theory (< 1 nm)
Describes the origin, the interaction, and the statistical thermodynamics of magnetic moments

Figure 2.22: Descriptive hierarchy of magnetically ordered materials. The levels are roughly distinguished with length scales. Figure adapted by the author from [176, 183].

where magnetization is uniform and coherent reversal takes place)\textsuperscript{57} from that where dipolar interaction dominates (\(L > l_{ex}\), where incoherent reversal of magnetization takes place through different processes like curling, buckling, and fanning), and can be in the range 1–100 nm [21, 68, 78, 169].\textsuperscript{58} The domain wall width parameter \(d_{DW}\)\textsuperscript{59} is determined by a competition of exchange and anisotropy, or exchange and dipolar (when anisotropy is weak), and depends on the sample geometry [82]. It usually falls in the range 1–100 nm [68, 78]. This parameter corresponds to the width of a Bloch wall that is found in materials where the main source of anisotropy is magnetocrystalline anisotropy (e.g., hard materials) [68]. In thin films of soft magnetic materials where surface charges are large (and are replaced by volume charges as suggested by Néel), the domain wall width parameter corresponds to a Néel wall. Finally, the critical single domain size \(d_{sd}\) can range from 5 nm for soft materials up to 1000 nm for hard ones [78]. Below this length, the magnet is single domain, whereas above it can exhibit a multidomain, or even vortex\textsuperscript{60} configuration. In general, the above parameters follow the inequalities below

\textsuperscript{57} A reversal is coherent (or homogeneous) when the moments remain strictly parallel throughout the process, independent of \(r\) [61, 78]. An incoherent (or inhomogeneous) reversal, on the other hand, might involve an intermediate state which is not uniformly magnetized.

\textsuperscript{58} Some authors [61, 78, 169] use a more strict measure for coherence reversal, a parameter called the \textit{coherence radius}, given roughly by the expression \(R_{coh} = \beta l_{ex}\), where \(\beta\) varies between 5.2 and 7.2. This gives the maximum size (i.e., upper bound) of coherent reversal of a uniformly magnetized particle and generally depends on the detailed shape as well as material parameters.

\textsuperscript{59} The \textit{domain wall width} is given by \(\pi d_{DW}\) [76, 78].

\textsuperscript{60} Also known as a swirl; a circular arrangement of magnetic moments.
Soft Material:
\[ d_{sd} \sim l_{ex} \ll d_{DW} \] (2.107)

Hard Material:
\[ d_{sd} \gg l_{ex} \geq d_{DW} \] (2.108)

2.3 Micromagnetism

Micromagnetism is a continuum theory to describe the magnetization distribution in mesoscopic magnetic structures [21]. Because the spintronic devices of interest are too small, a model solely based on Maxwell’s electrodynamics, though simple, is however inaccurate since it does not take into account many of the coupled mechanisms such as exchange interaction or anisotropy [187–189]. On the other hand, the devices are still too large for them to be considered 'atomistic', and hence, a pure quantum mechanical approach is of prohibitive difficulty and computationally expensive (and, in fact, would seem 'utopic') [189]. Micromagnetics is an intermediate solution; way beyond the range of classical electromagnetic theory, yet far from being considered an atomic scale theory. It includes effects on different spatial scales such as the long-range dipolar interaction and the short-range exchange interaction. Although it usually leads to complex nonlinear equations—for which only a few idealized cases result in analytic solutions—it bridges the gap and smoothly interpolates between the two approaches. It assumes a continuum magnetization configuration while, at the same time, uses results that have been derived from a quantum mechanical treatment (with a formalism appropriate for the limit of continuous material). The latter fact, coupled with an energy minimization approach and a dynamic formalism [158], forms the basic principles of micromagnetism.

The theory was originally developed in 1935 by Landau and Lifshitz [158] based on a variational principle, and later heavily contributed to by Brown with the rise of computational science in the 1940s [186, 190]. Brown coined the term 'Micromagnetics' in 1958 [190]. A classical treatment micromagnetics can be found in Brown’s early [191, 192] and late [193] books.

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61. Within the framework of the continuum theory in mechanics, a magnetizable specimen is composed of two interacting continua: lattice continuum and the spin continuum.

62. As long as any characteristic length is much larger than the size of a unit cell, the assumption of a continuous material is valid [186].

63. In particular, a semiclassical approach is invoked in which spins are replaced by classical vectors and quantum mechanical exchange interaction in the Heisenberg Hamiltonian by a classical exchange energy term [186].

64. This name could be misleading because in micromagnetism the microscopic structure (i.e., atomic nature of the material) is ignored.
2.3.1 Assumptions and Definitions

The semiclassical approach adopted by micromagnetism is based on the hypothesis that the average magnetization is a smoothly varying function of position with fixed magnitude. In particular

- The function $\mathbf{M}$ describes the magnetic structure in a continuous manner; it ignores the discrete nature of the atomic magnetic moments and replaces the ensemble of unpaired electron spins with a local averaged magnetization over a small volume $d\Omega_r$ of the ferromagnetic body (Fig. 2.23), where $\mathbf{r} \in \Omega$ is the position vector. Assuming the elemental volume $d\Omega_r$ contains enough magnetic moments so that: (a) Statistical and thermodynamical methods can be used to describe the properties, (b) fine-scale details and microscopic fluctuations average out, and (c) average magnetic moment varies smoothly $[169, 194, 195]$, we can define the net magnetic moment occupying a volume $d\Omega_r$ of a homogeneous medium by the product $\mathbf{M}(\mathbf{r}) d\Omega_r$, and hence define the magnetization vector as $[183]$

$$\mathbf{M}(\mathbf{r}) = \sum_i \frac{\mathbf{m}_i}{d\Omega_r}$$  \hspace{1cm} (2.109)

Figure 2.23: $d\Omega$ is the differential volume over which the magnetization is uniform.

- Within the sufficiently small averaging volume, one also assumes sufficiently low temperatures (well below $T_C$) such that thermal fluctuations still average out and exchange interaction prevails over all the other interactions in $d\Omega_r$ $[65, 157, 169, 183, 195, 196]$. Under this assumption, the ferromagnetic body is always locally

---

$^{65}$More precisely, the expectation value of the magnetic moment per unit volume due to spin and orbital angular momentum of unpaired electrons, averaged over a few lattice cells $[194]$. However, since we will be mostly dealing with 3d ferromagnets where orbital momentum is quenched, we will consider spin contribution only, and adjust some parameters later if we want to include the orbital contribution (e.g. adjusting the gyromagnetic ratio $[21, 194]$).

$^{66}$Not to be treated as the average magnetization $\mathbf{M} = \mathbf{B}/\mu_0 - \mathbf{H}$ used in classical electromagnetics, which is averaged over the whole volume of the ferromagnet $[194]$.

$^{67}$That still satisfies the continuum hypothesis.
saturated [157, 196], and we obtain the so-called fundamental constraint of micromagnetism

\[ |\mathbf{M}(r, t)| = M_s(T) \iff |\mathbf{m}(r, t)| = 1 \]  

(2.110)

where \( M_s \) is the saturation magnetization which depends on both the material and temperature.\(^{68}\)

Consider a ferromagnetic body (Fig. 2.24) at a temperature \( T \) occupying a bounded domain \( \Omega \subset \mathbb{R}^3 \) with a smooth boundary \( \partial \Omega \). From the previous assumptions, we can formally define the local magnetization at every point inside the body by the differentiable vector field \( \mathbf{M}(r, t) \) given as the map

\[ \mathbf{M} : (0, T) \times \Omega \to \{ \mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| = M_s \} \]  

(2.111D)

where \( M_s > 0 \) is the constant saturation magnetization at the temperature \( T \). The magnetization is assumed to vanish on \( \mathbb{R}^3 \setminus \Omega \) and for \( T \geq T_c \). Although the magnitude of \( \mathbf{M} \) is constant in space, its direction is allowed to vary. Thus we can write \( \mathbf{M} = M_s \mathbf{m} \), from which we define the reduced magnetization (or magnetic moment)\(^{69}\)

\[ \mathbf{m}(r, t) = \frac{\mathbf{M}(r, t)}{M_s} \]  

(2.112)

which can then formally be defined as

\[ \mathbf{m} : (0, T) \times \Omega \to \{ \mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| = 1 \} \]  

(2.113D)

Sometimes, one may write \( \mathbf{m} \) as

\[ \mathbf{m} : (0, T) \times \Omega \to S^2 \]  

(2.114D)

where \( S^2 \) denotes the unit sphere of \( \mathbb{R}^3 \).

\(^{68}\)The saturation magnetization vanishes above the Curie temperature \( T_C \) where phase transition takes place (a characteristic of each crystal type) [61, 71, 171, 173]. However, since we usually work with ferromagnets way below the Curie point and assume temperature to be uniform in space and constant in time, \( M_s \) can be taken as a material-dependent constant and therefore a single number when working with a single-crystal ferromagnet.

\(^{69}\)This is not the magnetic moment of the atom.
2.3.2 Micromagnetic Energy

2.3.2.1 Thermodynamics

A model of a magnetic medium is generally analyzed within a thermodynamic framework where the body is characterized in terms of its internal energy, and the temporal evolution of the involved variables (e.g., magnetization) is then determined under the goal of “total energy” minimization. For a unit volume $d\Omega$ of a material that is in contact with a thermal bath at temperature $T$, the principal thermodynamic laws are:

1st law of thermodynamics (energy conservation): When work $\delta W$ is performed on the system and heat $\delta Q$ is absorbed by it, the change in internal energy is given by the sum\footnote{The symbol $\delta$ usually denotes an inexact differential, a quantity which has a circulation that is not necessary zero, viz.} \[
dU = \delta W + \delta Q \tag{2.115}\]

For a state (i.e., extensive) variable $X$ describing some property of the system, and its conjugate (i.e., intensive) variable $Y_X$ describing some external action exerted on the system, one can always express the differential work as

\[
\delta W = Y_X dX \tag{2.116}\]

2nd law of thermodynamics (irreversible process): For an irreversible transformation in a non-isolated system, the entropy changes as

\[
dS \geq \frac{\delta Q}{T} \tag{2.117}\]

On the other hand, the special symbol $d$ is usually reserved for exact differentials (i.e., path-independent quantities) \[
\oint \delta A \neq 0
\]

\[
\oint dA = 0
\]
Under a reversible transformation, the equality holds and one has
\[ \delta Q = T \delta S \quad (2.118) \]
which in fact reveals that \( T \) and \( S \) are extensive and intensive variables, respectively (i.e., conjugate variables)\(^{71}\). The 2nd law can also be formulated as
\[ dS = \frac{\delta Q}{T} + dS_{irr} \quad (2.119) \]
where \( dS_{irr} \) is the amount of entropy generated by the irreversibility of the transformation. It is obvious that \( dS_{irr} \geq 0 \), where \( dS_{irr} = 0 \) holds for a reversible process.

Consider the general set of magnetic, mechanical, and thermal processes shown in Fig. 2.25. As pioneered by Massieu and Gibbs, one can analyze the static properties of any physical system by what we call thermodynamic potentials, which are state functions controlling how a transformation will evolve \([84, 169]\). There are four potentials of interest, each defined by fixing two variables and leaving the other two [61]. The potentials are: Internal Energy \( u(X,S) \), Enthalpy \( h(Y_X,S) \), Helmholtz Free Energy \( f(X,T) \), and Gibbs Free Energy \( g(Y_X,T) \); all in units of J·m\(^{-3}\) and each reaching a minimum at thermodynamic equilibrium and never increases under any transformation when the respective arguments are fixed [61, 169]. According to Fig. 2.25, the extensive variables are \( X = M, \varepsilon, S \), and the intensive variables are \( Y_X = H_a, \sigma, T \).

Consider an object in internal thermodynamic equilibrium at temperature \( T \). Although \( u(M,\varepsilon,S) \) is useful for studying adiabatic (isentropic) processes, in our case \( T \) is fixed and it is better to make a Legendre transformation to the variables \( (M,\varepsilon,T) \) and \( (H_a,\sigma,T) \). Thus the relevant potentials in this case are \( f(M,\varepsilon,T) \) and \( g(H_a,\sigma,T) \). With these potentials, we would measure the system’s ability to do work, i.e. find its free energy. The Helmholtz free energy density is given by the Legendre transformation
\[ f(M,\varepsilon,T) = u(M,\varepsilon,S) - TS \quad (2.120) \]
where the first term is related to all interaction energy terms within a magnet and the second term is constant at a given temperature [163]. In our case, the internal energy is determined by exchange interaction, crystalline anisotropy, magnetostatic, and magnetoelastic\(^{72}\) [199]. In fact, since the change in magnetomechanical work (due to

\(^{71}\)Equations (2.116) and (2.118) in fact reveal the symmetry between the extensive \((X,S)\) and intensive \((Y_X,T)\) variables involved: \( T \) and \( S \) are conjugate variables with respect to thermal energy, whereas \( Y_X \) and \( X \) are conjugate variables with respect to external work.

\(^{72}\)A change in magnetization may produce a deformation in the crystal lattice (and vice versa), a phenomenon known as magnetostriction [61, 82, 198].
The internal energy is

\[ du(M, \varepsilon, S) = \mu_0 H_a \cdot dM + \sigma d\varepsilon + T dS - T dS_{irr} \]  

(2.123)

Thus, the differential Helmholtz free energy becomes

\[ df(M, \varepsilon, T) = \mu_0 H_a \cdot dM + \sigma d\varepsilon - S dT - T dS_{irr} \]  

(2.124)

Since the body is not necessarily in external equilibrium with the applied field \( H_a \), and it is this field that we can control (in addition to temperature), the Gibbs free energy density is an appropriate state measure. It is given as the transformation \([61, 78, 199]\)

\[ g(H_a, \sigma, T) = f(M, \varepsilon, T) - \sigma \varepsilon - \mu_0 M \cdot H_a \]  

(2.125)

The Gibbs free energy has the differential

\[ dg(H_a, \sigma, T) = -\mu_0 M \cdot dH_a - \varepsilon d\sigma - S dT - T dS_{irr} \]  

(2.126)
which is a non-increasing function when its arguments are fixed, viz.

\[ dg(H_a, \sigma, T) = -TdS_{irr} \leq 0 \]  

(2.127)

since \( TdS_{irr} \geq 0 \). The minima of \( g \) gives the values \( M, \varepsilon, S \) to which the material converges as equilibria. The equilibrium equations are given by

\[
\begin{align*}
\frac{\partial g(H_a, \sigma, T)}{\partial \mathbf{M}} & = 0 \\
\frac{\partial g(H_a, \sigma, T)}{\partial \varepsilon} & = 0 \\
\frac{\partial g(H_a, \sigma, T)}{\partial S} & = 0
\end{align*}
\]

(2.128)  (2.129)  (2.130)

The above conditions are in fact equivalent to

\[
\begin{align*}
\mathbf{M} & = -\frac{1}{\mu_0} \left[ \frac{\partial g(H_a, \sigma, T)}{\partial H_a} \right]_{\sigma, T} \\
\varepsilon & = - \left[ \frac{\partial g(H_a, \sigma, T)}{\partial \sigma} \right]_{H_a, T} \\
S & = - \left[ \frac{\partial g(H_a, \sigma, T)}{\partial T} \right]_{H_a, \sigma}
\end{align*}
\]

(2.131)  (2.132)  (2.133)

The first equation in fact reveals that \( \mathbf{M} \) has to be expressed with the equation of state [61]

\[ \mathbf{M} = \mathbf{M}(H_a, \sigma, T) \]  

(2.134)

which, at thermodynamic equilibrium, and for a given \((H_a, \sigma, T)\), is uniquely determined. However, this is not the case for a ferromagnetic body: the variables \((H_a, \sigma, T)\) are not sufficient to uniquely determine the state of \( \mathbf{M} \). This is because the free energy will have many local minima (metastable equilibria, Fig. 2.26) [78]; a framework known as nonequilibrium thermodynamics [169]. This can be analyzed by a generalization of the Gibbs energy to the Landau-Gibbs free energy \( g_L \), given by [169]

\[
g_L(M; H_a, \sigma, T) = f(M, \varepsilon, T) - \sigma \varepsilon - \mu_0 \mathbf{M} \cdot \mathbf{H}_a
\]

(2.135)

\[
g_L(M; H_a, \sigma, T) = u(M, \varepsilon, S) - TS - \sigma \varepsilon - \mu_0 \mathbf{M} \cdot \mathbf{H}_a
\]

(2.136)

which coincides with the Gibbs energy (2.125) at thermodynamic equilibrium (except for the fact that \( g_L \) explicitly uses \( \mathbf{M} \), forcing it to take certain values and thus acting as if it was an external constraint) [61]. At equilibrium, \( g_L \) is at extremum [169]

\[
\left[ \frac{\partial g_L(M; H_a, \sigma, T)}{\partial \mathbf{M}} \right]_{H_a, T, \sigma} = 0
\]

(2.137)
For a fixed temperature $T \ll T_C$, we can neglect the entropy contribution. Ignoring magnetostriction too as well as any applied stress, we can write the total energy functional as\(^\text{73}\) [21, 78]

$$G_L(M, H_a) = \int_\Omega g_L dV = E_{\text{ex}} + E_{\text{an}} + E_m + E_a$$

(2.138)

where $E_{\text{ex}}$ is the exchange energy, $E_{\text{an}}$ the magnetocrystalline anisotropy energy, $E_m$ the magnetostatic (or dipolar) energy, and $E_a$ the applied field (or Zeeman) energy. The competition between the different energy terms determines the spontaneous magnetic domains configuration [15, 21, 78]. A schematic of the different interactions is shown in Fig. 2.27.

As mentioned previously, each energy term act at a different spatial scale. Exchange interaction is short-range (exponentially decaying [82]) and is involved in the nanoscopic resolution, whereas dipolar interaction is long-range (falls off as $1/r^3$, recall (2.82)) and thus works on the resolution of large samples [21, 70]. The anisotropy term, on the other hand, plays its role at an intermediate level\(^\text{74}\) where magnetic properties are mostly influenced by the size, shape, and boundary properties of grains. The latter statement reveals the complexity of the simulations that has to be performed for such structures, and thus one usually considers a single-crystal ferromagnet with a uniaxial or cubic symmetry, for example.

---

\(^{73}\)In general, we will ignore induced anisotropies (e.g., induced by annealing or stress) such as magnetoelastic and interfacial anisotropies, and only focus on magnetocrystalline anisotropy, which is the only intrinsic type of anisotropy [15, 61, 68]. Moreover, we will ignore the domain wall energy [15] and the effects of eddy currents; the latter is of course justified if one considers nonconducting materials [68, 78, 169, 196].

\(^{74}\)Though sometimes considered a short-range effect [21].
2.3.2.2 Energy Terms

Below, we discuss each energy term. Thermal effects will be included later.

- **Exchange Energy** $E_{\text{ex}}$
  In a solid, the electronic orbitals of contiguous atoms overlap, leading to a correlation between electrons. The result is that the “interatomic interaction” affects the total energy, introducing a dependency on the relative orientation of localized spins in neighboring atoms. Exchange energy is the energy required to rotate one spin with respect to its neighbors (overcoming the Pauli principle) [82, 173]. The interaction results from the electrostatic Coulomb repulsion between electrons, and the spin-dependency of the interaction arises from the requirement that the wave function of a pair of electrons is antisymmetric with respect to the interchange of electron coordinates and spin (Fig. 2.28) [70, 75, 76, 82].\(^{75}\) That is, when the electron spins are parallel, the wave function is antisymmetric in the coordinate part

$$\psi_{\sigma\sigma}(\mathbf{r}_1, \mathbf{r}_2) = -\psi_{\sigma\sigma}(\mathbf{r}_2, \mathbf{r}_1)$$  \hfill (2.139)

\(^{75}\)This comes from the indistinguishability of electrons which implies that exchange of two electrons should keep the total density of the electrons unchanged: $|\psi_{\sigma\sigma}(\mathbf{r}_1, \mathbf{r}_2)|^2 = |\psi_{\sigma\sigma}(\mathbf{r}_2, \mathbf{r}_1)|^2$ [61].

\(\text{Figure 2.27:}\) Four common types of magnetic energy. (a) Exchange. (b) Anisotropy. (c) Magnetostatic. (d) Zeeman.
which simply means the probability that two electrons are in close proximity is small (compared to the other case). This is in agreement with Pauli’s exclusion principle which essentially states that electrons with parallel spins tend to avoid each other spatially so that their wavefunctions do not overlap (i.e. not being in the same place) [14, 15]. As a consequence, the repulsive Coulomb energy is lowered, and this reduction in Coulomb energy is the exchange energy [15, 21, 75].

Figure 2.28: Symmetric and antisymmetric wavefunctions.

The “direct” exchange interaction is the sum of all of the different interactions: spin-spin, spin-orbit, etc. [82]. Usually, one only considers the spin-spin interaction between two contiguous spins and refer to it as a “direct” exchange interaction. In this case, the exchange energy is defined as the energy difference between parallel and antiparallel spin configuration. The exchange energy is typically given as the expectation value of the Heisenberg Hamiltonian. The latter, for example, is given for a two-spin system as [61, 78]

\[ \mathcal{H} = -2J \mathbf{s}_1 \cdot \mathbf{s}_2 \]  

(2.140)

where \( J \) is the exchange parameter which is positive for parallel spins (ferromagnetism) and negative for antiparallel spins (antiferromagnetism or ferrimagnetism)\(^{76}\) [68, 123]. The sign of \( J \) depends on the interatomic distances (i.e. orbital overlap), being negative if the atoms are closely spaced, and positive otherwise (Fig. 2.29).\(^{77}\) Here, \( \mathbf{s}_1 \) and \( \mathbf{s}_2 \) represent the localized electrons spins of adjacent atoms (in units of \( \hbar \)). The interaction is bilinear in spins and isotropic under rotation (guaranteed by the dot product).

\(^{76}\)Depending on the topology of the crystal lattice [61].
\(^{77}\)In the intermediate case, like in \( \gamma \)-Fe\(_2\)O\(_3\) and ferrites, the inter-atomic distance to the atomic size will result in ferrimagnetism [123].
The above expression is quantum mechanical. The classical counterpart can be written by replacing the operators with classical vectors. For many-electron system in a lattice, one can write [68, 78, 82]

\[ E_{ex} = -2J_{ij}s_i \cdot s_j \]  

(2.141)

where \( J_{ij} \) is the exchange parameter linking the \( i \)-th and \( j \)-th spins. Here Einstein’s summation convention is assumed.

The spin-spin exchange interaction penalizes spatial variations in \( M \) and leads to a preferential for large regions of uniform magnetization (magnetic domains) separated by thin transition regions (domain walls) [68, 196]. Exchange interaction is believed to be the main cause of ferromagnetism [78]. For small variations of \( M \) from point to point, one can expand the energy as a function of \( \nabla M \). Assuming a cubic crystal, a continuum (micromagnetic scale) approximation, and limiting to nearest neighbors, the exchange energy can be written by dropping the high order terms as [78, 82, 169, 196]

\[ E_{ex} = \frac{A}{M_i^2} \int \int \int_{\Omega} \left[ (\nabla M_x)^2 + (\nabla M_y)^2 + (\nabla M_z)^2 \right] dV \]  

(2.142)

where \( A = nJS^2/a \) is the exchange stiffness constant for a cubic crystal with one nonequivalent atom; a phenomenological positive material parameter that summarizes the (usually very) short-range exchange interaction. Here \( a \) is the lattice spacing, and \( n = 1 \) for simple cubic lattice, \( n = 2 \) for body-centered cubic (bcc) lattice, and \( n = 4 \) for face-centered cubic (fcc) [78]. Equation (2.142) can be written
more compactly as

\[ E_{ex} = A \frac{1}{M_s^2} \iiint_{\Omega} (\nabla M)^2 dV \]  

(2.143)

In the general case of a non-cubic and anisotropic medium, \( A \) is a tensor and one has

\[ E_{ex} = \frac{1}{M_s^2} \iiint_{\Omega} A_{kl} \frac{\partial M_i}{\partial x_k} \frac{\partial M_i}{\partial x_l} dV \]  

(2.144)

**Magnetocrystalline Anisotropy Energy \( E_{an} \)**

Magnetocrystalline anisotropy is related to the competition between spin-orbit coupling, and the local crystal electric field (single-ion) or the dipole-dipole interaction (two-ion), and thus manifests itself as the energy needed to overcome spin-orbit coupling\(^78\) [15, 21, 61, 68, 70, 82, 169]. The electronic structure induces \( \mathbf{M} \) to lie along certain preferred crystallographic directions, so-called easy-axes \([15, 68]\). The crystal anisotropy is generally determined by a globally non-negative anisotropy energy density functional, \( f_{an}(\mathbf{M}) : \mathbb{R}^3 \to \mathbb{R}^+ \) that depends on material parameters and symmetry of the crystalline lattice microstructure \([21, 171]\). The functional is globally Lipschitz continuous and vanishes (i.e., achieves its minima) on the set of unit vectors known as the easy-axes\(^79\) \([15, 82, 171]\). Using the energy density functional, the anisotropy energy is written as

\[ E_{an} = \iiint_{\Omega} f_{an}(\mathbf{M}) dV \]  

(2.145)

The functional is typically a polynomial possessing certain symmetry properties. In general, \( f_{an}(\mathbf{m}) \) is invariant under inversion of \( \mathbf{m} \) \([169]\). We consider two examples below.

**Uniaxial Anisotropy:** For uniaxial anisotropy, it is convenient to first express the magnetization components in spherical coordinates

\[ M_x = M_s \sin \theta \cos \phi \]  

(2.146)

\[ M_y = M_s \sin \theta \sin \phi \]  

(2.147)

\[ M_z = M_s \cos \theta \]  

(2.148)

---

\(^{78}\) This might also lead to surface anisotropy—breaking of inversion symmetry at the surface or interface—in very thin films \([68, 78, 200]\). Such anisotropy yields an energy of the form \( f_{an,s}(\mathbf{m}) = K_s (1 - \mathbf{m} \cdot \mathbf{a}_n) \) \([61, 78]\).

\(^{79}\) Saddle-points and maxima of \( f_{an}(\mathbf{M}) \) are attained at the medium-hard- and hard-axes, respectively \([169]\).
This gives the rescaled magnetization

\[
\begin{align*}
mx &= \sin \theta \cos \phi \\
m_y &= \sin \theta \sin \phi \\
m_z &= \cos \theta
\end{align*}
\] (2.149)

which only depends on direction. Now, since the anisotropy is symmetric with respect to the easy-axis (i.e., rotationally symmetric), we can write the anisotropy energy density as an even expansion in \(\sin \theta\) [78, 169]

\[
f_{an}(\mathbf{m}) = K_1 \sin^2 \theta + K_2 \sin^4 \theta + K_3 \sin^6 \theta + \cdots
\] (2.152)

where now \(f_{an}(\mathbf{m}) : S^2 \to \mathbb{R}^+\), since we used the rescaled magnetization. Here \(\theta\) is angle between \(\mathbf{m}\) and the easy-axis \(\mathbf{e}_{an}\), and \(K_i\)'s are the anisotropy constants. For simplicity, let us truncate the expansion and consider the first term [61, 68]

\[
f_{an}(\mathbf{m}) \simeq K_1 \sin^2 \theta
\] (2.153)

For \(K_1 > 0\), the energy minima are located on the easy-axis (for \(\theta = 0\) and \(\theta = \pi\)) whereas for \(K_1 < 0\), the minima are located on the easy-plane (for \(\theta = \pi/2\). The uniaxial energy functional can also be written as

\[
f_{an}(\mathbf{m}) \simeq K_1 \sin^2 \theta
\] (2.154)

\[
= K_1 \left[1 - \cos^2 \theta\right]
\] (2.155)

\[
= K_1 \left[1 - (\mathbf{e}_{an} \cdot \mathbf{m})^2\right]
\] (2.156)

Under the hypothesis of uniaxial anisotropy, (2.145) becomes

\[
E_{an} \simeq K_1 \iiint_{\Omega} \left[1 - (\mathbf{e}_{an} \cdot \mathbf{m})^2\right] dV
\] (2.157)

**Cubic Anisotropy:** For cubic anisotropy, we recall that the anisotropy energy density functional must satisfy the symmetry conditions. Namely, for this case it must be: (a) Invariant under any change of any two axes; (b) unaffected by any reversal of \(\mathbf{M}\) (which means it will be an expansion in the direction cosines). A function that satisfies these requirements is the expansion [76–78, 78]

\[
f_{an}(\mathbf{m}) = K_1 (m_x^2 m_y^2 + m_y^2 m_z^2 + m_z^2 m_x^2) + K_2 m_x^2 m_y^2 m_z^2 + \cdots
\] (2.158)

To lowest order

\[
f_{an}(\mathbf{m}) \simeq K_1 (m_x^2 m_y^2 + m_y^2 m_z^2 + m_z^2 m_x^2)
\] (2.159)
For $K_1 > 0$, one has six energy minima corresponding to $x$-, $y$-, and $z$-directions (both positive and negative) [169]. In fact, in total we have: cube edges $\langle 100 \rangle$ as easy-axes (minima), $\langle 110 \rangle$ as medium-hard-axes (saddle), and cube diagonals $\langle 111 \rangle$ as hard-axes (maxima). For $K_1 < 0$, a more complex situation results.\footnote{It can be shown that the roles interchange: there are now eight easy-axes, e.g. along $\langle 111 \rangle$. The $\langle 110 \rangle$ now correspond to medium-hard-axes (saddle points) whereas $\langle 100 \rangle$ are now the hard-axes (maxima) [169].}

**Magnetostatic energy $E_m$**

A magnetized sample generates its own magnetic field, which can be obtained by solving Maxwell’s equations (2.97) [198]. This ‘self-induced’ field is given different names in literature: stray field, demagnetizing field,\footnote{Although most people use the two names interchangably, some authors [61] technically refer to the field outside the sample as a stray field, and the one inside as a demagnetizing field.} dipolar field, or magnetostatic field. The energy associated with this field describes the nonlocal dipolar field term that favors a divergence-free configuration. The magnetostatic energy is given by [61, 78, 82, 169, 196, 198]

$$E_m = -\frac{\mu_0}{2} \iiint_{\Omega} \mathbf{M} \cdot \mathbf{H}_m dV = \frac{\mu_0}{2} \iiint_{\mathbb{R}^3} |\mathbf{H}_m|^2 dV \quad (2.160)$$

where $\mathbf{H} = -\nabla V_m$ in a current-free region with $V_m$ computed using the general solution (2.101). The factor $\frac{1}{2}$ accounts for the fact that this energy arises from the interaction of the magnetization with the magnetic field it produces, thus avoiding double counting the contribution of each differential $\delta \mathbf{m}$ (as a source and as a moment) [61, 78].

The calculation of the magnetostatic field is usually the most computationally difficult and time consuming task in the micromagnetic problem. Fortunately, one can simplify things when the sample is uniformly magnetized. This can be the case, for example, in nanoscopic particles where magnets are mostly single domain, or for ellipsoidal\footnote{Sometimes called a tri-axial or scalene ellipsoid.} particles (and its degenerate shapes: spheroid, long rod, disk, etc.) or perpendicularly magnetized infinite thin films. In this special case, $\mathbf{M}$ is divergenceless and the first integral in (2.101) vanishes, yielding [82, 169]

$$V_m = \frac{1}{4\pi} \mathbf{M} \cdot \iint_{\Sigma} \frac{\mathbf{a}_n}{|\mathbf{r} - \mathbf{r}'|} dS' \quad (2.161)$$

where one can immediately see the proportionality between the potential and the magnetization. Moreover, the potential is merely determined by the geometrical shape of the body [169]. In fact, this is a character of the dipolar field which, due to its long-range interaction, generally depends on the shape. For example, if one considered a spherical particle with no magnetocrystalline anisotropy, then the magnetization has no preferred direction. However, for an ellipsoidal particle, the...
magnetization will align along the longest axis, and thus the effect is sometimes called *shape anisotropy* [21, 61].

In general, for a uniformly magnetized sample of ellipsoidal shape, the demagnetizing field will also be uniform and can be written as \(^{83}[61, 78, 163, 171, 186, 202]\)

\[
H_m = -NM \tag{2.163}
\]

where \(N\) is the ellipsoid demagnetization rank-2 tensor; a real symmetric \(3 \times 3\) matrix

\[
N = \begin{bmatrix}
N^{11} & N^{12} & N^{13} \\
N^{21} & N^{22} & N^{23} \\
N^{31} & N^{32} & N^{33}
\end{bmatrix} \tag{2.164}
\]

of unit trace (i.e., \(N^{11} + N^{22} + N^{33} = 1\)) and non-negative diagonal elements \([169, 202]\). The negative sign indicates the tendency of this field to 'demagnetize' the specimen.

The elements of the demagnetization tensor are still difficult to compute. In the particular case when \(M\) is parallel to one of the principal axes of the ellipsoid, \(N\) is a diagonal matrix

\[
N = \begin{bmatrix}
N_a & 0 & 0 \\
0 & N_b & 0 \\
0 & 0 & N_c
\end{bmatrix} \tag{2.165}
\]

where the subscripts \(a, b,\) and \(c\) denotes the ellipsoid semi-principal axes, and the condition \(N_a + N_b + N_c = 1\) still holds.\(^{84}\) In this case \(H_m\) is related to \(M\) along each direction by a single number; typically called in literature a *demagnetization factor* \([186]\). Using this matrix, one can use the first integral in (2.160) with (2.163) and write the magnetostatic energy as \([78, 169]\)

\[
E_m = \frac{1}{2} \mu_0 V \left( N_a M_x^2 + N_b M_y^2 + N_c M_z^2 \right) \tag{2.166}
\]

Below we show the demagnetization factors for some special (limiting) cases.

**Spheroid (Ellipsoid of Revolution):** The result (2.166) can be simplified even further if one considered an ellipsoid with rotational symmetry, where two of the

---

\(^{83}\)For an arbitrarily shaped sample that is uniformly magnetized (an assumption that exactly holds if the applied field intensity is infinite \([201]\); and a fairly good assumption for finite bodies in large applied fields, or for any applied field if the particles are too small such that exchange interaction prevails and magnetization rotates coherently \([202]\)), the demagnetizing field will generally be non-uniform \([169]\) but can however be expressed similarly. One such expression is in terms of a point-function demagnetization tensor \([202]\)

\[
H_m (r) = -N_p (r) M \tag{2.162}
\]

\(^{84}\)Sometimes we might interchangeably use the subscripts \(x, y,\) and \(z.\)
Figure 2.30: Ellipsoid.

principal axes are equal (e.g., $a = b$), representing the transverse axes, and the third (i.e., $c$), representing the rotation symmetry axis. In this case, the demagnetization factors of the transverse and symmetry axes are respectively written as $N_a = N_b = N_\perp$ and $N_c = N_\parallel$. With this notation, we write the demagnetization tensor as

$$N = \begin{bmatrix} N_\perp & 0 & 0 \\ 0 & N_\perp & 0 \\ 0 & 0 & N_\parallel \end{bmatrix}$$  \hspace{1cm} (2.167)$$

where $N_\parallel + 2N_\perp = 1$ \cite{61}. Using this matrix, we can write (2.166) as \cite{78, 169}

$$E_m = \frac{1}{2} \mu_0 M_s^2 V \left( N_\perp \sin^2 \theta + N_\parallel \cos^2 \theta \right)$$  \hspace{1cm} (2.168)$$

where $\theta$ is the angle between the magnetization and the rotational symmetry axis. The factors can be found in terms of the ratio $r = \frac{c}{a} > 1$ for the three special spheroids as \cite{78, 169}

**Prolate (Elongated) Spheroid:** $r > 1$, which means the ellipse is rotated about its major axis.

$$N_\parallel = \frac{1}{r^2 - 1} \left[ \frac{r}{\sqrt{r^2 - 1}} \ln \left( r + \sqrt{r^2 - 1} \right) - 1 \right]$$  \hspace{1cm} (2.169)$$

which, for $r \gg 1$, can be approximated as

$$N_\parallel \approx \frac{\ln (2r) - 1}{r^2}$$  \hspace{1cm} (2.170)$$

Here, $N_\parallel < \frac{1}{3}$, $N_\perp > N_\parallel$, and we have an easy-axis anisotropy along the symmetry axis of the spheroid.

**Oblate (Flattened) Spheroid:** $r < 1$, which means the ellipse is rotated about its minor axis.

$$N_\parallel = \frac{1}{1 - r^2} \left[ 1 - \frac{r}{\sqrt{1 - r^2}} \sin^{-1} \left( \sqrt{1 - r^2} \right) \right]$$  \hspace{1cm} (2.171)$$
Here, $N_\parallel > \frac{1}{3}$, $N_\perp < N_\parallel$, and we have an easy-plane anisotropy in the plane perpendicular to the symmetry axis of the spheroid.

*Sphere:* $r = 1$. In this case, all directions are equivalent and thus all of the demagnetizing factors has to be equal. Hence

$$N = \begin{bmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{bmatrix}$$  \hspace{1cm} (2.172)$$

**Figure 2.31:** Sphere-like, or spheroid, shapes. The arrows indicate the symmetry axis. (a) Prolate ($c > a = b$). (b) Oblate ($c < a = b$). (c) Sphere ($c = a = b$).

**Infinite Cylinder:** For an infinite cylinder (or rod) extending along the $z$-axis and having a circular cross-section in the $xy$-plane, only the perpendicular components demagnetize the magnet

$$N = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$  \hspace{1cm} (2.173)$$

**Figure 2.32:** Cylinder.
**Infinite Sheet:** For an infinite sheet lying in the \(xz\)-plane, only the perpendicular component actually enters into account and one has

\[
N = \begin{bmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0
\end{bmatrix}
\] (2.174)

![Figure 2.33: Sheet.](image)

- **External Field Energy** \(E_a\)
  The external field energy (also known as Zeeman energy) reflects the tendency of a specimen to have its magnetization \(M\) aligned with \(H_a\). This interaction energy is given by [61]

\[
E_a = -\mu_0 \iint_{\Omega} M \cdot H_a dV
\] (2.175)

2.3.2.3 Brown’s Equation

Given the energy terms derived above, one can write the Landau-Gibbs free energy as [78, 194]

\[
G_L(M; H_a) = \iiint_{\Omega} \left[ \frac{A}{M_s^2} \langle \nabla M \rangle^2 + f_{an}(M) - \frac{\mu_0}{2} M \cdot H_m - \mu_0 M \cdot H_a \right] dV
\] (2.176)

The micromagnetic problem is concerned with finding the direction of \(M(r)\) at all points inside the FM. Associated with a given magnetization is the micromagnetic energy functional (2.176). It is well-known from thermodynamics that in equilibrium and after a sufficient time, a closed system with fixed entropy will reach a state with minimum total energy (minimum energy principle) [196]. Hence, in equilibria and under the influence of an applied field \(H_a\), an observable metastable state of magnetization will result in extrema of the Landau-Gibbs free energy [158, 196]. The problem can then be mathematically characterized as local (or global) minimizers of the free energy functional...
subject to the constraint \((2.110)\). The micromagnetic equilibrium condition will result in a set of equations known as Brown’s equations.

As stated above, the equilibrium distribution of magnetization will result in extrema of \((2.176)\). By means of variational calculus, one can find the set of local extrema. At each point inside the FM, the magnetization vector \(\mathbf{M}(\mathbf{r})\) will be varied, and we denote this variation by the small quantity \(\delta \mathbf{M}(\mathbf{r})\) (subject to the constraint \((2.110)\), namely that \(|\mathbf{M} + \delta \mathbf{M}| = M_s\)). In response to that, the energy functional will vary, and we denote this variation by \(\delta G_L(\mathbf{M}; \mathbf{H}_a)\). We want the equilibrium distribution that will result in the minimum value of energy. From variational calculus, we know that the sufficient conditions are: for the first variation to be zero \(\delta G_L(\mathbf{M}; \mathbf{H}_a) = 0\) and for the second variation to be strongly positive \(\delta^2 G_L(\mathbf{M}(\cdot), \mathbf{H}_a) > 0\) \([169]\). Applying the rules of variational calculus, one finds the first variation in the energies as follows:

- **Variation in the Exchange Energy** \(\delta E_{ex}:\)

\[
\delta E_{ex} = E_{ex}(\mathbf{M} + \delta \mathbf{M}) - E_{ex}(\mathbf{M}) = \frac{2A}{M_s^2} \iiint_\Omega \nabla \mathbf{M} \cdot \nabla \delta \mathbf{M} dV \tag{2.177}
\]

Consider the \(i\)-th component \(M_i\)

\[
\iiint_\Omega \nabla M_i \cdot \nabla \delta M_i dV = \iiint_\Omega \nabla \cdot (\delta M_i \nabla M_i) dV - \iiint_\Omega \delta M_i \nabla \cdot (\nabla M_i) dV
\]

\[
= \iiint_\Omega \delta M_i \frac{\partial M_i}{\partial n} dS - \iiint_\Omega \delta M_i \nabla \cdot (\nabla M_i) dV \tag{2.178}
\]

where we have used \((A.155)\) and \((A.139)\). Thus the variation becomes

\[
\delta E_{ex} = -\frac{2A}{M_s^2} \iiint_\Omega \nabla \cdot (\nabla \mathbf{M}) \cdot \delta \mathbf{M} dV + \frac{2A}{M_s^2} \iiint_\Sigma \frac{\partial \mathbf{M}}{\partial n} \cdot \delta \mathbf{M} dS \tag{2.179}
\]

- **Variation in the Anisotropy Energy** \(\delta E_{an}:\)

\[
\delta E_{an} = E_{an}(\mathbf{M} + \delta \mathbf{M}) - E_{an}(\mathbf{M}) = \iiint_\Omega \frac{\partial f_{an}(\mathbf{M})}{\partial \mathbf{M}} \cdot \delta \mathbf{M} dV \tag{2.180}
\]

- **Variation in the Magnetostatic Energy** \(\delta E_{m}:\)

\[
\delta E_m = E_m(\mathbf{M} + \delta \mathbf{M}) - E_m(\mathbf{M}) = -\frac{\mu_0}{2} \iiint_\Omega \delta \mathbf{M} \cdot \mathbf{H}_m dV - \frac{\mu_0}{2} \iiint_\Omega \mathbf{M} \cdot \delta \mathbf{H}_m dV \tag{2.181}
\]

However, by the reciprocity theorem \([166]\), the two integrals are identical. Thus

\[
\delta E_m = -\mu_0 \iiint_\Omega \delta \mathbf{M} \cdot \mathbf{H}_m dV \tag{2.182}
\]

\(^{83}\)One of the difficulties is that the minimization will be carried out in an infinite-dimensional functional space of all possible vector fields \([169]\).
• Variation in the Zeeman Energy $\delta E_a$:

$$\delta E_a = E_a(M + \delta M) - E_a(M) = -\mu_0 \iint \delta M \cdot H_a dV$$  \hspace{1cm} (2.183)

Combining the first-order variations above, one finds

$$\delta G_L(M; H_a) = \delta E_{ex} + \delta E_{an} + \delta E_m + \delta E_a$$  

$$= -\mu_0 \iint \left( \frac{2A}{\mu_0 M_s^2} \nabla \cdot (\nabla M) - \frac{1}{\mu_0} \frac{\partial f_{an}(M)}{\partial M} + H_m + H_a \right) \cdot \delta M dV$$

$$- \frac{2A}{\mu_0 M_s^2} \iint_{\Sigma} \frac{\partial M}{\partial n} \cdot \delta M dS$$  \hspace{1cm} (2.184)

which can be written as [196]

$$\delta G_L(M; H_a) = -\mu_0 \iint \iint_{\Omega} H_{eff} \cdot \delta M dV - \frac{2A}{\mu_0 M_s^2} \iint_{\Sigma} \frac{\partial M}{\partial n} \cdot \delta M dS$$  \hspace{1cm} (2.185)

where the local effective field $H_{eff}$ is given by

$$\mathbf{H}_{eff} = -\frac{1}{\mu_0} \frac{\delta^2 G_L}{\delta M^2} = \frac{2A}{\mu_0 M_s^2} \nabla \cdot (A \nabla \mathbf{M}) - \frac{1}{\mu_0} \frac{\partial f_{an}(M)}{\partial M} + \mathbf{H}_m + \mathbf{H}_a$$  \hspace{1cm} (2.186)

The field can then be written as the sum

$$\mathbf{H}_{eff} = \mathbf{H}_{ex} + \mathbf{H}_{an} + \mathbf{H}_m + \mathbf{H}_a$$  \hspace{1cm} (2.187)

where each term is given by [196]

- Exchange field $\mathbf{H}_{ex}$ [194]:

$$\mathbf{H}_{ex} = \frac{2A}{\mu_0 M_s^2} \nabla^2 \mathbf{M}$$  \hspace{1cm} (2.188)

- Anisotropy field $\mathbf{H}_{an}$:

$$\mathbf{H}_{an} = -\frac{1}{\mu_0} \frac{\partial f_{an}(M)}{\partial M}$$  \hspace{1cm} (2.189)

If we consider uniaxial anisotropy

$$f_{an}(M) \simeq K_1 \left[ 1 - \frac{(e_{an} \cdot M)^2}{M_s^2} \right]$$  \hspace{1cm} (2.190)

then the anisotropy field is given by

$$\mathbf{H}_{an} = \frac{H_K}{M_s} (e_{an} \cdot M) e_{an}$$  \hspace{1cm} (2.191)

where $H_K = 2K_1/\mu_0 M_s$ [78].

Not to be interpreted as a magnetic field in the sense of Maxwell’s equations [169].
Magnetostatic field $H_m$: Can be found by solving the magnetostatic Maxwell equations [196]

\[
\begin{align*}
\nabla \cdot H_m &= \begin{cases} 
\nabla \cdot M, & r \in \Omega \\
0, & r \in \mathbb{R}^3 \setminus \Omega 
\end{cases} \\
\n\nabla \times H_m &= 0
\end{align*}
\]  
(2.192)

subject to following boundary conditions at the FM surface

\[
\begin{align*}
\mathbf{a}_n \cdot H_m &= \mathbf{a}_n \cdot M \\
\mathbf{a}_n \cdot H_m &= 0
\end{align*}
\]  
(2.194)
(2.195)

In the special case of uniform magnetization (e.g., ellipsoidal particles) or perpendicularly magnetized infinite thin films, one can write

\[
H_m = -NM
\]  
(2.196)

where $N$ is the demagnetization tensor which satisfies $N_x + N_y + N_z = 1$.

Applied field $H_a$: Produced by external sources and can be assumed to be a given vector field of space and time.

Now, $\delta M$ is always perpendicular to $M$ (since the magnitude of $M$ is conserved) [158], and thus we can write the variation as the rotation $\delta M = M \times \delta W$, where $W$ is a space-dependent vector; this is the most general variation compatible with (2.110) [169, 196]. Plugging this in (2.185) and using (A.145) for both integrands, one finds

\[
\delta G_L (M; H_a) = -\mu_0 \left[ \iiint_{\Omega} \delta W \cdot (H_{eff} \times M) dV - \frac{2A}{\mu_0 M_s} \iint_{\Sigma} \delta W \cdot \left( \frac{\partial M}{\partial n} \times M \right) dS \right]
\]  
(2.197)

At equilibrium, $\delta G_L (M; H_a) = 0$ for any arbitrary $\delta M$ consistent with (2.110) [158, 196]. This means that any term multiplying $\delta M$ has to be zero. Imposing this condition in (2.197), we obtain two important equations. The first, known as **Brown’s equation**

\[
M \times H_{eff} = 0, \quad \forall r \in \Omega
\]  
(2.198)

essentially states that the magnetization vector experiences zero torque at equilibrium [191, 192]. The second is the **homogeneous boundary condition**

\[
M \times \frac{\partial M}{\partial n} = 0 \iff \frac{\partial M}{\partial n} = 0, \quad \forall r \text{ on } \Sigma
\]  
(2.199)
where $\leftrightarrow$ indicates an equivalence (resulting from the constraint (2.110)) [78]. The Neumann boundary condition above is valid only when no surface anisotropy is present [196].

Brown’s equation (2.198) determine all possible magnetization equilibria, regardless of their stability [169, 196]. That is, the extrema are not necessarily minima of (2.176) (corresponding to metastable equilibria). The nature of the equilibria can be found by computing the second variation of (2.176) or checking $\delta G_L \geq 0$ for an arbitrary small variation of the solution [169].

### 2.4 Deterministic Dynamic Equations

Ferromagnets are typically bistable [198], and one can switch between magnetization states using either applied magnetic fields or the more novel solution so-called spin-transfer torque (STT). In this section, we briefly describe the dynamics of a FM subject to external excitations.

When $\mathbf{M} \times \mathbf{H}_{\text{eff}} \neq 0$, the magnetization experiences a local torque exerted by the effective field and will evolve in time according to a dynamic equation [21, 196]. The state of a FM will now be, of course, a function of both space and time $\mathbf{M}(\mathbf{r}, t)$. The most used magnetization evolution equation is the Landau-Lifshitz (LL) equation and Landau-Lifshitz-Gilbert (LLG) equations, both of which adequately model the dynamics under low-energy excitations (i.e., spin waves or magnons) [29].

#### 2.4.1 Landau-Lifshitz (LL)

The undamped dynamic equation of a magnetic moment is a simple first order partial differential equation describing the precession of $\mathbf{M}(\mathbf{r}, t)$ as a 'free' moment about $\mathbf{H}_{\text{eff}}$ [61, 158, 196]

\[
\frac{\partial \mathbf{M}}{\partial t} = -\gamma_{LL} \mathbf{M} \times \mathbf{H}_{\text{eff}}, \quad \mathbf{M}(\mathbf{r}, 0) = \mathbf{M}_0(\mathbf{r})
\]  

(2.200)

where $\gamma_{LL}$ is the LL gyromagnetic ratio, usually taken to be the gyromagnetic ratio associated with the electron spin (i.e., $\gamma_{LL} \approx 2.21 \times 10^5 \frac{\text{rad}}{\text{s}}$) [158]. Such a precession is typically called Larmor precession and is characterized by the Larmor frequency $\omega = \ldots$}

\[\gamma_{LL} = \mu_0 |\gamma_S| = \mu_0 \left| -g_S \frac{\mu_B}{\hbar} \right| \approx \mu_0 \left| -2 \frac{\mu_B}{\hbar} \right| \approx 221019 = 2.21 \times 10^5 \frac{m}{A \cdot s} \]

\[\gamma_{LL} = \mu_0 |\gamma_L| = \mu_0 \left| -g_L \frac{\mu_B}{\hbar} \right| = \mu_0 \left| -1 \frac{\mu_B}{\hbar} \right| \approx 110509 = 1.10 \times 10^5 \frac{m}{A \cdot s} \]

\[\gamma_{LL} = \mu_0 |\gamma_L| = \mu_0 \left| -g_L \frac{\mu_B}{\hbar} \right| = \mu_0 \left| -1 \frac{\mu_B}{\hbar} \right| \approx 110509 = 1.10 \times 10^5 \frac{m}{A \cdot s} \]

\[\gamma_{LL} = \mu_0 |\gamma_L| = \mu_0 \left| -g_L \frac{\mu_B}{\hbar} \right| = \mu_0 \left| -1 \frac{\mu_B}{\hbar} \right| \approx 110509 = 1.10 \times 10^5 \frac{m}{A \cdot s} \]
Before delving further, we present a brief account of the phenomenological derivation of the undamped equation.

**Classical picture:** From mechanics, we know that the angular momentum of an object with a moment of inertia tensor $I$ and angular velocity $\omega$ is given by $L = I\omega = r \times p$, where $r$ the moment arm and $p$ the linear momentum. Taking the temporal derivative of $L$ leads to
\[
\frac{dL}{dt} = \frac{d}{dt} (r \times p) = \frac{dr}{dt} \times p + r \times \frac{dp}{dt}
\]  

(2.201)

If the axis of rotation is fixed, $\frac{dr}{dt} = \mathbf{v}$ and thus $\frac{dr}{dt} \times p = \mathbf{v} \times p = \mathbf{v} \times (m\mathbf{v}) = 0$. Hence (2.201) becomes
\[
\frac{dL}{dt} = r \times \frac{dp}{dt} = r \times \mathbf{F} = \tau
\]  

(2.202)

where we used Newton’s 2nd law of motion $\frac{dp}{dt} = \mathbf{F}$ with $\mathbf{F}$ being the force and $\tau$ the torque experienced. If we consider (semi-classically) an electron orbiting the nucleus, then we can associate the electron with the dipole moment given by (2.81). However, a magnetic moment $\mathbf{m}$ immersed in a magnetic field $\mathbf{B}_{eff} = \mu_0 \mathbf{H}_{eff}$ experiences a torque given by (B.15). Plugging this relation into (2.202) and using the definition of classical orbital gyromagnetic ratio $m = \gamma_L L$, one finds
\[
\frac{dm}{dt} = \mu_0 \gamma_L \mathbf{m} \times \mathbf{H}_{eff}
\]  

(2.203)

Usually, we would like to see a negative sign in front. Since $\gamma_L < 0$, we use $|\gamma_L|$ and invoke the relation $\gamma_{LL} = \mu_0 |\gamma_L|$ to obtain
\[
\frac{dm}{dt} = -\gamma_{LL} \mathbf{m} \times \mathbf{H}_{eff}
\]  

(2.204)

which can be written in terms of the volume averaged magnetization $\mathbf{M}$ to obtain the desired result.

**Quantum picture:** Consider the spin operator $\hat{S} = \hat{S}_x a_x + \hat{S}_y a_y + \hat{S}_z a_z$. The equation of motion can be derived from the quantum-mechanical commutator [21, 203]
\[
\frac{d\hat{S}_x}{dt} = -\frac{i}{\hbar} \left[ \hat{S}_x, \hat{H} \right]
\]  

(2.205)

where $\alpha \in \{x, y, z\}$ and $\hat{H}$ is the Hamiltonian of the system. To first order in $\hbar$, one can write the equation of motion as
\[
\frac{d\hat{S}_x}{dt} = -\frac{i}{\hbar} \hat{H} \left[ \hat{S}_x, \hat{S}_{\beta} \right] + O(\hbar)
\]  

(2.206)

In general, instead of using either of the g-factors alone, one can use an effective g-factor $g^*$ that includes both and which in general depends on the material [21, 29, 194].
where Einstein’s summation convention is implied (see A.1.1.1). From the properties of the spin operator, we can write

\[ [\hat{S}_\alpha, \hat{S}_\beta] = i\hbar \varepsilon_{\alpha\beta\gamma} \hat{S}_\gamma \]  

(2.207)

where \( \varepsilon_{\alpha\beta\gamma} \) is the antisymmetrical unit tensor (Levi-Civita symbol (A.5)). Invoking the last property in the equation of motion, one obtains

\[ \frac{d\hat{S}_\alpha}{dt} = \frac{d\hat{H}}{\hat{S}_\beta} \varepsilon_{\alpha\beta\gamma} \hat{S}_\gamma + O(\hbar) \]  

(2.208)

However, from the properties of the Levi-Civita symbol, we know that

\[ [A \times B]_\alpha = \varepsilon_{\alpha\beta\gamma} A_\beta B_\gamma \]  

(2.209)

Therefore, we can write (2.208) as

\[ \frac{d\hat{S}}{dt} = -\hat{S} \times \frac{d\hat{H}}{d\hat{S}} + O(\hbar) \]  

(2.210)

In the semiclassical limit as \( \hbar \to 0 \) [200]

\[ \frac{d\langle \hat{S} \rangle}{dt} = -\langle \hat{S} \rangle \times \mathbf{H}_{\text{eff}} \]  

(2.211)

where

\[ \mathbf{H}_{\text{eff}} = \frac{1}{\mu_0 |\gamma_S|} \left\langle \frac{d\hat{H}}{d\hat{S}} \right\rangle \]  

(2.212)

or in the semiclassical approximation

\[ \mathbf{H}_{\text{eff}} = \frac{1}{\mu_0} \frac{dE}{dm} \]  

(2.213)

The last two equations imply that \( m = -g_S\mu_B \langle \hat{S} \rangle / \hbar \), where we have used \( |\gamma_S| = g_S\mu_B / \hbar \). Hence, for classical spins

\[ \frac{dm}{dt} = -\gamma_{LL} m \times \mathbf{H}_{\text{eff}} \]  

(2.214)

where \( \gamma_{LL} = \mu_0 |\gamma_S| \). The last equation can be written in terms of the volume averaged magnetization \( M \) to obtain the desired result.

The above approach can in fact be simplified: In analogy with the relation between the magnetic moment \( m \) and the orbital angular momentum \( L \) of a moving electron, one can relate the magnetic moment with the spin angular momentum. In fact, (2.202) still
holds if we interpret every quantity as an operator in Hilbert space (i.e., $\hat{\mathbf{L}}$ and $\hat{\mathbf{\tau}}$) [194]. Thus one can extend this to spin systems by merely replacing $\hat{\mathbf{L}}$ with $\hat{\mathbf{S}}$ in (2.202) so that

$$\frac{d\hat{\mathbf{S}}}{dt} = \hat{\mathbf{\tau}} \quad (2.215)$$

Then the analogy between the classical and quantum pictures can be applied if one takes the expectation value of the spin angular momentum operator $\mathbf{\hat{S}}$ using appropriate quantum states or a density matrix [194]. The equation can then be converted into a dynamic equation for magnetization by using the definition $\mathbf{\hat{m}} = \gamma_S \mathbf{\hat{S}}$ along with (B.15) so that upon using $\mathbf{m} = \langle \mathbf{\hat{m}} \rangle$ we obtain

$$\frac{d\mathbf{m}}{dt} = -\gamma_{LL} \mathbf{m} \times \mathbf{H}_{\text{eff}} \quad (2.216)$$

where we have used $\gamma_{LL} = \mu |\gamma_S|$. The equation can again be written in terms of the volume averaged magnetization $\mathbf{M}$ to obtain the desired result.

The dynamic equation (2.200) has to be consistent with the micromagnetic constraint (2.110). Dotting both sides of (2.200) with $\mathbf{M}$

$$\mathbf{M} \cdot \frac{\partial \mathbf{M}}{\partial t} = -\gamma_{LL} \mathbf{M} \cdot (\mathbf{M} \times \mathbf{H}_{\text{eff}})$$

and using the fact that $\mathbf{M} \cdot (\partial \mathbf{M} / \partial t) = (1/2) \frac{d}{dt} |\mathbf{M}|^2$ along with the invariance property of triple scalar product under cyclic permutation (A.145), we obtain

$$\frac{1}{2} \frac{\partial}{\partial t} |\mathbf{M}|^2 = -\gamma_{LL} \mathbf{H}_{\text{eff}} \cdot (\mathbf{M} \times \mathbf{M}) = 0 \quad (2.217)$$

from which we conclude that the magnitude is conserved.

Experimentally, a precession decays in time towards an energy minimum. The dynamic equation (2.200) is not dissipative and thus cannot describe any approach to equilibrium [196]. This can be shown by taking the temporal derivative of (2.185) and using (2.199) for the second term to obtain

$$\frac{dG_L}{dt} = -\mu_0 \iiint_\Omega \mathbf{H}_{\text{eff}} \cdot \frac{\partial \mathbf{M}}{\partial t} dV - \mu_0 \iiint_\Omega \mathbf{M} \cdot \frac{\partial \mathbf{H}_a}{\partial t} dV \quad (2.219)$$

Alternatively

$$\frac{dG_L}{dt} = \iiint_\Omega \left[ \delta G_L \frac{\partial \mathbf{M}}{\partial t} + \delta G_L \frac{\partial \mathbf{H}_a}{\partial t} \right] dV = -\mu_0 \iiint_\Omega \mathbf{H}_{\text{eff}} \cdot \frac{\partial \mathbf{M}}{\partial t} dV - \mu_0 \iiint_\Omega \mathbf{M} \cdot \frac{\partial \mathbf{H}_a}{\partial t} dV \quad (2.218)$$
Substituting (2.200) and assuming a DC external field (so that $\partial\mathbf{H}_a/\partial t = 0$), one finds

$$\frac{dG_L}{dt} = \mu_0\gamma_{LL} \iiint_{\Omega} \mathbf{H}_{\text{eff}} \cdot (\mathbf{M} \times \mathbf{H}_{\text{eff}}) \, dV = 0$$

where we used the identity (A.145). Thus, the dynamics are non-dissipative but in fact conservative [198]. Therefore, a damping term has to be added to the equation for it to describe a realistic situation. The damping term will take into account the transfer (or loss) of energy from the macroscopic local magnetization to the microscopic thermal motion (i.e., thermal bath) [194, 196]. However, due to the complexity in describing the interactions between the magnetic moment and the crystal lattice vibration, crystal defects (e.g., voids, interstitial atoms, etc.), magnons, or eddy currents, the damping is usually added as a phenomenological term since it is difficult to separately account for these mechanisms or even connect it with the energy dissipation rate measured experimentally (e.g., using FMR) [157, 194].

![Figure 2.34: Magnetization precession and damping torques.](image)

In 1935, Landau and Lifshitz introduced the basic damped dynamics equation for magnetization in their pioneering work about the phenomenological evaluational of the permeability tensor in FMs [158]. Landau and Lifshitz originally described damping in a phenomenological approach by adding a term directed toward $\mathbf{H}_{\text{eff}}$ and perpendicular to $\mathbf{M}$

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma_{LL} \mathbf{M} \times \mathbf{H}_{\text{eff}} + \gamma_{LL} \lambda M_s \left( \mathbf{H}_{\text{eff}} - \frac{\mathbf{M} \cdot \mathbf{H}_{\text{eff}}}{M_s^2} \mathbf{M} \right), \quad \mathbf{M}(\mathbf{r}, 0) = \mathbf{M}_0(\mathbf{r})$$

where $\lambda$ is a dimensionless phenomenological damping constant.

The form above is rarely used in literature. In fact, one may notice that the second term can be obtained by using the identity (A.146) as follows

$$\mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}}) = (\mathbf{M} \cdot \mathbf{H}_{\text{eff}}) \mathbf{M} - (\mathbf{M} \cdot \mathbf{M}) \mathbf{H}_{\text{eff}} = (\mathbf{M} \cdot \mathbf{H}_{\text{eff}}) \mathbf{M} - M_s^2 \mathbf{H}_{\text{eff}}$$

(2.221)
which implies

$$H_{eff} - \frac{(M \cdot H_{eff})}{M_s} M = -\frac{1}{M_s^2} M \times (M \times H_{eff}) \quad (2.222)$$

Hence we can rewrite the LL equation (2.221) in the more admissible form [78, 196]

$$\frac{\partial M}{\partial t} = -\gamma_{LL} M \times H_{eff} - \gamma_{LL} \frac{\lambda}{M_s} M \times (M \times H_{eff}), \quad M(r, 0) = M_0(r) \quad (2.223)$$

The precession and damping terms are schematically shown in Fig. 2.35 below.

![Figure 2.35: Magnetization precession and damping torques in the LL equation.]

Now we check if the dynamics are dissipative. Using (2.223) in the general relation (2.219) while still assuming DC external fields, we obtain

$$\frac{dG_L}{dt} = -\mu_0 \iint_{\Omega} H_{eff} \cdot \left[-\gamma_{LL} M \times H_{eff} - \gamma_{LL} \frac{\lambda}{M_s} M \times (M \times H_{eff})\right] dV$$

$$= \mu_0 \gamma_{LL} \iint_{\Omega} H_{eff} \cdot (M \times H_{eff}) dV + \mu_0 \gamma_{LL} \frac{\lambda}{M_s} \iint_{\Omega} H_{eff} \cdot [M \times (M \times H_{eff})] dV$$

$$= 0 + \mu_0 \gamma_{LL} \frac{\lambda}{M_s} \iint_{\Omega} (M \times H) \cdot (H \times M) dV$$

$$= -\mu_0 \gamma_{LL} \frac{\lambda}{M_s} \iint_{\Omega} |M \times H|^2 dV \quad (2.224)$$

where we have used (2.220) and (A.145) throughout. The last equation shows that energy is a decreasing function of time and thus dissipative. In fact, by numerically integrating the LL equation, we can plot the damped motion of the moment as in Fig. 2.36.

Before concluding the subsection, we write the LL equation (2.223) in terms of the rescaled magnetization by dividing both sides by $M_s$ to obtain

$$\frac{\partial m}{\partial t} = -\gamma_{LL} m \times H_{eff} - \gamma_{LL} \lambda m \times (m \times H_{eff}), \quad m(r, 0) = m_0(r) \quad (2.225)$$
2.4.2 Landau-Lifshitz-Gilbert (LLG)

In 1955, and based on a Lagrangian formalism of the precession equation with damping added using the so-called Rayleigh dissipation function, Gilbert [194] introduced a viscous damping term into the undamped LL equation. In particular, he started with a Lagrangian formulation of the damped equation of motion starting from the Euler-Lagrange equation for conservative dynamics

\[
\frac{d}{dt} \left( \frac{\delta \mathcal{L}}{\delta \dot{\mathbf{M}}} \right) - \frac{\delta \mathcal{L}}{\delta \mathbf{M}} = 0
\]  

(2.226)

where \( \mathcal{L} [\mathbf{M}, \dot{\mathbf{M}}] \) is the Lagrangian. He then included a nonconservative force using the Rayleigh dissipation function

\[
\frac{d}{dt} \left( \frac{\delta \mathcal{L}}{\delta \dot{\mathbf{M}}} \right) - \frac{\delta \mathcal{L}}{\delta \mathbf{M}} + \frac{d\mathcal{R}[\dot{\mathbf{M}}]}{d\mathbf{M}} = 0
\]

(2.227)

where the Rayleigh dissipation functional \( \mathcal{R} [\dot{\mathbf{M}}] \) is given by

\[
\mathcal{R} [\dot{\mathbf{M}}] = \frac{\eta}{2} \iiint_{\Omega} \left| \dot{\mathbf{M}}(t, \mathbf{r}) \right|^2 dV
\]

(2.228)

where \( \alpha = \eta \gamma_G M_s \) is the Gilbert damping, \( \eta \) is a damping parameter, and \( \gamma_G \) is the Gilbert gyromagnetic ratio. The Gilbert damping depends on temperature and the impurity/defect composition of the material [151] and can be a tensor in general [29].

Using the dissipation functional, the LLG can be shown to be [78, 194, 196]

\[
\frac{\partial \mathbf{M}}{\partial t} = -\gamma_G \mathbf{M} \times \mathbf{H}_{eff} + \frac{\alpha}{M_s} \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t}, \quad \mathbf{M}(\mathbf{r}, 0) = \mathbf{M}_0(\mathbf{r})
\]

(2.229)

The precession and damping terms are schematically shown in Fig. 2.37 below.

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89 Although I should probably refer to [204], Gilbert’s original paper was never published, I believe. However, Gilbert later published his Ph.D. thesis, and [194] is based on chapters II and III of his thesis, with little modifications.
Figure 2.37: Magnetization precession and damping torques in the LLG equation.

The LLG equation was the first phenomenological equation to describe the magnetization dynamics in the whole dissipation range [157]. The Gilbert form of damping was merely introduced since the damped LL equation encountered problems for large damping, producing unphysical solutions [157, 194]. If one considers $\lambda$ in (2.223) as a parameter proportional to the energy dissipation in the system, then in the overdamped regime ($\lambda \geq 1$) the dissipation term dominates and the equation will predict faster relaxation for larger damping, an obvious contradiction to the physical picture of damping [157]. In fact, it was pointed by Landau and Lifshitz themselves [158] that the damping term introduced by them is neither the only possible nor most general and one may use their equation in the precession-dominated regime ($\lambda \ll 1$) only [157].

To check if the dynamics are dissipative. It is convenient to rewrite (2.229) as

$$\frac{\partial \mathbf{M}}{\partial t} = -\gamma G \mathbf{M} \times \left( \mathbf{H}_{\text{eff}} - \frac{\alpha}{\gamma G M_s} \frac{\partial \mathbf{M}}{\partial t} \right)$$

(2.230)

which in fact reveals the nature of the damping term: Directly subtracted from the effective field, and having a magnitude proportional to the relaxation speed (analogous to a hydrodynamical viscous damping) [157, 196].

The LLG equation can straightforwardly be shown to be magnitude conserving. To check if it is dissipative, we dot both sides of (2.230) by $(\mathbf{H}_{\text{eff}} - (\alpha/\gamma G M_s) \partial \mathbf{M}/\partial t)$

$$\left( \mathbf{H}_{\text{eff}} - \frac{\alpha}{\gamma G M_s} \frac{\partial \mathbf{M}}{\partial t} \right) \cdot \frac{\partial \mathbf{M}}{\partial t} = -\gamma G \left( \mathbf{H}_{\text{eff}} - \frac{\alpha}{\gamma G M_s} \frac{\partial \mathbf{M}}{\partial t} \right) \left[ \mathbf{M} \times \left( \mathbf{H}_{\text{eff}} - \frac{\alpha}{\gamma G M_s} \frac{\partial \mathbf{M}}{\partial t} \right) \right] = 0$$

(2.231)

where the second term vanishes as evident from (A.145). Therefore from (2.231), it is obvious that

$$\mathbf{H}_{\text{eff}} \cdot \frac{\partial \mathbf{M}}{\partial t} = \frac{\alpha}{\gamma G M_s} \left| \frac{\partial \mathbf{M}}{\partial t} \right|^2$$

(2.232)
Using (2.232) in (2.219) while assuming static external field $H_a$, we obtain

$$
\frac{dG_L}{dt} = -\mu_0 \int \int \int_{\Omega} H_{eff} \cdot \frac{\partial M}{\partial t} \, dV = -\frac{\mu_0 \alpha}{\gamma G M_s} \int \int \int_{\Omega} \left| \frac{\partial M}{\partial t} \right|^2 \, dV
$$

(2.233)

which implies that the LLG dynamics are always decreasing and thus dissipative. The last equation expresses the so-called Lyapunov structure of the LLG equation.

The native form of the LLG equation (2.229) is an implicit differential equation, which is inconvenient to implement in numerical computations. Fortunately, it can be casted into an explicit form. Taking the cross product of $M$ with the LL equation (2.223)

$$
M \times \frac{\partial M}{\partial t} = -\gamma_{LL} M \times M \times H_{eff} - \gamma_{LL} \frac{\alpha}{M_s} M \times [M \times (M \times H_{eff})]
$$

(2.234)

But from the identities (A.145) and (A.146), we find $M \times [M \times (M \times H_{eff})] = -M_s^2 M \times H_{eff}$. Therefore

$$
M \times \frac{\partial M}{\partial t} = -\gamma_{LL} M \times (M \times H_{eff}) + \gamma_{LL} \lambda M_s M \times H_{eff}
$$

(2.235)

or equivalently

$$
\gamma_{LL} M \times (M \times H_{eff}) = -M \times \frac{\partial M}{\partial t} + \gamma_{LL} \lambda M_s M \times H_{eff}
$$

(2.236)

Substituting (2.236) back into (2.223) and collecting like terms, we obtain

$$
\frac{\partial M}{\partial t} = -\gamma_{LL} \left(1 + \lambda^2\right) M \times H_{eff} + \frac{\lambda}{M_s} M \times \frac{\partial M}{\partial t}, \quad M(r, 0) = M_0(r)
$$

(2.237)

where the last equation transforms into the LLG equation upon substituting [21]

$$
\gamma_{LL} = \frac{\gamma G}{1 + \alpha^2}
$$

(2.238)

$$
\lambda = \alpha
$$

(2.239)

The relations above can also be used in (2.223) to cast the Gilbert equation into the archetypal LL form (which, from now on, we call the combined LLG equation or just LLG equation)

$$
\frac{\partial M}{\partial t} = -\frac{\gamma G}{1 + \alpha^2} M \times H_{eff} - \frac{\gamma G}{1 + \alpha^2} \frac{\alpha}{M_s} M \times (M \times H_{eff}), \quad M(r, 0) = M_0(r)
$$

(2.240)

The last equation for zero damping ($\alpha = 0$) is related to the symplectic flow of harmonic maps and is also known as the Schrödinger map equation [198]. For high damping ($\alpha \to \infty$), the equation is related to the heat flow of harmonics maps [198].
The equivalence between (2.223) and (2.229) is not a coincidence; it turned out that the LL equation is universal and is the most general equation of damped motion for magnetic moments [157, 196]. Consider the 1st-order dynamic equation

\[
\frac{\partial \mathbf{M}}{\partial t} = \mathbf{F}(\mathbf{M}, \mathbf{H}_{\text{eff}}), \quad \mathbf{M}(\mathbf{r}, 0) = \mathbf{M}_0(\mathbf{r}) \tag{2.241}
\]

At every instant of time, one can decompose the vector field \( \mathbf{F}(\mathbf{M}, \mathbf{H}_{\text{eff}}) \) along three mutually orthogonal vectors and hence write it as a linear combination of the basis vectors. In particular, one can write [196]

\[
\frac{\partial \mathbf{M}}{\partial t} = c_1 \mathbf{M} + c_2 \mathbf{M} \times \mathbf{a} + c_3 \mathbf{M} \times (\mathbf{M} \times \mathbf{a}) \tag{2.242}
\]

where \( \mathbf{a} \) is some unknown vector. We can then determine the unknowns by using the fundamental micromagnetic constraint (2.110) and Brown’s equation (2.198) at equilibria. The former can be utilized by dotting both sides of (2.242) by \( \mathbf{M} \) to obtain

\[
\frac{1}{2} \frac{\partial |\mathbf{M}|^2}{\partial t} = c_1 |\mathbf{M}|^2 \tag{2.243}
\]

where the other terms vanishes after one uses (A.145) and (A.146). For (2.110) to hold, we must have \( c_1 = 0 \). This should not be surprising since the restriction (2.110) implies that \( \mathbf{M} \) can only rotate and that any change \( \Delta \mathbf{M} \) must be perpendicular to \( \mathbf{M} \) [157]. In this sense, the equation

\[
\frac{\partial \mathbf{M}}{\partial t} = c_2 \mathbf{M} \times \mathbf{a} + c_3 \mathbf{M} \times (\mathbf{M} \times \mathbf{a}) , \quad \mathbf{M}(\mathbf{r}, 0) = \mathbf{M}_0(\mathbf{r}) \tag{2.244}
\]

can be thought as the general equation of magnetization dynamics; an expansion of \( \partial \mathbf{M}/\partial t \) over the two orthogonal vectors \( \mathbf{M} \times \mathbf{a} \) and \( \mathbf{M} \times (\mathbf{M} \times \mathbf{a}) \) which span the plane perpendicular to \( \mathbf{M} \) over which \( \partial \mathbf{M}/\partial t \) lies [157]. Now at equilibrium, (2.244) becomes

\[
0 = c_2 \mathbf{M} \times \mathbf{a} + c_3 \mathbf{M} \times (\mathbf{M} \times \mathbf{a}) \tag{2.245}
\]

which implies that \( \mathbf{M} \times \mathbf{a} = 0 \) (since the two terms on the right are mutually orthogonal). This equation is equivalent to Brown’s condition when \( \mathbf{a} = \mathbf{H}_{\text{eff}} \). In fact, (2.242) reduces to the LL equation (2.200) with \( c_2 = -\gamma_{\text{LL}}, c_3 = -\gamma_{\text{LL}} \frac{\mu}{M_s} \) and to the combined LLG equation (2.240) with \( c_2 = -\frac{\gamma_0}{1+\alpha^2}, c_3 = -\frac{\gamma_0}{1+\alpha^2} \frac{\alpha}{M_s} \). This implies that all dynamic equations are reducible to the LL equation (having the general form (2.244)), with the possibility of having different coefficients [196]. Although (2.223) and (2.229) are in this sense mathematically equivalent (as also evident from the resulting equation: (2.240)), they may not be regarded as physically equivalent when one tries to interpret the precession and damping terms [157, 194, 196]. The two equation have identical damping
terms, and only differ in the dimensionless damping parameter \([194]\). For \(\alpha^2 \ll 1\), \((2.240)\) obviously coincides with \((2.223)\) \([194]\), and one can then safely interpret \(\alpha\) as a damping parameter proportional to the dissipation energy in the LL form as well (which is not true for large damping) \([157]\). It is worth noting at this point that the coefficients \(\gamma_{LL}, \lambda, \) etc. need not to be constant or time-independent, and can be functions of the state of the system and can also be tensors \([157, 196]\).

Before concluding, we write the LLG equation \((2.229)\) and the combined LLG equation \((2.240)\) in terms of the rescaled magnetization by dividing both sides by \(M_s\) to obtain

\[
\frac{\partial \mathbf{m}}{\partial t} = -\gamma_G \mathbf{m} \times \mathbf{H}_{eff} + \alpha \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial t}, \quad \mathbf{m}(r, 0) = m_0(r)
\]  

\[(2.246)\]
and

\[
\frac{\partial \mathbf{m}}{\partial t} = -\frac{\gamma_G}{1 + \alpha^2} \mathbf{m} \times \mathbf{H}_{eff} - \frac{\gamma_G}{1 + \alpha^2} \alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{H}_{eff}), \quad \mathbf{m}(r, 0) = m_0(r)
\]  

\[(2.247)\]

### 2.4.3 Dimensionless Equations

It is instructive to write \((2.176)\) and \((2.187)\) in a normalized (dimensionless) form. If the magnetization and magnetic fields are normalized in units of \(M_s\)

\[
\mathbf{m} = \frac{M}{M_s}
\]  

\[(2.248)\]

\[
\mathbf{h}_{eff} = \frac{H_{eff}}{M_s} = \mathbf{h}_{ex} + \mathbf{h}_{an} + \mathbf{h}_m + \mathbf{h}_a
\]  

\[(2.249)\]

then the free energy \((2.176)\) can be normalized as follows \([78, 196]\)

\[
g_L(\mathbf{m}(\cdot), \mathbf{h}_a) = \frac{G_L(M(\cdot), H_a)}{\mu_0 M_s^2 V} = \frac{1}{V} \iiint_{\Omega} \left[ \frac{A}{\mu_0 M_s^2} (\nabla \mathbf{m})^2 + \frac{1}{\mu_0 M_s^2} f_{an}(M) - \frac{1}{2} \mathbf{m} \cdot \mathbf{h}_m - \mathbf{m} \cdot \mathbf{h}_a \right] dV
\]  

\[(2.250)\]

This can also be rewritten in terms of the exchange length \(l_{ex} = \sqrt{\frac{2A}{\mu_0 M_s^2}}\) \([21, 78]\) and the normalized anisotropy energy \(\varphi_{an}(\mathbf{m}) = \frac{f_{an}(M)}{\mu_0 M_s^2}\) as \([196]\)

\[
g_L(\mathbf{m}(\cdot), h_a) = \frac{1}{V} \iiint_{\Omega} \left[ \frac{l_{ex}^2}{2} (\nabla \mathbf{m})^2 + \varphi_{an}(\mathbf{m}) - \frac{1}{2} \mathbf{m} \cdot \mathbf{h}_m - \mathbf{m} \cdot \mathbf{h}_a \right] dV
\]  

\[(2.251)\]

If we normalize \(\mathbf{r}\) in units of \(l_{ex}\), we can write

\[
g_L(\mathbf{m}(\cdot), h_a) = \frac{1}{V} \iiint_{\Omega} \left[ \frac{1}{2} (\nabla \mathbf{m})^2 + \varphi_{an}(\mathbf{m}) - \frac{1}{2} \mathbf{m} \cdot \mathbf{h}_m - \mathbf{m} \cdot \mathbf{h}_a \right] dV
\]  

\[(2.252)\]
where now \( \nabla \) operates with respect to the normalized position vector \( \mathbf{r}/l_{ex} \). In this case, the first variation (2.185) becomes

\[
\delta g_L (m(\cdot), h_a) = -\frac{1}{V} \iiint_{\Omega} \mathbf{h}_{eff} \cdot \delta \mathbf{m} dV + \frac{l_{ex}}{V} \iint_{\Sigma} \frac{\partial \mathbf{m}}{\partial n} \cdot \delta \mathbf{m} dS \tag{2.253}
\]

where the normalized local effective field \( \mathbf{h}_{eff} \) is given by

\[
\mathbf{h}_{eff} = -\frac{\delta g_L}{\delta \mathbf{m}} = \nabla \cdot (\nabla m) - \frac{\partial \varphi_{an} (m)}{\partial m} + \mathbf{h}_m + h_a \tag{2.254}
\]

The field can then be written as sum

\[
\mathbf{h}_{eff} = \mathbf{h}_{ex} + \mathbf{h}_{an} + \mathbf{h}_m + h_a \tag{2.255}
\]

where each term is given by [196]

- Normalized exchange field \( \mathbf{h}_{ex} \):
  \[
  \mathbf{h}_{ex} = \nabla^2 m \tag{2.256}
  \]

- Normalized anisotropy field \( \mathbf{h}_{an} \):
  \[
  \mathbf{h}_{an} = -\frac{\partial \varphi_{an} (m)}{\partial m} \tag{2.257}
  \]

If we consider uniaxial anisotropy

\[
\varphi_{an} (M) \simeq \frac{K_1}{\mu_0 M_s^2} \left[ 1 - (e_{an} \cdot \mathbf{m})^2 \right] \tag{2.258}
\]

then the normalized anisotropy field is given by

\[
\mathbf{h}_{an} = \frac{H_K}{M_s} (e_{an} \cdot \mathbf{m}) e_{an} \tag{2.259}
\]

where \( H_K = \frac{2K_1}{\mu_0 M_s} \) [78].

- Normalized magnetostatic field \( \mathbf{h}_m \): Can be found by solving the magnetostatic Maxwell equations [196]

\[
\nabla \cdot \mathbf{h}_m = \begin{cases} 
\nabla \cdot \mathbf{m}, & \mathbf{r} \in \Omega \\
0, & \mathbf{r} \in \mathbb{R}^3 \setminus \Omega \end{cases} \tag{2.260}
\]

\[
\nabla \times \mathbf{h}_m = 0 \tag{2.261}
\]
subject to following boundary conditions at the FM surface

\[ \mathbf{a}_n \cdot h_m = \mathbf{a}_n \cdot \mathbf{m} \tag{2.262} \]
\[ \mathbf{a}_n \cdot h_m = 0 \tag{2.263} \]

In the special case of uniform magnetization (e.g., ellipsoidal particles) or perpendicularly magnetized infinite thin films, one can write

\[ h_m = -N \mathbf{m} \tag{2.264} \]

where \( N \) is the demagnetization tensor which satisfies \( N_x + N_y + N_z = 1 \).

- Normalized Applied field \( h_a \): Produced by external sources and can be assumed to be a given vector field of space and time.

Using a similar approach to that in 2.3.2, we write the variation in \( \mathbf{m} \) as \( \delta \mathbf{m} = \mathbf{m} \times \delta \mathbf{w} \), where \( \mathbf{w} \) is a space-dependent vector. Plugging this in (2.253) and using (A.145) for both integrands, we find

\[
\delta g_L (\mathbf{m} (\cdot), h_a) = -\mu_0 \left[ \iiint_\Omega \delta \mathbf{w} \cdot (h_{\text{eff}} \times \mathbf{m}) dV - \frac{2A}{\mu_0 M_s^2} \iint_\Sigma \delta \mathbf{w} \cdot \left( \frac{\partial \mathbf{m}}{\partial n} \times \mathbf{m} \right) dS \right]
\tag{2.265}
\]

At equilibrium, \( \delta g_L (\mathbf{m} (\cdot), a_a) = 0 \) for any arbitrary \( \delta \mathbf{m} \) consistent with (2.110). Imposing this condition in (2.265), we obtain two important equations. The first is the normalized Brown equation [196]

\[ \mathbf{m} \times h_{\text{eff}} = 0, \quad \forall \mathbf{r} \in \Omega \tag{2.266} \]

The second is the normalized homogeneous boundary condition [196]

\[ \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial n} = 0 \Leftrightarrow \frac{\partial \mathbf{m}}{\partial n} = 0, \quad \forall \mathbf{r} \text{ on } \Sigma \tag{2.267} \]

which is valid only when no surface anisotropy is present [196].

In the dimensionless case, the dynamics are governed by normalized forms of the LL (2.225) and LLG (2.246) equations. By noting that \( \mu_0 |\gamma| M_s \) has the units \( \frac{\text{A}}{\text{s} \cdot \text{m}} = \frac{1}{8} \), we identify the reciprocal \( \frac{1}{\mu_0 |\gamma| M_s} \) as a time constant, and we denote it by \( \tau \). Therefore we can write the time constants of the LL and LLG equations as

\[ \tau_{LL} = \frac{1}{\gamma_{LL} M_s} \tag{2.268} \]
\[ \tau_G = \frac{1}{\gamma_G M_s} \tag{2.269} \]
Multiplying each of (2.225) and (2.229) by its own time constant, we obtain
\[
\frac{\tau_{LL}}{\tau_L} \frac{\partial m}{\partial t} = -m \times h_{eff} - \alpha m \times (m \times h_{eff}) \tag{2.270}
\]
\[
\frac{\tau_G}{\tau_G} \frac{\partial m}{\partial t} = -m \times h_{eff} + \alpha \tau_G m \times \frac{\partial m}{\partial t} \tag{2.271}
\]

If we define the normalized time-spans \( t_{LL} = \frac{t}{\tau_{LL}} \) and \( t_G = \frac{t}{\tau_G} \), then their differentials are given by
\[
\frac{\partial t_{LL}}{\tau_{LL}} = \frac{\partial t}{\tau_{LL}} \Leftrightarrow \partial t = \tau_{LL} \partial t_{LL} \tag{2.272}
\]
\[
\frac{\partial t_G}{\tau_G} = \frac{\partial t}{\tau_G} \Leftrightarrow \partial t = \tau_G \partial t_G \tag{2.273}
\]

Plugging these in (2.270) and (2.271), respectively, one obtains
\[
\frac{\partial m}{\partial t_{LL}} = -m \times h_{eff} - \alpha m \times (m \times h_{eff}) \tag{2.274}
\]
\[
\frac{\partial m}{\partial t_G} = -m \times h_{eff} + \alpha m \times \frac{\partial m}{\partial t_G} \tag{2.275}
\]

or just simply (after dropping the time subscripts)
\[
\frac{\partial m}{\partial t} = -m \times h_{eff} - \alpha m \times (m \times h_{eff}), \quad m(r, 0) = m_0(r) \tag{2.276}
\]
\[
\frac{\partial m}{\partial t} = -m \times h_{eff} + \alpha m \times \frac{\partial m}{\partial t}, \quad m(r, 0) = m_0(r) \tag{2.277}
\]

Following a similar approach to that in 2.4.1 and 2.4.2, the associated energy balance equations for the normalized LL and LLG equations above are given respectively by [196]
\[
\frac{dg_L}{dt} = -\frac{\alpha}{V} \iiint_{\Omega} [m \times h_{eff}]^2 dV - \frac{1}{V} \iiint_{\Omega} m \cdot \frac{\partial h_a}{\partial t} dV \tag{2.278}
\]
\[
\frac{dg_L}{dt} = -\frac{\alpha}{V} \iiint_{\Omega} \left| \frac{\partial m}{\partial t} \right|^2 dV - \frac{1}{V} \iiint_{\Omega} m \cdot \frac{\partial h_a}{\partial t} dV \tag{2.279}
\]
which are, of course, decreasing functions of time at equilibrium.

If one prefers the combined LLG equation (2.247), then a renormalization of (2.247) can be applied by using the procedure above but with the time constant \( \tau_{G,e} = \frac{1+\alpha^2}{\tau_G M_s^2} \) to arrive at (2.276) with \( \partial t = \tau_{G,e} \partial t_{G,e} \).
2.4.4 Toward the Nanoscale—The Macrospin Approximation

As discussed in 2.2.5, modern spintronic devices involve magnets with dimensions in the nanoscopic (1 – 100 nm) scale [68, 78]. At such reduced dimensions, magnetostatic interaction is weak, and at temperatures well below the Curie point, the strong exchange interaction aligns all spins together so that spins rotate in unison, effectively creating a spatially uniform magnetization, i.e. a giant *macrospin* [21, 29, 78, 196, 205, 206]. In this case, a magnetic sample is said to be *single domain* (or *monodomain*)

\[ L < d_{sd} \]  

That is, one now has the effective field

\[ H_{eff} = H_{an} + H_m + H_a \]  

(2.280)

In general, one has a spatially uniform solution when the following hold [78, 196, 208]:

1. The initial distribution is given by \( m(r, 0) = m_0 \), where \( m_0 \) is a spatially uniform (i.e., space-independent) vector;
2. The magnet is of some special shape, for example ellipsoidal;
3. The effective field \( H_{eff} \) is spatially uniform.

**2.4.4.1 Statics: The Stoner-Wohlfarth Model**

The first static model (and the one mostly used) to describe the magnetization of small particles is the Stoner-Wohlfarth model developed in 1948 [209]. This model is valid for \( T = 0 \) K only, but can be generalized for any temperature [78]. In this model, the main character of a single domain particle is hysteresis (through magnetization reversal), in which the magnetization of the so-called Stoner particle coherently reverses and can achieve a maximum coercivity [68, 78].

\[ \text{Strictly when } L < R_{coh}, \text{ where } R_{coh} = \beta l_{ex}. \text{ Otherwise, magnetization reversal may not necessarily be coherent [61], but can exhibit curling, buckling, and fanning.} \]

\[ \text{In what is sometimes known as } \text{Néel rotation. Small particles that are free to rotate as a whole are said to exhibit } \text{Brown rotation [78].} \]

\[ \text{This was first suggested by Dorfman [207] in 1930.} \]

\[ \text{This is also obvious as there are no domain walls to form [82].} \]

\[ \text{The coercivity in a single domain particle is larger than in multidomain particle since it is energetically more difficult to overcome the anisotropy energy than to nucleate (on inhomogeneities and defects) or move a DW [61]. Thus, single domain particles are magnetically hard due to their high coercivity and remanence.} \]
The model assumes a homogeneously magnetized, single domain, elongated rotationally symmetric ellipsoid, with uniaxial anisotropy along some axis. For simplicity, we take the $z$-axis as the easy-axis. In this case, the Landau-Gibbs free energy becomes

$$G_L(M; H_a) = V \left\{ K_1 \left[ 1 - \left(\frac{e_{an} \cdot M}{M_s^2}\right)^2 \right] + \frac{\mu_0 M \cdot (N M) - \mu_0 M \cdot H_a}{2} \right\}$$

$$= V \left\{ K_1 \left[ 1 - m_z^2 \right] + \frac{\mu_0 M_s^2}{2} \left[ N_\perp (1 - m_z^2) + N_\parallel m_z^2 \right] - \mu_0 M_s m \cdot H_a \right\}$$

$$= V \left\{ K_1 + \frac{\mu_0 M_s^2}{2} N_\perp + \left[ \frac{\mu_0 M_s^2}{2} (N_\parallel - N_\perp) - K_1 \right] m_z^2 - \mu_0 M_s m \cdot H_a \right\}$$

(2.281)

where we have used (2.110). If $\theta$ is the angle between the $M$ and the easy-axis (which coincides with the major axis of the ellipse), $\phi$ the angle between $H_a$ (which lies on the $xz$-plane) and the easy-axis, and $\psi$ the angle the projection of $M$ makes on $xy$-plane with the $x$-axis, then

$$G_L(M; H_a) = V \left\{ K_1 + \frac{\mu_0 M_s^2}{2} N_\perp + \left[ \frac{\mu_0 M_s^2}{2} (N_\parallel - N_\perp) - K_1 \right] m_z^2 \cos^2 \theta \right.$$

$$- \left. \mu_0 M_s H_a (\sin \theta \cos \psi \sin \phi + \cos \theta \cos \phi) \right\}$$

(2.282)

Figure 2.38: Geometry of the Stoner-Wohlfarth (SW) problem.

---

*Which could result from the shape, or the sum of crystal and shape effects [68, 78]. In general, anisotropy is determined from shape (magnetostatic), crystalline structure (magnetocrystalline), residual strain (magnetoelastic), and various surface/interface effects due to the broken translation symmetry at an interface.*
When $H_a = 0$, $\mathbf{M}$ points along the anisotropy axis. When $H_a \neq 0$, $\mathbf{M}$ rotates away from the easy-axis (toward $\mathbf{H}_a$). Because of symmetry, $\mathbf{M}$ will lie on the plane containing $\mathbf{e}_{an}$ and $\mathbf{H}_a$, and one has $\psi = 0$ (planar problem on the $xz$-plane) [169]. Thus [78]

$$G_L (\mathbf{M}; H_a) = V \left[ K_1 \sin^2 \theta + \frac{\mu_0 M_s^2}{2} \left( N_\perp \sin^2 \theta + N_\parallel \cos^2 \theta \right) - \mu_0 M_s H_a \cos (\phi - \theta) \right]$$

or

$$G_L (\mathbf{M}; H_a) = V \left[ K_1 + \frac{\mu_0 M_s^2}{2} \left( N_\perp - N_\parallel \right) \right] \sin^2 \theta + \frac{\mu_0 M_s^2}{2} N_\parallel - \mu_0 M_s H_a \cos (\phi - \theta)$$

$$= V \left[ K_1 + K_d \right] \sin^2 \theta + \frac{\mu_0 M_s^2}{2} N_\parallel - \mu_0 M_s H_a \cos (\phi - \theta)$$

$$= V \left[ K_{eff} \sin^2 \theta + \frac{\mu_0 M_s^2}{2} N_\parallel - \mu_0 M_s H_a \cos (\phi - \theta) \right]$$

where $K_{eff} = K_1 + K_d = K_1 + \mu_0 M_s^2 \left( N_\perp - N_\parallel \right) / 2$ is the effective anisotropy constant which takes both magnetocrystalline and shape anisotropy into account [78, 169, 210]. The direction of equilibrium magnetization is determined by the condition [77, 78, 210]

$$\frac{\partial G_L}{\partial \theta} = 0$$

(2.285)

Imposing this condition, one finds

$$\frac{\partial G_L}{\partial \theta} = V \left[ 2K_{eff} \sin \theta \cos \theta - \mu_0 M_s H_a \sin (\phi - \theta) \right] = 0$$

(2.286)

or

$$\frac{2K_{eff}}{\mu_0 M_s} \sin \theta \cos \theta - H_a \sin (\phi - \theta) = 0$$

(2.287)

or even more compactly as

$$H_{K,eff} \sin \theta \cos \theta - H_a \sin (\phi - \theta) = 0$$

(2.288)

where $H_{K,eff} = 2K_{eff} / \mu_0 M_s$ is the effective anisotropy field, also known as the Stoner-Wohlfarth field (or the negative of the nucleation field in this context) [78]. A magnetic field of intensity $H_{K,eff}$ is sufficient to rotate the magnetization, and thus, it is also equal to the coercivity of the material. The above equation can be used to find the height of the energy barrier separating the two anisotropy energy minima. For example, for $\phi = 0$,
and in the absence of the demagnetizing field

\[ [H_K \cos \theta + H_a] \sin \theta = 0 \]  
(2.290)

where \( H_K = 2K_1/\mu_0 M_s \). The equation has the three solutions

\[ \theta = 0 \]  
(2.291)

\[ \theta = \pi \]  
(2.292)

\[ \theta = \cos^{-1} \left( -\frac{H_a}{H_K} \right) \]  
(2.293)

The first two solutions correspond to \( G_{L,\text{min}} \), whereas the third solution correspond to \( G_{L,\text{max}} \) when \( H_a/H_K \leq 1 \). Since \( \cos (H_a/H_K) \leq 1 \), a field of intensity \( H_K \) is sufficient to rotate the magnetization. The height of the energy barrier can be found from the difference

\[ E_b = G_{L,\text{max}} - G_{L,\text{min}} = K_1 V \left( 1 - \frac{H_a}{H_K} \right)^2 \]  
(2.294)

which disappears at \( H_a = H_K \).

Now, stable equilibrium is ensured only if the second derivative is strongly positive, viz. \([77, 78, 210]\)

\[ \frac{\partial^2 G_L}{\partial \theta^2} > 0 \]  
(2.295)

This derivative can be found and set to zero (since switching occurs when the energy minimum becomes unstable \([61]\))

\[ H_{K,\text{eff}} \cos 2\theta + H_a \cos (\phi - \theta) = 0 \]  
(2.296)

Thus equations (2.288) and (2.296) give the system

\[ \frac{1}{2} H_{K,\text{eff}} \sin 2\theta - H_a \sin (\phi - \theta) = 0 \]  
(2.297)

\[ H_{K,\text{eff}} \cos 2\theta + H_a \cos (\phi - \theta) = 0 \]  
(2.298)

which, after defining \( H_z = H_a \cos \phi, H_x = H_a \sin \phi \), can be rewritten as

\[ \frac{1}{2} H_{K,\text{eff}} \sin 2\theta - H_x \cos \theta + H_z \sin \theta = 0 \]  
(2.299)

\[ H_{K,\text{eff}} \cos 2\theta + H_x \cos \theta + H_z \cos \theta = 0 \]  
(2.300)

fluctuations, resulting in what is commonly known as Brown’s Paradox \([61, 68, 78]\). In general, Brown’s Theorem in micromagnetics states that the coercive field satisfies the inequality \([61, 169]\)

\[ H_c \geq H_K - N M_s = -H_N \]  
(2.289)
The two equations can be manipulated to get the parametric expressions

\[ H_x = H_{K,eff} \sin^3 \theta \]  
\[ H_z = -H_{K,eff} \cos^3 \theta \]  

which can be combined (by taking the cubic root and summing the squares) to give the equation of an asteroid

\[ H_x^{2/3} + H_z^{2/3} = H_{K,eff}^{2/3} \]  

This asteroid separates the region where the system has one single minimum from that with two stable minima [77].

![Switching asteroid obtained by plotting (2.303).](image)

**Figure 2.39:** Switching asteroid obtained by plotting (2.303).

### 2.4.4.2 Dynamics

The dynamics of a macrospin can be computed from the LLG equation

\[
\frac{d\mathbf{m}}{dt} = -\frac{\gamma G}{1 + \alpha^2} \mathbf{m} \times \mathbf{H}_{eff} - \frac{\gamma G}{1 + \alpha^2} \alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{H}_{eff}), \quad \mathbf{m}(r, 0) = \mathbf{m}_0
\]  

To find the form of the effective field, we write Landau-Gibbs free energy

\[
G_L(\mathbf{m}; H_a) = V \left\{ K_1 - K_1 (\mathbf{e}_{an} \cdot \mathbf{m})^2 + \frac{\mu_0 M_s^2}{2} \mathbf{m} \cdot (N \mathbf{m}) - \mu_0 M_s \mathbf{m} \cdot \mathbf{H}_a \right\}
\]

The effective field can be found from the derivative

\[
\mathbf{H}_{eff} = -\frac{1}{\mu_0 V M_s} \frac{\delta G_L}{\delta \mathbf{m}} = -\frac{1}{\mu_0 M_s} \frac{\delta}{\delta \mathbf{m}} \left[ K_1 - K_1 (\mathbf{e}_{an} \cdot \mathbf{m})^2 + \frac{\mu_0 M_s^2}{2} \mathbf{m} \cdot (N \mathbf{m}) - \mu_0 M_s \mathbf{m} \cdot \mathbf{H}_a \right]
\]
But from the rules of matrix calculus

$$\frac{\delta}{\delta \mathbf{m}} (\mathbf{e}_{an} \cdot \mathbf{m})^2 = 2(\mathbf{e}_{an} \cdot \mathbf{m}) \mathbf{e}_{an}$$  \hspace{1cm} (2.307)

$$\frac{\delta}{\delta \mathbf{m}} \mathbf{m} \cdot (N \mathbf{m}) = \frac{\delta}{\delta \mathbf{m}} \mathbf{m}^T N \mathbf{m} = (N + N^T) \mathbf{m} = 2N \mathbf{m}$$  \hspace{1cm} (2.308)

$$\frac{\delta}{\delta \mathbf{m}} \mathbf{m} \cdot \mathbf{H}_a = \frac{\delta}{\delta \mathbf{m}} \mathbf{m}^T \mathbf{H}_a = \mathbf{H}_a$$  \hspace{1cm} (2.309)

where we used the fact that $N$ is symmetric. Thus

$$\mathbf{H}_{eff} = \mathbf{H}_K (\mathbf{e}_{an} \cdot \mathbf{m}) \mathbf{e}_{an} - M_s N \mathbf{m} + \mathbf{H}_a$$  \hspace{1cm} (2.310)

where $H_K = 2K_1/\mu_0 M_s$.

### 2.4.5 Landau-Lifshitz-Gilbert-Slonczewski (LLGS)

The Landau-Lifshitz-Gilbert-Slonczewski (LLGS) is the LLG equation (2.246) with the STT term added.

![Figure 2.40: Magnetization precession and damping torques in the LLGS equation.](image)

From our discussion in 2.1.6, we know that for each electron (with $q = -e$ and a spin angular momentum $\pm \hbar/2$), the loss in the transverse spin angular momentum at a NM/FM interface is [29]

$$-\frac{1}{e} \left[ \mathbf{I}_S \cdot \mathbf{m} \right] = -\frac{1}{e} \left[ \mathbf{I}_S - (\mathbf{I}_S \cdot \mathbf{m}) \mathbf{m} \right]$$  \hspace{1cm} (2.311)

where $\mathbf{I}_S$ is the spin current (in units of A). For sufficiently small nanomagnets, the macrospin approximation holds and all spins rotate in unison. In this case, the torque has to be shared with all the spins and thus can simply be divided by $M_s V$ [21, 29]. In addition, this torque has to be scaled by the appropriate gyromagnetic ratio ($\gamma_S$ in this
case) for it to be included in the equation of dynamics,\(^98\) namely

\[
- \gamma_S \frac{1}{M_s V} \left[ I_S - (I_S \cdot m) \right] m 
\]

(2.312)

However, \(\gamma_S = -g_S \mu_B / \hbar \cong -2\mu_B / \hbar\) and thus we can write the STT torque as

\[
\tau_{STT} = - \gamma_S \frac{1}{M_s V} \left[ I_S - (I_S \cdot m) \right] m = \frac{\mu_B}{e M_s V} \left[ I_S - (I_S \cdot m) \right] m = \frac{1}{e N_s} \left[ I_S - (I_S \cdot m) \right] m 
\]

where we identified \(N_s = M_s V / \mu_B\) as the number of Bohr magnetons comprising the FM [47]. Now, using (A.146), we can write

\[
m \times (I_S \times m) = (m \cdot m) I_S - (I_S \cdot m) m = I_S - (I_S \cdot m) m 
\]

(2.313)

and the STT torque becomes

\[
\tau_{STT} = \frac{1}{e N_s} m \times (I_S \times m) 
\]

(2.314)

The LLGS equation thus reads

\[
\frac{d m}{d t} = -\gamma_G m \times H_{eff} + \alpha m \times \frac{d m}{d t} + \tau_{STT}, \quad m(r, 0) = m_0 
\]

(2.315)

where \(\tau_{STT} = (1/e N_s) m \times (I_S \times m)\). The competition between the damping and STT terms is shown in Fig. 2.41.

---

\(^98\)Something like

\[
\frac{d m}{d t} = \gamma \tau
\]
The LLGS equation is a transcendental equation. It can be casted in the LL form by plugging the derivative in the right-hand side

\[
\frac{dm}{dt} = -\gamma G (m \times H_{eff}) + \alpha \left( m \times \left[ -\gamma \mu_0 (m \times H_{eff}) + \alpha \left( m \times \frac{dm}{dt} \right) + \tau_{STT} \right] \right) + \tau_{STT}
\]

\[
= -\gamma G (m \times H_{eff}) - \alpha \gamma G [m \times (m \times H_{eff})] + \alpha^2 \left[ m \times \left( m \times \frac{dm}{dt} \right) \right] + \alpha (m \times \tau_{STT}) + \tau_{STT}
\]

(2.316)

However, from (A.146), we can write

\[
m \times \left( m \times \frac{dm}{dt} \right) = m \left( m \cdot \frac{dm}{dt} \right) - \frac{dm}{dt} (m \cdot m) = 0 - \frac{dm}{dt} |m|^2 = -\frac{dm}{dt} \tag{2.317}
\]

where we have used (2.110). Therefore

\[
\frac{dm}{dt} = -\gamma G (m \times H_{eff}) - \gamma G \alpha [m \times (m \times H_{eff})] - \alpha^2 \frac{dm}{dt} + \alpha (m \times \tau_{STT}) + \tau_{STT}
\]

(2.318)

or, after collecting like terms, the LLGS finally becomes

\[
\frac{dm}{dt} = -\frac{\gamma G}{1 + \alpha^2} m \times H_{eff} - \frac{\gamma G}{1 + \alpha^2} \alpha m \times (m \times H_{eff}) + \frac{1}{1 + \alpha^2} \alpha m \times \tau_{STT} + \frac{1}{1 + \alpha^2} \tau_{STT}, \quad m(r, 0) = m_0 \tag{2.319}
\]

where \(\tau_{STT} = (1/eN_s) m \times (I_s \times m)\) and \(m \times \tau_{STT} = (1/eN_s) m \times I_s\).\(^{99}\)

\[\text{2.5 Stochastic Dynamic Equations}\]

\[\text{2.5.1 Thermal Noise in Nanomagnets}\]

The equations discussed so far model the magnetization dynamics at 0 K [198]. When \(T \neq 0\), a ferromagnet will experience the unavoidable thermal noise due to the interaction with the thermal bath [211]. In modern magnetized media (which lie in the mesoscopic or nanoscopic scale), thermal agitation is significant, and magnetization (though macroscopically have constant magnitude) fluctuates in direction [78, 196, 199]. Fig. 2.42 shows the effect of temperature on magnetization trajectories. In general, this thermal

\[\text{\(\^99\)Easily obtained from}\]

\[
m \times \tau_{STT} = \frac{1}{eN_s} m \times [I_s - (I_s \cdot m) m] = \frac{1}{eN_s} [m \times I_s - (I_s \cdot m) m \times m] = \frac{1}{eN_s} m \times I_s
\]
fluctuation is caused by the coupling of the magnetic moment with the microscopic degrees of freedom of its environment such as phonons, conducting electrons, nuclear spins, etc. [206, 212].

![Possible stochastic trajectories for damped motion obtained by numerically integrating the stochastic LLG equation. (a) $T = 4.2$ K. (b) $T = 77$ K. (c) $T = 300$ K.]

As discussed previously, modern spintronic devices utilize FMs which tend to be monodomain. The magnetic energy of these small magnets depends on the magnetic moment orientation, which, because of anisotropy, has a number of preferred stable directions or energy minima (defined by the easy-axes), separated by an energy barrier $E_b$ that is in general proportional to the effective anisotropy and volume of the sample. Namely, $E_b = K_{eff}V$ in the absence of an applied field, or in general [16, 78, 198, 206]

$$E_b = K_{eff}V \left(1 - \frac{H_a}{H_{K}}\right)^2$$

(2.320)

At $T = 0$ K, one has the anisotropy field $H_{K,eff} = 2K_{eff}/\mu_0M_s$, whereas at $T \neq 0$ K, one has [78, 169]

$$H_{K,eff} = \frac{2K_{eff}}{\mu_0M_s} \left[1 - \left(\frac{d_{sp}}{d}\right)^{3/2}\right] = \frac{2K_{eff}}{\mu_0M_s} \left[1 - \left(\frac{25k_B T}{K_{eff}V}\right)^{1/2}\right]$$

(2.321)

where $d_{sp} = (25k_B T/\alpha K_{eff})^{3}$ is the critical superparamagnetic diameter,\textsuperscript{101} $V = \alpha d^3$ is the volume of the particle, and $\alpha$ is a geometrical factor that depends on the shape of the particle [78, 169]. The above anisotropy field formula is valid in the range $0 \leq T \leq K_{eff}V/25k_B$.

Using the concept of an energy barrier, one can quantify the stability of the magnet under thermal fluctuations by the ratio of the energy barrier to the thermal activation

---

\textsuperscript{100} Defined as the difference between the energies at the saddle and minimum points.

\textsuperscript{101} A superparamagnet behaves like a Langevin paramagnet; presenting a giant classical moment ($10^4$ times larger than individual atomic moment), hence the name [61].
energy, $\Delta = E_b/k_B T$, usually called the *thermal stability factor*\cite{15,16}.\footnote{For example, the thermal stability limit for magnetic recording is typically taken as $\Delta > 25$. This is usually considered the limit at which transition to superparamagnetism in most particles takes place (although it could vary between 20 - 25)\cite{61,68,78}.} If the thermal energy is comparable to or larger than the energy barrier, the system is unstable and will oscillate between energy minima, presenting superparamagnetism\cite{15,61,68,78,82}. Superparamagnetism is typically characterized by zero coercivity, zero remanence, and a blocking temperature $T_B$ above which a FM order disappears\cite{68}. If the thermal energy is smaller than the energy barrier, the system behaves as a paramagnet, and the magnetization will stay in a local minimum and will precess for many periods until thermal fluctuations cause magnetization reversal from one stable state to another by surmounting the energy crest separating the two valleys (Fig. 2.43)\cite{68}. This switching phenomenon occurs on physically relevant timescales and is known as the thermal fluctuation after-effect (or just thermal-activation), one of the after-effects inherent to FMs\cite{61,206}.

Assume $H_a = 0$. Most of the time, one has $E_b/k_B T \gg 1$, and switching due to thermal fluctuations rarely occurs. However, there is still a finite probability of such unwanted events, and one can calculate the mean time between two flips. In literature, this retention time is called the Néel relaxation time\cite{213} of magnetization, and it can be approximated in the high-barrier regime using the Néel-Brown law\cite{68,199}.

\begin{equation}
\tau_N = \tau_0 e^{E_b/k_B T} \tag{2.322}
\end{equation}

\footnote{Sometimes called the Arrhenius-Néel law, since it resembles an Arrhenius type activation law.}
where \( \tau_0 \) is the attempt time, a characteristic of the material that usually falls in the range \( 10^{-12} \text{ to } 10^{-9} \, \text{s} \) [78]. The relaxation time \( \tau_N \) is the inverse of the relaxation frequency (frequency of jumps or inversions), whereas \( \tau_0 \) is inverse of the attempt frequency (the number of attempts to surmount the energy barrier). If one denotes the measurement time (or time window) by \( t_m \), then for \( t_m \gg \tau_N \) the magnetization will flip several times during the measurement, and the magnet is in a superparamagnetic state with zero average magnetization [78, 206]. If, on the other hand, \( t_m \ll \tau_N \), the magnetization will not flip during the measurement and will be blocked in its initial state, resulting in nonzero spontaneous magnetization [78, 206]. In between, a nonequilibrium phenomena accompanied with magnetic relaxation occurs [206]. The blocking temperature is defined as the temperature at which \( t_m = \tau_N \). Imposing this condition in (2.322), one finds [169]

\[
T_B = \frac{E_b}{k_B \ln \left( \frac{\tau_N}{\tau_0} \right)}
\]

Under this temperature, the particle is blocked (ferromagnet): hysteresis will appear and superparamagnetism will disappear; while above it, the particle is unblocked and the information is lost [68, 78, 82].

### 2.5.2 Stochastic LLG (sLLG)

The dynamic equations associated with a thermally disturbed system are the stochastically perturbed dynamic equations [192]. The effect of thermal noise can be added as an extra random thermal field to the effective field given by (2.187) [199, 206, 214, 215]. The thermal field will be assumed to be Gaussian because \( \mathbf{m} \) interacts with a large number of independent (or weakly coupled) microscopic degrees of freedom with equivalent statistical properties [196, 206]. The stochastically perturbed LLG equation is a stochastic differential equation (SDE) of the Langevin type with multiplicative noise, namely [198, 199, 212]

\[
\frac{d\mathbf{m}}{dt} = -\frac{\gamma G}{1 + \alpha^2} \mathbf{m} \times (\mathbf{H}_{eff} + \mathbf{H}_T) - \frac{\gamma G}{1 + \alpha^2} \alpha \mathbf{m} \times [\mathbf{m} \times (\mathbf{H}_{eff} + \mathbf{H}_T)], \quad \mathbf{m}(r, 0) = \mathbf{m}_0
\]

(2.324)

where \( \mathbf{H}_T \) is the thermal field defined as \( \mathbf{H}_T = \sigma \dot{\mathbf{W}} \). Here, \( \dot{\mathbf{W}} \) is the derivative of a Wiener process that represents the effect of thermal fluctuations. It is an uncorrelated

\(^{104}\text{Central limit theorem [196, 211, 216].}\)
and independent Gaussian white noise\textsuperscript{105} characterized by the two moments\textsuperscript{106} \cite{198, 199}

\[
\langle \dot{W}_i (t) \rangle = 0 \tag{2.325}
\]

\[
\langle \dot{W}_i (t) \dot{W}_j (t + \tau) \rangle = 2D\delta_{ij}\delta (\tau) \tag{2.326}
\]

where \(D\) is a measure of the fluctuating field strength (typically determined by the fluctuation-dissipation theorem). Here \(\sigma^2 = 2D\) is the variance. In addition, \(\langle \rangle\) denotes an average taken over different realizations of the thermal field \cite{206, 212}. The zero first moment expresses the fact the average thermal field taken over different realizations vanishes in all directions \(i \in \{x, y, z\}\). In the second moment, the Kronecker delta \(\delta_{ij}\) expresses the assumption that the different components of the thermal field are uncorrelated, whereas the Dirac delta \(\delta (\tau)\) expresses the assumption that the correlation time of the thermal field is much shorter then the response time of the system, i.e. the noise has negligible correlation time ("white noise") \cite{196, 212}.

The magnetization trajectory can be obtained by integrating (2.324), which now has a stochastic contribution in addition to the deterministic one. In the stochastic term, the thermal field \(H_T\) enters in a multiplicative way (through the cross product \(m \times (\cdot)\)), which needs a little extra care when handling since for a white multiplicative noise any Langevin equation must be supplemented by an interpretation rule to properly define it \cite{206, 217}. The two dominant interpretations will lead to either Itô \cite{218} or Stratonovich \cite{219} calculus, which, due to different drift terms, will yield different dynamical properties \cite{212}. The Itô interpretation relies upon the Markovian and Martingale properties and is usually used when one wants to employ general results of probability theory, whereas the Stratonovich interpretation (which does not invoke the Martingale property) is typically preferred in physical applications since it preserves the standard rules of ordinary calculus (e.g., chain rule) \cite{206, 217, 220}. Regarding the equation at hand, it turned out that (2.324) should be interpreted in the Stratonovich sense since in the Itô interpretation the magnetization would not only not be preserved in magnitude but will also blow up in a finite time \cite{198}.\textsuperscript{107} The Stratonovich interpretation of the LLG equation will thus lead to correct thermal properties, in contrast to the Itô interpretation \cite{196, 206}. In general, the white noise interpretation of at least scalar SDEs should be handled in the Stratonovich sense \cite{217, 220}.

From a numerical integration point of view, the multiplicative white noise in the Langevin equation also introduces difficulties in developing high-order schemes \cite{221}.

\begin{footnotesize}
\begin{itemize}
\item[\textsuperscript{105}] Formally defined as the derivative of a Wiener process, see A.2.
\item[\textsuperscript{106}] Recall that the first two moments determine a Gaussian process.
\item[\textsuperscript{107}] Brown \cite{199} who first described the spins dynamics using Langevin equations (and others; e.g. Kubo \cite{215} who on the other hand considered generic classical spins) have in general employed the Stratonovich calculus.
\end{itemize}
\end{footnotesize}
This presents an issue since, in addition to the fact that a mere translation of a numerical scheme in the deterministic case might not be convergent in the stochastic case (to either calculus), the order of convergence is typically lower than in the deterministic scheme [206].

To analyze the problem and find an expression for $D$, let us start by separating the deterministic and stochastic parts of (2.324) as

$$
\frac{d\mathbf{m}}{dt} = -\frac{\gamma G}{1 + \alpha^2} \mathbf{m} \times \mathbf{H}_{\text{eff}} - \frac{\gamma G}{1 + \alpha^2} \alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{H}_{\text{eff}})
- \frac{\gamma G}{1 + \alpha^2} \mathbf{m} \times \mathbf{H}_T - \frac{\gamma G}{1 + \alpha^2} \alpha \mathbf{m} \times (\mathbf{m} \times \mathbf{H}_T)
$$

(2.327)

which in fact reveals that it is a Langevin type SDE with multiplicative noise (cf. A.2.4). The dynamic equation can be casted into the form of a general system of Langevin equations

$$
d\mathbf{m} = a(t, \mathbf{m}) \, dt + B(t, \mathbf{m}) \circ \mathbf{H}_T(t) \, dt, \quad \mathbf{m}(t_0) = \mathbf{m}_0
$$

(2.328)

where the symbol “$\circ$” indicates a Stratonovich interpretation (cf. A.2). The equation can be written component-wise, viz.

$$
dm_i = a_i(t, \mathbf{m}) \, dt + b_{ik}(t, \mathbf{m}) \circ \mathbf{H}_{T,k}(t) \, dt, \quad m_i(t_0) = m_{i,0}
$$

(2.329)

for $i \in \{x, y, z\}$. Now, if we use the antisymmetrical unit tensor $\varepsilon_{ijk}$ (Levi-Civita symbol (A.5)), we can write

$$
[A \times B]_i = \varepsilon_{ijk} A_j B_k
$$

(2.330)

and\footnote{It might be also easy use (A.146).}

$$
[A \times (B \times C)]_i = \varepsilon_{ijn} A_j \varepsilon_{nmk} B_m C_k \\
= \varepsilon_{ijn} \varepsilon_{nmk} A_j B_m C_k \\
= \varepsilon_{ijn} \varepsilon_{mkn} A_j B_m C_k \\
= (\delta_{in} \delta_{jk} - \delta_{ik} \delta_{jn}) A_j B_m C_k \\
= (\delta_{in} A_m \delta_{jk} B_j - \delta_{ik} \delta_{jn} A_j B_m) C_k \\
= (A_i B_k - \delta_{ik} A_m B_m) C_k
$$

(2.331)
where Einstein summation convention is assumed throughout (see A.1.1.1). Using (2.335) and (2.330) with \(A = \mathbf{m}, B = \mathbf{m}, C = \mathbf{H}_{\text{eff}}\), we obtain

\[
[m \times \mathbf{H}_{\text{eff}}]_i = \varepsilon_{ijk}m_j\mathbf{H}_{\text{eff},k}
\]

(2.332)

\[
[m \times (m \times \mathbf{H}_{\text{eff}})]_i = (m_i m_k - \delta_{ik}m_m^2)\mathbf{H}_{\text{eff},k} = (m_i m_k - \delta_{ik})\mathbf{H}_{\text{eff},k}
\]

(2.333)

Using the last equations, we find [206, 212]

\[
a_i(t, \mathbf{m}) = -\frac{\gamma G}{1 + \alpha^2}[\varepsilon_{ijk}m_j + \alpha(m_i m_k - \delta_{ik})]H_{\text{eff},k}
\]

(2.334)

\[
b_{ik}(t, \mathbf{m})H_{T,k} = -\frac{\gamma G}{1 + \alpha^2}[\varepsilon_{ijk}m_j + \alpha(m_i m_k - \delta_{ik})]H_{T,k}
\]

(2.335)

Now, to find \(D\), we use the Fokker-Planck equation (FPE) which describes the temporal evolution of the probability density of a stochastic process expressed by the Langevin equation (2.329) [206, 222]. The equation describes the evolution of the entire distribution function on the spherical surface rather than the evolution under individual thermal kicks. The FPE reads [199]

\[
\frac{\partial p}{\partial t} = -\frac{\partial}{\partial m_i} \left[ \left(a_i + D\frac{\partial b_{ik}}{\partial m_j} \right) p \right] + \frac{\partial^2}{\partial m_i \partial m_j} [(D b_{ik} b_{jk}) p]
\]

(2.336)

By taking the \(m_j\) derivatives on the right-hand side, one can cast the FPE in the form of a continuity equation for the probability distribution [206]

\[
\frac{\partial p}{\partial t} = -\frac{\partial}{\partial m_i} \left[ \left(a_i - D b_{ik} \frac{\partial b_{ik}}{\partial m_j} - D b_{ik} b_{jk} \frac{\partial}{\partial m_j} \right) p \right]
\]

(2.337)

Let us start by considering the second term. Using (2.335), we write

\[
\frac{\partial b_{ik}}{\partial m_j} = \frac{\partial}{\partial m_j} \left[ -\frac{\gamma G}{1 + \alpha^2}[\varepsilon_{ijk}m_j + \alpha(m_i m_k - \delta_{ik})]H_{T,k} \right]
\]

\[
= -\frac{\gamma G}{1 + \alpha^2}[\varepsilon_{ijk}m_j + \alpha(m_i m_k - \delta_{ik})] \cdot \frac{\partial}{\partial m_j} [\varepsilon_{ijk}m_j + \alpha(m_i m_k - \delta_{ik})]
\]

\[
= -\frac{\gamma G}{1 + \alpha^2}[\varepsilon_{ijk} + \alpha(\delta_{ij}m_k + m_i \delta_{jk} - 2\delta_{ik}m_j)]
\]

(2.338)

Contracting the index \(i\)

\[
\frac{\partial b_{jk}}{\partial m_j} = -\frac{\gamma G}{1 + \alpha^2}[\varepsilon_{jjk} + \alpha(\delta_{jj}m_k + m_j \delta_{jk} - 2\delta_{jk}m_j)]
\]

\[
= -\frac{\gamma G}{1 + \alpha^2}[0 + \alpha(3m_k + m_k - 2m_k)]
\]

\[
= -\frac{\gamma G}{1 + \alpha^2}(2\alpha m_k)
\]

(2.339)
Therefore
\[
\begin{align*}
 b_{ik} \frac{\partial b_{jk}}{\partial m_j} &= \left\{ -\frac{\gamma G}{1+\alpha^2} [\varepsilon_{ijk} m_j + \alpha (m_i m_k - \delta_{ik})] \right\} \left\{ -\frac{\gamma G}{1+\alpha^2} (2\alpha m_k) \right\} \\
 &= \left( \frac{\gamma G}{1+\alpha^2} \right)^2 2\alpha [\varepsilon_{ijk} m_j + \alpha (m_i m_k - \delta_{ik})] m_k \\
 &= \left( \frac{\gamma G}{1+\alpha^2} \right)^2 2\alpha [\varepsilon_{ijk} m_j m_k + \alpha (m_i m_k m_k - \delta_{ik} m_k)] \\
 &= \left( \frac{\gamma G}{1+\alpha^2} \right)^2 2\alpha [0 + \alpha (m_i - m_i)] \\
 &= 0
\end{align*}
\] (2.340)

and thus the second term vanishes. Consider the third term
\[
\begin{align*}
 b_{ik} b_{jk} &= \left\{ -\frac{\gamma G}{1+\alpha^2} [\varepsilon_{ijk} m_j + \alpha (m_i m_k - \delta_{ik})] \right\} \left\{ -\frac{\gamma G}{1+\alpha^2} [\varepsilon_{jik} m_j + \alpha (m_j m_k - \delta_{jk})] \right\} \\
 &= \left( \frac{\gamma G}{1+\alpha^2} \right)^2 \alpha [\varepsilon_{ijk} m_j + \alpha (m_i m_k - \delta_{ik})] (m_j m_k - \delta_{jk}) \\
 &= \left( \frac{\gamma G}{1+\alpha^2} \right)^2 \alpha [\varepsilon_{ijk} m_j m_k - \varepsilon_{ijk} m_j \delta_{jk} + \alpha m_i m_k m_j m_k - \alpha m_i m_k \delta_{jk} - \alpha m_j m_k \delta_{ik} + \alpha \delta_{ik} \delta_{jk}] \\
 &= \left( \frac{\gamma G}{1+\alpha^2} \right)^2 \alpha [\varepsilon_{ijk} m_k - \varepsilon_{ijk} m_k + \alpha m_i m_j - \alpha m_i m_j = \alpha m_j m_i + \alpha \delta_{ij}] \\
 &= \left( \frac{\gamma G}{1+\alpha^2} \right)^2 \alpha^2 [-m_j m_i + \delta_{ij}]
\end{align*}
\] (2.341)

which can be compared to (2.333) to reveal that
\[
\begin{align*}
 b_{ik} b_{jk} \frac{\partial p}{\partial m_j} &= -\left( \frac{\gamma G}{1+\alpha^2} \right)^2 (1+\alpha^2) \left[ m \times \left( m \times \frac{\partial p}{\partial m_j} \right) \right]_i
\end{align*}
\] (2.342)

Finally, using (2.334), (2.340) and (2.342) in (2.337), one can write the FPE as
\[
\begin{align*}
 \frac{\partial p}{\partial t} &= -\frac{\partial}{\partial m_i} \left[ \left( -\frac{\gamma G}{1+\alpha^2} m \times H_{eff} - \frac{\gamma G}{1+\alpha^2} \alpha m \times (m \times H_{eff}) \right) \right]_i \\
 &\quad + D \frac{\gamma G^2}{1+\alpha^2} \left[ m \times \left( m \times \frac{\partial p}{\partial m_j} \right) \right]_i
\end{align*}
\] (2.343)

or
\[
\begin{align*}
 \frac{\partial p(t,\mathbf{m})}{\partial t} &= -\frac{\partial}{\partial \mathbf{m}} \left\{ \left[ -\frac{\gamma G}{1+\alpha^2} \mathbf{m} \times H_{eff} - \frac{\gamma G}{1+\alpha^2} \alpha \mathbf{m} \times (\mathbf{m} \times H_{eff}) \right] \right. \\
 &\quad \left. + \frac{1}{2\tau_N} \mathbf{m} \times \left( \mathbf{m} \times \frac{\partial p}{\partial \mathbf{m}} \right) \right\}
\end{align*}
\] (2.344)

where
\[
\frac{1}{\tau_N} = 2D \frac{\gamma G^2}{1+\alpha^2}
\] (2.345)
is the reciprocal of the Néel relaxation time. Now, in order to ensure that the stationary properties coincide with the proper thermal equilibrium properties, the FPE is forced to have the Boltzmann distribution as a stationary solution, namely

\[ p_0(m) = p_0(m_0), \]

where

\[ p_0(m_0) = \frac{1}{e^{E/k_B T}}, \]

so that the FPE (2.344) becomes

\[
0 = -\frac{\partial}{\partial m} \left\{ \left[ -\frac{\gamma G}{1 + \alpha^2} m \times H_{eff} - \frac{\gamma G}{1 + \alpha^2} \alpha m \times (m \times H_{eff}) \right] \right\}
+ \frac{1}{2 \tau_N} m \times \left( m \times \frac{\partial}{\partial m} \right) p_0.
\]

(2.347)

where we have set \( \partial p_0(m) / \partial t = 0 \). Moreover

\[
\frac{\partial p_0}{\partial m} = -\frac{1}{k_B T} \frac{\partial E}{\partial m} p_0.
\]

(2.348)

However, for a magnet of volume \( V \), the energy is given by

\[
E = (-\mu_0 M \cdot H_{eff}) V = -\mu_0 VM_S m \cdot H_{eff}
\]

(2.349)

Thus

\[
\frac{\partial E}{\partial m} = -\mu_0 VM_S H_{eff}
\]

(2.350)

from which we find

\[
\frac{\partial p_0}{\partial m} = \frac{\mu_0 VM_S}{k_B T} H_{eff} p_0.
\]

(2.351)

And thus the first term of the FPE becomes

\[
\frac{\partial}{\partial m} \left\{ \left[ -\frac{\gamma G}{1 + \alpha^2} m \times H_{eff} p_0 \right] \right\}
= -\frac{\gamma G}{1 + \alpha^2} \alpha m \times \left( \frac{k_B T}{\mu_0 VM_S} \frac{\partial p_0}{\partial m} \right)
= -\frac{\gamma G}{1 + \alpha^2} \frac{k_B T}{\mu_0 VM_S} \frac{\partial}{\partial m} \left( \frac{\partial p_0}{\partial m} \right)
\]

(2.352)

which has the \( i \)-th component

\[
\left[ \frac{\partial}{\partial m} \left( m \times \frac{\partial p_0}{\partial m} \right) \right]_i = \frac{\partial}{\partial m_i} \left( \varepsilon_{ijk} m_j \frac{\partial p_0}{\partial m_k} \right) = 0
\]

(2.353)

\(^{109}\) Also known as the free-diffusion time [206].
Thus the FPE (2.347) becomes

\[
0 = -\frac{\partial}{\partial m} \cdot \left[ -\frac{\gamma G}{1 + \alpha^2} \alpha m \times (m \times H_{eff}) p_0 + \frac{1}{2\tau_N} m \times \left( m \times \frac{\partial}{\partial m} p_0 \right) \right]
\]

\[
= -\frac{\partial}{\partial m} \cdot \left[ -\frac{\gamma G}{1 + \alpha^2} \alpha m \times (m \times H_{eff}) p_0 + \frac{1}{2\tau_N} m \times \left( m \times \frac{\mu_0 V M_S}{k_B T} H_{eff} p_0 \right) \right]
\]

\[
= -\frac{\partial}{\partial m} \cdot \left[ -\frac{\gamma G}{1 + \alpha^2} \alpha m \times (m \times H_{eff} p_0) + \frac{\mu_0 V M_S}{k_B T} \frac{1}{2\tau_N} m \times (m \times H_{eff} p_0) \right]
\]

\[
= -\left( -\frac{\gamma G}{1 + \alpha^2} \alpha + \frac{\mu_0 V M_S}{k_B T} \frac{1}{2\tau_N} \right) \frac{\partial}{\partial m} \cdot \left[ m \times (m \times H_{eff} p_0) \right]
\]

(2.354)

One can then see that it suffice to set

\[
-\frac{\gamma G}{1 + \alpha^2} \alpha + \frac{\mu_0 V M_S}{k_B T} \frac{1}{2\tau_N} = 0
\]

(2.355)

from which we find

\[
\frac{1}{\tau_N} = 2 \frac{\gamma G}{1 + \alpha^2} \frac{\alpha k_B T}{\mu_0 V M_S}
\]

(2.356)

Comparing this to (2.345), we obtain the strength of the thermal field

\[
D = \frac{\alpha k_B T}{\gamma G \mu_0 V M_S}
\]

(2.357)

which is the well-known fluctuation-dissipation relation. The above expression is for the LLG formulation. If one wishes to use the LL form, the substitution (2.238) is needed. In fact, using this we obtain the field strength for the LL and LLG equations [206, 222]

\[
D_{LL} = \frac{1}{1 + \frac{\lambda^2}{\gamma_{LL} \mu_0 V M_s}} \frac{\lambda k_B T}{1 + \frac{\lambda^2}{\gamma_{LL} \mu_0 V M_s}}
\]

(2.358)

\[
D_G = \frac{\alpha k_B T}{\gamma_G \mu_0 V M_s}
\]

(2.359)

Although these quantities will definitely yield different trajectories for the magnetization, the averaged quantities obtained from either the LL or LLG are the same [206].
2.5.3 Stochastic LLGS (sLLGS)

The stochastic LLGS (sLLGS) is the stochastically perturbed LLGS equation [223–225], viz.

\[
\frac{d\mathbf{m}}{dt} = -\frac{\gamma G}{1 + \alpha^2} \mathbf{m} \times (H_{\text{eff}} + H_T) - \frac{\gamma G}{1 + \alpha^2} \alpha \mathbf{m} \times [\mathbf{m} \times (H_{\text{eff}} + H_T)]
\]
\[
+ \frac{1}{1 + \alpha^2} \alpha \mathbf{m} \times \tau_{\text{STT}} + \frac{1}{1 + \alpha^2} \tau_{\text{STT}}, \quad \mathbf{m}(r, 0) = \mathbf{m}_0
\]  

(2.360)

where \(\tau_{\text{STT}} = (1/eN_s) \mathbf{m} \times (I_S \times \mathbf{m})\) and \(\mathbf{m} \times \tau_{\text{STT}} = (1/eN_s) \mathbf{m} \times I_S\). Here, the thermal field is again given by \(H_T = \sigma \dot{\mathbf{W}}\), where

\[
\langle \dot{W}_i(t) \rangle = 0
\]
\[
\langle \dot{W}_i(t) \dot{W}_j(t + \tau) \rangle = 2D \delta_{ij} \delta(\tau)
\]  

(2.361, 2.362)

The main assumption in the above formulation is that the STT term does not contain a fluctuating field, which is a good assumption considering the fact that the transport properties of the conduction electrons are less affected by the thermal field since they have much higher Fermi level than the thermal energy [225].

Similar to the previous subsection, one may start by casting the sLLGS into a vector Langevin equation

\[
d\mathbf{m} = a(t, \mathbf{m}) \, dt + B(t, \mathbf{m}) \circ H_T(t) \, dt, \quad \mathbf{m}(t_0) = \mathbf{m}_0
\]  

(2.363)

and write the FPE

\[
\frac{\partial \rho(t, \mathbf{m})}{\partial t} = -\frac{\partial}{\partial \mathbf{m}} \cdot \left\{ -\frac{\gamma G}{1 + \alpha^2} \mathbf{m} \times H_{\text{eff}} - \frac{\gamma G}{1 + \alpha^2} \alpha \mathbf{m} \times (\mathbf{m} \times H_{\text{eff}}) + \frac{1}{1 + \alpha^2} \alpha \mathbf{m} \times \tau_{\text{STT}}
\]
\[
+ \frac{1}{1 + \alpha^2} \tau_{\text{STT}} + D \frac{\gamma G^2}{1 + \alpha^2} \mathbf{m} \times \left( \mathbf{m} \times \frac{\partial}{\partial \mathbf{m}} \right) \right\} \rho \right\}
\]  

(2.364)

where now only the deterministic term is altered. If \(I_S = 0\) (i.e., no STT action), then we are in the same situation arrived at the previous subsection: \(\rho\) takes the form of the Boltzmann distribution, and one can find the strength of the fluctuating field, \(D\). However, when \(I_S \neq 0\), one can show that the Boltzmann distribution is no more a solution of the FPE. The reason is that the system is now out of equilibrium; it is open (due to the applied current) with no minimum free energy, which breaks down the concept of thermal equilibrium [225].
However, following [225], we can still try to obtain a stationary solution of the equation, namely, setting $\partial p_0 (m)/\partial t = 0$ so that

$$0 = -\frac{\partial}{\partial m} \left\{ \left[ -\frac{\gamma G}{1 + \alpha^2} m \times H_{eff} - \frac{\gamma G}{1 + \alpha^2} \alpha m \times (m \times H_{eff}) + \frac{1}{1 + \alpha^2} \alpha m \times \tau_{STT} + \frac{1}{1 + \alpha^2} \tau_{STT} \right] + D \frac{\gamma G^2}{1 + \alpha^2} m \times \left( m \times \frac{\partial}{\partial m} \right) \right\} \right) \right\} \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) \right) 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2.5.4 Numerical Scheme: Heun’s Method

Also referred to as the modified (or improved) Euler method. It is an example of a predictor-corrector method (a sort of two-stage Runge-Kutta scheme). It has been found to be a good compromise between numerical stability and computational complexity, and converges quadratically when one interprets the integral of the Langevin equations (2.327) in the Stratonovich sense [212]. In fact, the main reason for using Heun’s scheme is that Stratonovich solutions are obtained without altering the deterministic drift term \( a_i (t, m) \) which is actually integrated with a second order accuracy [206, 212]. Below we show the stochastic generalization of Heun’s method [206].

**Algorithm 2.1 (Heun’s Method)**

Given the SDE

\[
\frac{d m_i}{dt} = a_i (t, m) dt + b_{ik} (t, m) \circ H_{T,k} (t) dt, \quad m_i (t_0) = m_{i,0}
\]

for \( i \in \{x, y, z\} \), Heun’s predictor-corrector scheme is given by

\[
\begin{align*}
\tilde{m}_{i,n+1} &= m_i^n + a_i (t^n, m^n) \Delta t + b_{ik} (t^n, m^n) \Delta W^n_k \\
\tilde{m}_{i,n+1} &= m_i^n + \Delta t \left[ a_i (t^n, m^n) + a_i (t^{n+1}, \tilde{m}^{n+1}) \right] \\
&\quad + \Delta W^n_k \left[ b_{ik} (t^n, m^n) + b_{ik} (t^{n+1}, \tilde{m}^{n+1}) \right]
\end{align*}
\]

where \( n = 1, 2, \ldots, N \) and \( N = (t_{final} - t_0) / \Delta t \). Here

\[
\Delta W^n_k = \int_t^{t+\Delta t} H_{T,k} (s) \, ds
\]

are Gaussian random numbers with the following statistical properties

\[
\begin{align*}
\langle \Delta W_i \rangle &= 0 \\
\langle \Delta W_i \Delta W_j \rangle &= 2D \delta_{ij} \Delta t
\end{align*}
\]

where the variance is given by

\[
2D = 2 \frac{\alpha k_B T}{\gamma G \mu_0 V M_S} \quad (2.373)
\]

We note that since Euler’s integration scheme does not preserve the norm of the vector—which is preserved by (2.110) and hence lives in the sphere \( \mathbb{S}^2 \)—one has to normalize the vector after every time step, or otherwise the solution may blow up in a
finite time. Moreover, for an efficient algorithm to generate the Gaussian random numbers the reader is referred to Appendix C.

2.5.5 Randomizing The Initial Angle

Since the initial angle of a FM is thermally distributed, then for consistency one has to randomize this angle before starting the integration scheme. To find the most probable angle deviation under thermal perturbation, we follow \[123\] and use the *equipartition theorem* from statistical mechanics. \[112\] Consider the total energy of a uniformly magnetized FM in the absence of external fields

\[
E = -\mu_0 M \cdot H_{eff} V \\
= \left( K_1 \left[ 1 - \left( \frac{e_{an} \cdot M}{M_s^2} \right)^2 \right] + \frac{\mu_0}{2} M \cdot (NM) \right) V \\
= \left( K_{eff} \sin^2 \theta_0 + \frac{\mu_0 M_s^2}{2} N_{\parallel} \right) V
\]

(2.374)

where \( K_{eff} = K_1 + K_d = K_1 + \mu_0 M_s^2 \left( N_\perp - N_{\parallel} \right) / 2 \) is the effective anisotropy constant which takes both magnetocrystalline and shape anisotropy into account (see 2.4.4.1). Here, \( \theta_0 \) is the initial angle in root-mean-square (RMS). Since we care about energy changes, we can drop the constant term for now and just write

\[
E = K_{eff} V \sin^2 \theta_0
\]

(2.375)

Now, the equipartition theorem states that in thermal equilibrium, every degree of freedom of a system has, \[113,114\] most probably, an average energy equal to \((1/2) k_B T\). \[115\] Therefore \[123\]

\[
K_{eff} V \sin^2 \theta_0 = \frac{1}{2} k_B T
\]

(2.376)

\[110\] In general, it is well-known that first-order methods fail to describe the magnetization dynamics [226].

\[111\] Although this naive approach is sometimes criticized because it changes the time evolution of magnetization in a nonlinear manner.

\[112\] Also known as the law of equipartition, equipartition of energy, or just equipartition. It is a general formula that relates the average energies of a system to its temperature. One of its original statements was that in thermal equilibrium, energy is shared equally among all of its various forms.

\[113\] A degree of freedom is any part of the system that is able to store energy.

\[114\] In general, for a FM there are two degrees of freedom: (1) Rotation out of the plane, and (2) rotation in the plane. However, due to the large demagnetizing fields, which tend to keep the magnetization in the plane, the out of plane component is usually small compared to the latter and thus most of the time neglected [123].

\[115\] In fact, for quadratic energies \( AX^2 \), where \( A \) is a constant and \( X \) the degree of freedom, the equipartition theorem states that in thermal equilibrium, the average energy is equal to \((1/2) k_B T\). For example, for an LC-circuit in thermal equilibrium, the energies stored in the components are most probably \((1/2) CV_N^2 = (1/2) k_B T \) and \((1/2) LI_N^2 = (1/2) k_B T \), where \( V_N \) and \( I_N \) are the RMS noise voltage and current, respectively [123].
or

\[ \sin \theta_0 = \sqrt{\frac{k_B T}{2K_{eff} V}} \]  

(2.377)

This can be written in terms of the effective anisotropy field \( H_{K_{eff}} = 2K_{eff}/\mu_0 M_s \) as

\[ \sin \theta_0 = \sqrt{\frac{k_B T}{H_{K_{eff}} \mu_0 M_s V}} \]  

(2.378)

Alternatively, we can write it in terms of the energy barrier \( E_b = K_{eff} V \)

\[ \sin \theta_0 = \sqrt{\frac{k_B T}{2E_b}} \]  

(2.379)

or in terms of the thermal stability factor \( \Delta = E_b/k_B T \)

\[ \sin \theta_0 = \sqrt{\frac{1}{2\Delta}} \]  

(2.380)
Chapter 3

Spin Circuit Theory

In this chapter, we discuss the elementary concepts of magnetoelectronics and diffusive spin transport for the general case of noncollinear spins. In addition, we introduce the four-component spin circuit formalism which naturally extends Kirchhoff’s laws, circuit variables, and circuit techniques to Pauli spin space.
3.1 Magnetoelectronics

Magnetoelectronics deals with the transport in circuits when FM elements are incorporated [71, 227, 228]. The magnetoelectronic problem is best treated with the unified semiclassical circuit theory pioneered by Brataas et al. [124, 145] which assumes diffusive transport in the bulk and applies quantum mechanical boundary conditions at the interfaces [29]. Consider the FM/NM multilayer shown in Fig. 3.1.

![Figure 3.1: Noncollinear FM/NM/FM trilayer with voltage applied across the structure.](image)

The formal procedure is to divide the FM/NM multilayer into [71, 106, 124, 145]:

1. **Nodes (Low Impedance Interconnectors):** Each node can be a FM or a NM, and is characterized by a generalized distribution function, namely a $2 \times 2$ distribution matrix in spin space $\hat{f}$.\(^1\) One can assume the nodes to be large and/or irregular in shape with a sufficient number of randomly distributed scatterers so that the distribution matrix is isotropic in $\mathbf{k}$-space and therefore depends only on energy (i.e., $\hat{f} \equiv \hat{f}(E)$) [71, 124, 145]. Otherwise, if, say, the node size is larger than the spin-diffusion length, one has to use spatially-dependent spin distribution functions [106, 124, 145]. Finally, the charge and spin conservation laws have to be applied at each node, viz. [145]

$$\sum_i \hat{I}_{ij} = \left( \frac{\partial \hat{f}_j}{\partial t} \right)_{\text{relaxation}} (3.1)$$

where $\hat{I}_{ij}$ is the current matrix from node (or reservoir) $\alpha$ to node (or reservoir) $\beta$. The term on the right-hand side describes the spin-relaxation, and can be set to zero when the current is conserved (e.g., when $t \ll \tau_{sf}$) [145].

2. **Reservoirs (Voltage Sources):** A reservoir can be a FM or a NM, and is characterized by a chemical potential $\mu$. The reservoirs are assumed to be large and in thermal equilibrium with $\mu$ so that the $2 \times 2$ distribution matrix is diagonal in spin space with each component of the matrix given by the Fermi-Dirac distribution, that is $\hat{f} \equiv \hat{\mathbf{1}} f_F(E, \mu)$ where $\hat{\mathbf{1}}$ is the unit matrix and $f_F(E, \mu)$ is the Fermi-Dirac distribution.

\(^1\)The hat $\hat{}$ denotes a $2 \times 2$ matrix in spin-space.
3. Contacts (Resistive Elements): The current-limiting elements. They connect the nodes to each other and to the reservoirs and are characterized by the microscopic scattering matrices of the Landauer-Büttiker formalism [229–232]. The contacts are assumed to have much higher resistance than the nodes, that is

\[ R_{\text{contact}} \gg R_{\text{node}} \] (3.2)

which is clearly satisfied when the contact have a much smaller cross-sectional area or when it is are in the tunneling regime [124]. The above simple theory above will fail when (3.2) does not hold [106].

As mentioned, a contact can be described in terms of the scattering matrices. In particular, in terms of the \(2 \times 2\) conductance tensor composed of [71]

\[
G_{\sigma} = \frac{e^2}{\hbar} \left[ M - \sum_{nm} |r_{\sigma}^{nm}|^2 \right] = \frac{e^2}{\hbar} \left[ \sum_{nm} |r_{\sigma}^{nm}|^2 \right]
\]

(3.3)

\[
G_{\sigma,-\sigma} = \frac{e^2}{\hbar} \left[ M - \sum_{nm} r_{\sigma}^{nm} (r_{-\sigma}^{nm})^* \right]
\]

(3.4)

where \(G_{\sigma}\) is the spin-dependent conductance and \(G_{\sigma,-\sigma}\) is the spin-mixing conductance. Here \(r_{\sigma}^{nm}\) (\(r_{-\sigma}^{nm}\)) is the reflection coefficient between the transverse modes \(n\) and \(m\) at the Fermi level of an electron with spin \(\sigma\) \((-\sigma)\) in the NM that is connected to the FM. In addition, \(M\) is the number of modes at the NM side and is given by \(M = k_f A/4\pi\), where \(k_f\) is the wave-vector in the NM. The spin-mixing conductance is only relevant for the noncollinear case and is responsible for the rotation of spins around the magnetization axis [106, 124]. That is, the transport of spins that are noncollinear to the magnetization is determined by \(G_{\sigma,-\sigma}\), and hence the spin-transfer torque is only determined by it [150]. For the collinear case, the transport of spins is only determined by \(G_{\sigma}\) [106, 124]. The spin-mixing and spin-dependent conductances can be shown to satisfy the inequality [145]

\[
\text{Re} \{G_{\sigma,-\sigma}\} \leq \frac{G_{\sigma} + G_{-\sigma}}{2}
\]

(3.5)

The conductances can be computed for diffusive, ballistic, and a tunnel contacts [145]. Some calculations of \(G_{\sigma,-\sigma}\) can be found in [150, 151].
3.2 Carrier Transport

Below we show the carrier transport model in diffusive samples, i.e. those for which \( L > \lambda \), where \( \lambda \) is the mean-free path between scattering events.\(^2\) In particular, we employ the drift-diffusion model derived from the transparent and coherent thermodynamic approach as presented in [84], and also make use of the derivations in [43, 79, 109] regarding charge and spin transport along with the classical works of Valet-Fert [104] and Johnson-Silsbee [113]. In our formalism, we assume high enough temperatures to dispel the question of diffusion, and also ignore spin-orbit (SO) coupling\(^3\). We assume all transport is governed by differences in electric fields (drift) or density gradients (diffusion). Moreover, we assume particles cannot be created or destroyed\(^4\); a fact summarized in the normalization condition [79]

\[
N_0 = \iiint_{\mathbb{R}^3} n(t, \mathbf{r}) \, dV
\]

(3.6)

where \( N_0 \) is the total number of particles, which is fixed. However, we will allow for slow spin relaxation processes to establish correct equilibrium polarization [109].

Let \( X \) be a balanceable\(^5\) quantity that is associated with a local density \( x \) and a local current density \( \mathbf{J}_{x} \). Every such quantity has to obey a continuity equation [84]

\[
\frac{\partial x(t, \mathbf{r})}{\partial t} + \nabla \cdot \mathbf{J}_{x}(t, \mathbf{r}) = \Sigma_{x}(t, \mathbf{r})
\]

(3.7)

where \( \Sigma_{x} \) is the \( X \)-generation rate per volume. For conserved quantities, \( \Sigma_{x} = 0 \). For charged particles (in the absence of external magnetic fields), we do not use the local chemical potential \( \mu \),\(^6\)\(^7\) but rather the local electrochemical potential \( \bar{\mu} = \mu + qV_C \) to quantify energy changes required for adding or removing charged particles. Thus \( V_C \) gives the electrostatic contribution to the energy term for the local increase in charge

\(^2\)In other words, those for which the Knudsen number satisfies

\[ K_n = \frac{\lambda}{L} < 1 \]

\(^3\)Otherwise, full quantum transport formalisms like the nonequilibrium Green’s function (NEGF) [233] or scattering theory [71] has to be applied.

\(^4\)Unless in semiconductors where electrons can recombine with holes.

\(^5\)Not necessarily conserved (e.g., spin).

\(^6\)The key point behind the assumption of “local equilibrium” is that carriers are in equilibrium with the other carriers in the same local region. This assumption generally holds as long as the subvolume considered is greater than \( \lambda^3 \) [84].

\(^7\)Measured relative to \( E_c \) (bottom of conduction band) for electrons, or relative to \( E_v \) (top of valence band) for holes.
density from $n_0(\mu)$ \textsuperscript{8}. Thus, for the transport of electric charges we choose $\bar{\mu}$ as an independent variable and this parameter should enter all the thermodynamic relations (instead of $\mu$). In the linear low-field regime, one has the current density\textsuperscript{9}

\[ \mathbf{J}_x = -D \nabla x (t, \mathbf{r}) + \frac{\sigma}{q} \mathbf{E}(t, \mathbf{r}) \]  

(3.9)

where $\mathbf{E} = -\nabla V_C$, $D$ is the diffusivity (or diffusion coefficient), and is the $\sigma$ the conductivity. The first term represents diffusion, whereas the second term represents drift.

**Charge Transport:** Letting $X = N$, we obtain the continuity equation

\[ \frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J}_n = 0 \]  

(3.10)

where we have set $\Sigma_n = 0$. The particle current density is given by

\[ \mathbf{J}_n = -D \nabla n - \frac{\sigma}{e} \mathbf{E} \]  

(3.11)

where $\sigma = e\bar{\mu}n$, $\bar{\mu}$ being the mobility. The charge current density can be found from $\mathbf{J}_C = -e\mathbf{J}_n$ as

\[ \mathbf{J}_C = e D \nabla n + \sigma \mathbf{E} \]  

(3.12)

\[ = e D \frac{\partial n_0}{\partial \mu} \nabla \mu - \sigma \nabla V_C \]  

(3.13)

where we have used the fact that we are in near-equilibrium (i.e., $|eV_C| \leq k_B T$) so that we can write $\nabla n (\mathbf{r}) = \frac{\partial n_0}{\partial \mu} \nabla \mu = \frac{\partial n_0}{\partial \mu} \nabla (\bar{\mu} + eV_C)$ \textsuperscript{[79, 109]}. Under global equilibrium, $\bar{\mu}$ is constant and the current vanishes \textsuperscript{[79, 84, 109]}. Thus

\[ 0 = e D \frac{\partial n_0}{\partial \mu} (0 + e\nabla V_C) - \sigma \nabla V_C \]  

(3.14)

or

\[ \sigma = e^2 D \frac{\partial n_0}{\partial \mu} \]  

(3.15)

which is the general form of *Einstein’s Relation*. The factor $\partial n_0/\partial \mu$ is called the charge compressibility (also known as the thermodynamic DOS) and is usually denoted by $\chi_c$

\textsuperscript{8}Recall that at equilibrium $n_0 = \int_{-\infty}^{\mu} g(E) f_F(\mu - E) dE$ (if the minimum energy of the band energy is $E = 0$), where $g(E)$ is the DOS and $f_F(\mu - E)$ the Fermi-Dirac distribution given by

\[ f_F(\mu - E) = \frac{1}{1 + e^{\frac{E - \mu}{k_B T}}} \]  

(3.8)

\textsuperscript{9}This can be derived from the classical Boltzmann equation in the limit where the density and external potentials are slowly varying on the scale of $\lambda$ \textsuperscript{[79, 84, 104, 109]}. 
Using Einstein’s relation [61, 78, 84, 109]

\[ \mathbf{J}_C = \frac{e}{\hbar} \nabla \bar{\mu} \]  

(3.16)

where we clearly see that current flow is driven by a gradient in the electrochemical potential [61].\(^{12}\) Note that authors sometimes call the electrochemical potential \(\bar{\mu}\) the quasi-chemical potential. In fact, in the same way as one calls the “equilibrium” chemical potential the Fermi level, one can also call the quasi-chemical potential (the electrochemical potential) the quasi-Fermi level. Moreover, we note that both (3.16) and (3.12) are equivalent in the linear regime and can be used to find the current density. The two are related by Einstein’s relation (3.15).

**Spin Transport:** Labeling electrons with up- and down-spin with the spin index \(\sigma = \uparrow, \downarrow\), we write the total electron density as

\[ n = n_{\uparrow} + n_{\downarrow} = (n_{0,\uparrow} + \delta n_{\uparrow}) + (n_{0,\downarrow} + \delta n_{\downarrow}) = (n_{0,\uparrow} + n_{0,\downarrow}) + (\delta n_{\uparrow} + \delta n_{\downarrow}) = n_0 + \delta n \]  

(3.17)

where \(\delta n_{\uparrow} = n_{\uparrow} - n_{0,\uparrow}\) and \(\delta n_{\downarrow} = n_{\downarrow} - n_{0,\downarrow}\) are the deviations of the up- and down-densities from their equilibrium values, respectively. The continuity equations can then be simply extended as [65, 109]

\[ \frac{\partial n_{\uparrow}}{\partial t} - \frac{1}{e} \nabla \cdot \mathbf{J}_{\uparrow} = -\left( \frac{\delta n_{\uparrow}}{\tau_{\uparrow\downarrow}} - \frac{\delta n_{\downarrow}}{\tau_{\downarrow\uparrow}} \right) \]  

(3.18)

\[ \frac{\partial n_{\downarrow}}{\partial t} - \frac{1}{e} \nabla \cdot \mathbf{J}_{\downarrow} = -\left( \frac{\delta n_{\downarrow}}{\tau_{\downarrow\uparrow}} - \frac{\delta n_{\uparrow}}{\tau_{\uparrow\downarrow}} \right) \]  

(3.19)

where \(1/\tau_{\uparrow\downarrow}\) is the rate at which a spin \(\uparrow\) is flipped to \(\downarrow\), and \(1/\tau_{\downarrow\uparrow}\) the rate at which spin \(\downarrow\) is flipped to \(\uparrow\).\(^{13}\) The terms on the right-hand side represent the generation rates \(\Sigma_{n_{\uparrow}}\) and \(\Sigma_{n_{\downarrow}}\) which are now nonzero due to the non-conserving spin scattering events (e.g., electron-magnon collisions, or spin-orbit interactions on defects and impurities.

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\(^{10}\)This quantity is related to the microscopic length scale in a Mott insulator known as the screening length, given by \(\delta = \left( \frac{e^2}{\hbar^2 c^2} \right)^{-1/2}\). This is the length over which any charge imbalance is effectively screened out [109]. The spreading of the local charge accumulation roughly occurs during the very short time scale known as the dielectric relaxation time given by \(\tau_d = \varepsilon/\sigma\) [60]. This is the reason diffusion is usually neglected in metals. In contrast to metals, in doped semiconductors the electron-hole packets are charge-neutral and can therefore be long-lived and result in density inhomogeneity, making diffusion important.

\(^{11}\)For degenerate Fermi gas (\(\mu \approx E_F\)), \(g(E_F) \approx \frac{3}{2} \pi^2 \frac{n}{m} \propto n^{1/3}\) where \(E_F = \frac{h^2 (3e^2 n)^{2/3}}{2m}\), yielding \(\chi_c = g(E_F)\). This can also be obtained from fact that the Fermi-Dirac distribution for a degenerate Fermi gas resembles a step function \(\frac{\partial g}{\partial \mu} \approx \delta (E - \mu)\) so that \(\frac{\partial n}{\partial \mu} = g(E_F)\). For a nondegenerate Fermi gas (\(E - \mu \gg k_B T\)), one has \(\chi_c = \frac{1}{\sqrt{2\pi}}\) [79, 84].

\(^{12}\)Note that in general \(\sigma \equiv \sigma (\mu)\). Thus for low carrier density materials (e.g., semiconductors) where large deviations of the local charge density can occur, it is better to separate \(\sigma\) into the carrier density and mobility, as the latter depends less on \(\mu\) and thus can be better analyzed [109].

\(^{13}\)For degenerate Fermi gas (\(\mu \approx E_F\)), \(\tau_{\uparrow\downarrow} g_{\uparrow} (E_F) = \tau_{\downarrow\uparrow} g_{\downarrow} (E_F)\). For a nondegenerate Fermi gas (\(E - \mu \gg k_B T\)), one has \(\tau_{\uparrow\downarrow} n_{\downarrow} = \tau_{\downarrow\uparrow} n_{\uparrow}\) [65].
Adding the above two equation yields the charge continuity equation (3.10). On the other, we can define the spin density as the difference

\[ s = n^\uparrow - n^\downarrow = (n_{0,\uparrow} + \delta n^\uparrow) - (n_{0,\downarrow} + \delta n^\downarrow) = (n_{0,\uparrow} - n_{0,\downarrow}) + (\delta n^\uparrow - \delta n^\downarrow) = s_0 + \delta s \]  

(3.20)

where \( \delta s = n^\uparrow - n^\downarrow = \delta n^\uparrow - \delta n^\downarrow \) is the spin accumulation. Now subtracting the equations yields the continuity equation for the spin current density

\[ \frac{\partial}{\partial t} s - \frac{1}{e} \nabla \cdot J_S = -2 \left( \frac{\delta n^\uparrow}{\tau_{\uparrow}} - \frac{\delta n^\downarrow}{\tau_{\downarrow}} \right) \]  

(3.21)

For times \( t > \tau_d \), the system can be considered locally charge neutral, namely \( n = n_0 \) so that \( \delta n = \delta n^\uparrow + \delta n^\downarrow = 0 \) (giving for a system that is charge-neutral at equilibrium \( \rho = -e\delta n \) a divergenceless electric field \( \nabla \cdot \mathbf{E} = \rho/\varepsilon = 0 \) [109]. The last fact implies the only the spin accumulation matters. In fact, now we have \( \delta n^\uparrow = -\delta n^\downarrow = \frac{\delta s}{\tau_{sf}} \). Thus

\[ \frac{\partial}{\partial t} s - \frac{1}{e} \nabla \cdot J_S = -\frac{\delta s}{\tau_{sf}} \]  

(3.22)

where \( \tau_{sf} = (1/\tau_{\uparrow} + 1/\tau_{\downarrow})^{-1} \) is the average spin-flip (or spin-relaxation) time [71].

In a FM conductor, the different DOSs at the Fermi level along with the different Fermi velocities of majority and minority spins result in spin-dependent properties. Thus, now we may define the spin-resolved properties, for example, as [79, 109]

\[ g = g^\uparrow + g^\downarrow \quad g_s = g^\uparrow - g^\downarrow \]  

(3.23)

\[ \sigma = \sigma^\uparrow + \sigma^\downarrow \quad \sigma_s = \sigma^\uparrow - \sigma^\downarrow \]  

(3.24)

\[ D = \frac{1}{2} (D^\uparrow + D^\downarrow) \quad D_s = \frac{1}{2} (D^\uparrow - D^\downarrow) \]  

(3.25)

In addition, by allowing for spin-dependent quasi-chemical potentials, we may write

\[ \bar{\mu}^\uparrow = \mu^\uparrow - eV_C, \quad \mu^\uparrow = \mu + \mu_s \]  

(3.26)

\[ \bar{\mu}^\downarrow = \mu^\downarrow - eV_C, \quad \mu^\downarrow = \mu - \mu_s \]  

(3.27)

we can write the charge and spin quasi-chemical potentials as

\[ \bar{\mu} = \frac{1}{2} (\bar{\mu}^\uparrow + \bar{\mu}^\downarrow) \quad \bar{\mu}_s = \frac{1}{2} (\bar{\mu}^\uparrow - \bar{\mu}^\downarrow) \]  

(3.28)

---

14 Although this name sometimes refers to the half-difference in the quasi-chemical potentials [79]. Recall the discussion in 2.1.4.
Similarly, Einstein’s relation would be
\[ J_{\uparrow} = eD_{\uparrow} \nabla n_{\uparrow} + \sigma_{\uparrow} E \]
\[ J_{\downarrow} = eD_{\downarrow} \nabla n_{\downarrow} + \sigma_{\downarrow} E \]
(3.29)
(3.30)
where we have used \( \nabla n_{\uparrow} = \frac{\partial n_{0,\uparrow}}{\partial \mu_{\uparrow}} \nabla \mu_{\uparrow} \) and \( \nabla n_{\downarrow} = \frac{\partial n_{0,\downarrow}}{\partial \mu_{\downarrow}} \nabla \mu_{\downarrow} \).
Similarly, Einstein’s relation can be generalized in a non-homogeneous equilibrium state (where the spin currents vanish and electrochemical potentials are constant [84]), yielding\(^{16,17}\) [109]
\[ \sigma_{\uparrow} = e^2 D_{\uparrow} \frac{\partial n_{0,\uparrow}}{\partial \mu_{\uparrow}} \]
\[ \sigma_{\downarrow} = e^2 D_{\downarrow} \frac{\partial n_{0,\downarrow}}{\partial \mu_{\downarrow}} \]
(3.34)
(3.35)
These relations allow us to write the spin current densities more compactly as [104]
\[ J_{\uparrow} = \frac{\sigma_{\uparrow}}{e} \nabla \mu_{\uparrow} \]
\[ J_{\downarrow} = \frac{\sigma_{\downarrow}}{e} \nabla \mu_{\downarrow} \]
(3.36)
(3.37)
which is just an extension of the charge transport result by allowing for different quasi-chemical potentials. Using the last two equations along with the definitions stated at the beginning, and after some algebra, we can write the current densities as [79]
\[ J_{C} = J_{\uparrow} + J_{\downarrow} = \frac{\sigma_{\uparrow}}{e} \nabla \mu_{\uparrow} + \frac{\sigma_{\downarrow}}{e} \nabla \mu_{\downarrow} \]
\[ J_{S} = J_{\uparrow} - J_{\downarrow} = \frac{\sigma_{\uparrow}}{e} \nabla \mu_{\uparrow} + \frac{\sigma_{\downarrow}}{e} \nabla \mu_{\downarrow} \]
(3.38)
(3.39)
\(^{15}\)For degenerate Fermi gas (\( \mu \approx E_F \)), \( \nabla n_{\uparrow} = g_{\uparrow}(E_F) \nabla \mu_{\uparrow} \) and \( \nabla n_{\downarrow} = g_{\downarrow}(E_F) \nabla \mu_{\downarrow} \). For a nondegenerate Fermi gas (\( E - \mu \gg k_B T \)), one has \( \nabla n_{\uparrow} = \frac{\sigma_{\uparrow} T}{\partial \mu_{\uparrow}} \nabla \mu_{\uparrow} \) and \( \nabla n_{\downarrow} = \frac{\sigma_{\downarrow} T}{\partial \mu_{\downarrow}} \nabla \mu_{\downarrow} \) [65].
\(^{16}\)If one includes electron-electron interactions between different spin populations (i.e. spin Coulomb drag [234]), then \( \sigma, D \) and other spin-dependent parameters like the susceptibility \( \chi \) all extend to \( 2 \times 2 \) tensors in spin space. For example [109]
\[ e, ecJ_{\uparrow} = e(D_{\uparrow\uparrow} \nabla n_{\uparrow} + D_{\uparrow\downarrow} \nabla n_{\downarrow}) + (\sigma_{\uparrow\uparrow} + \sigma_{\uparrow\downarrow}) E \]
\[ J_{\downarrow} = e(D_{\downarrow\uparrow} \nabla n_{\uparrow} + D_{\downarrow\downarrow} \nabla n_{\downarrow}) + (\sigma_{\downarrow\uparrow} + \sigma_{\downarrow\downarrow}) E \]
(3.31)
(3.32)
and Einstein’s relation would be
\[ \begin{pmatrix} \sigma_{\uparrow\uparrow} & \sigma_{\uparrow\downarrow} \\ \sigma_{\downarrow\uparrow} & \sigma_{\downarrow\downarrow} \end{pmatrix} = e^2 \begin{pmatrix} D_{\uparrow\uparrow} & D_{\uparrow\downarrow} \\ D_{\downarrow\uparrow} & D_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} \frac{\partial n_{0,\uparrow}}{\partial \mu_{\uparrow}} \\ \frac{\partial n_{0,\downarrow}}{\partial \mu_{\downarrow}} \end{pmatrix} \]
(3.33)
Thus the Coulomb interaction is responsible for the appearance of the off-diagonal elements.
\(^{17}\)In a simple two-band model \( D_{\uparrow} = \frac{1}{2} v_{F,\uparrow} \lambda_{\uparrow} = \frac{1}{2} v_{F,\uparrow}^2 \tau_{\uparrow} \) and \( D_{\downarrow} = \frac{1}{2} v_{F,\downarrow} \lambda_{\downarrow} = \frac{1}{2} v_{F,\downarrow}^2 \tau_{\downarrow} \), where \( d = 1, 2, 3 \) is the spatial dimension [71].
which in fact reveals that a spin current can be generated even in a NM ($\sigma_s = 0$) as long as there is an accumulation of spins.

The above formulation is for spins along a single axis (i.e., collinear spins). For the general case in a systems consisting of noncollinear spins, one can write the transport equation for each spin component, viz.

$$\frac{\partial s_k}{\partial t} - \frac{1}{e} \nabla \cdot \mathbf{J}_{S,k} = -\frac{\delta s_k}{\tau_{sf}}$$  (3.40)

where $k$ is used to denote the spin-polarization along the $k$-th axis. The current density along each spin-polarization direction is given by

$$\mathbf{J}_{S,k} = eD\nabla \delta s_k + e\bar{\mu}_k \mathbf{E}$$  (3.41)

The equations can be combined (while still assuming local charge neutrality) to obtain the spin drift-diffusion equation (SDDE)

$$\frac{\partial \mathbf{s}}{\partial t} - D\nabla^2 \mathbf{s} - \bar{\mu} (\mathbf{E} \cdot \nabla) \mathbf{s} = -\frac{\delta \mathbf{s}}{\tau_{sf}}$$  (3.42)

3.3 Four-Component Circuit Formalism

3.3.1 Total Voltage and Current

Following [47] and the similar implementation in [45, 48, 52, 60], we generalize the current and voltage circuit variables as follows

$$\mathbf{I} = \begin{bmatrix} I_C \\ I_{S,x} \\ I_{S,y} \\ I_{S,z} \end{bmatrix} = \begin{bmatrix} I_C \\ I_{S,x} \\ I_{S,y} \\ I_{S,z} \end{bmatrix}$$  (3.43)

$$\mathbf{V} = \begin{bmatrix} V_C \\ V_{S,x} \\ V_{S,y} \\ V_{S,z} \end{bmatrix} = \begin{bmatrix} V_C \\ V_{S,x} \\ V_{S,y} \\ V_{S,z} \end{bmatrix}$$  (3.44)
where $I_C$ is the charge current, $I_S$ the vector spin current, $V_C$ the charge voltage, $V_S$ the vector spin voltage\(^{18}\).

### 3.3.2 Generalized Ohm’s Law

Assuming a linear relationship between the total voltage and current,\(^{19}\) the two can be related by a conductance tensor \([45, 47, 48, 52, 60]\)

$$
\begin{bmatrix}
I_C \\
I_{S,x} \\
I_{S,y} \\
I_{S,z}
\end{bmatrix}
= 
\begin{bmatrix}
G^{11} & G^{12} & G^{13} & G^{14} \\
G^{21} & G^{22} & G^{23} & G^{24} \\
G^{31} & G^{32} & G^{33} & G^{34} \\
G^{41} & G^{42} & G^{43} & G^{44}
\end{bmatrix}
\begin{bmatrix}
V_C \\
V_{S,x} \\
V_{S,y} \\
V_{S,z}
\end{bmatrix}
$$

(3.45)

Thus Ohm’s law naturally generalizes to

$$
\mathbf{I} = \mathbf{G} \mathbf{V}
$$

(3.46)

where $\mathbf{G} = \mathbf{R}^{-1}$, the inverse of the resistance matrix.

### 3.3.3 Generalized Kirchoff’s Circuit Laws

In spin circuits, Kirchoff’s conservation laws should take spin dissipation (due to spin-flipping events) into account \([47, 48, 52, 124, 145]\).

**Kirchoff’s Current Law (KCL):** At any node (junction) in a spin circuit, the sum of the vector currents flowing into the node is equal to total dissipated vector spin current at that node. That is

$$
\sum_{k=1}^{n} \mathbf{I}_k = \mathbf{I}_{dissipated}
$$

(3.47)

where $\mathbf{I}_k$ is the vector current flowing from branch $k$ into the node, $n$ the total number of branches, and $\mathbf{I}_{dissipated}$ the dissipated vector spin current in that node.\(^{20}\)

\(^{18}\) This relation is for 1D flow. Recall that the spin current is a tensor of the form

$$
\mathbf{J}_S = 
\begin{bmatrix}
J_{Sx}^x & J_{Sy}^x & J_{Sz}^x \\
J_{Sx}^y & J_{Sy}^y & J_{Sz}^y \\
J_{Sx}^z & J_{Sy}^z & J_{Sz}^z
\end{bmatrix}
$$

so the spin circuit variables we will define could correspond to any of the rows of this matrix (which correspond to different directions of flow and not spin quantization).

\(^{19}\) The assumption of a linear relationship between voltage and current is valid at least in metals where electron density is high and $\mathbf{E}$ varies slower than the scattering time; for a better accuracy, one can take the branches/nodes on which computation is performed to be sufficiently small \([48, 79]\).

\(^{20}\) This is essentially an equation of the form (3.1). The dissipated spin current is handled by sinking it to a “virtual” ground terminal \([45, 52]\).
**Kirchoff’s Voltage Law (KVL):** The sum of the vector voltage differences around any closed circuit is zero. That is

\[ \sum_{k=1}^{n} V_k = 0 \quad (3.48) \]

where \( V_k \) is the \( k \)-th voltage difference and \( n \) the total number of voltages.

### 3.3.4 Generalized Modified Nodal Analysis

In circuit theory, the nodal analysis is a widely used method to obtain the unknown voltages using KCL. Though simple, the method has some shortcomings, in particular for algorithm implementation and when handling voltage sources, current-dependent elements, and the direct evaluation of branch currents. The modified nodal analysis (MNA) [235] is an extension of the nodal analysis, which, in contrast to the latter, also determines some branch currents. Although it results in a larger system to be solved, it is more systematic and better suited for computer implementation. Below we briefly state the rules of MNA and definitions of the matrices/vectors involved and then naturally extend MNA to spin space as made in [48].

Given a linear circuit with \( n \) nodes (excluding ground) and \( m \) voltage sources, the MNA algorithm proceeds as follows:

1. Select a reference node (usually ground).
2. Label the variables: (i) The nodal voltages \( V_1, V_2, \ldots, V_n \), and (ii) the currents through the voltage sources as \( I_{\text{source},1}, I_{\text{source},2}, \ldots, I_{\text{source},m} \).
3. Write KCL at every node.
4. Write an equation for the voltage of each voltage source.
5. Solve for the \( n + m \) unknowns.

In general, the algorithm above will result in the linear system

\[ A \mathbf{x} = \mathbf{b} \quad (3.49) \]

where \( A \in \mathbb{R}^{(n+m)\times(n+m)} \), \( \mathbf{x} \in \mathbb{R}^{(n+m)\times1} \), and \( \mathbf{b} \in \mathbb{R}^{(n+m)\times1} \). The definitions and entries of the matrix and vectors are as follows:

- **\( A \):** Related to the connection of the passive elements. It can generally be written in terms of some block matrices as

\[
A = \begin{bmatrix}
G & B \\
C & D
\end{bmatrix} \quad (3.50)
\]
where

- \( G \in \mathbb{R}^{n \times n} \): Related to the interconnection between the passive elements where the entries can be found as follows
  \[
  G^{ij} = \begin{cases} 
  \text{negative the conductance between nodes } i \text{ and } j, & i \neq j \\
  \text{sum of the conductances connected to node } i \text{ (j),} & i = j 
  \end{cases} \quad (3.51)
  \]
  The definition clearly implies that \( G = G^T \).

- \( B \in \mathbb{R}^{n \times m} \): Related to the connection between the passive elements and the voltage sources where the entries can be found as follows
  \[
  B^{ij} = \begin{cases} 
  1, & \text{if node } i \text{ is connected to the positive terminal of the } j\text{-th voltage source} \\
  -1, & \text{if node } i \text{ is connected to the negative terminal of the } j\text{-th voltage source} \\
  0, & \text{if node } i \text{ is not connected to the } j\text{-th voltage source}
  \end{cases} \quad (3.52)
  \]

- \( C \in \mathbb{R}^{m \times n} \): In the special case in which the circuit has only independent voltage sources, the matrix is related to \( B \) by \( C = B^T \).\(^{21}\)

- \( D \in \mathbb{R}^{m \times m} \): In the special case in which the circuit has only independent voltage sources, the matrix is the zero matrix, i.e. \( D = O \).

- **\( \mathbf{b} \):** Composed of the known node voltages and branch currents and it has the form
  \[
  \mathbf{b} = \begin{bmatrix} \mathbf{i} \\
  \mathbf{e} \end{bmatrix} \quad (3.53)
  \]
  where

- \( \mathbf{i} \in \mathbb{R}^{n \times 1} \): Related to the independent current sources where the entries can be found as follows
  \[
  i_k = \begin{cases} 
  0, & \text{if no current into node } k \\
  I_{\text{independent},k}, & \text{if the independent current } I_{\text{independent},k} \text{ is going into node } k
  \end{cases} \quad (3.54)
  \]

- \( \mathbf{e} \in \mathbb{R}^{m \times 1} \): Related to the independent voltage sources where the entries can be found as follows
  \[
  e_k = V_{\text{independent},k} \quad (3.55)
  \]

\(^{21}\)We will only consider this case here. For the more general case the reader is referred to [236].
• **x**: Composed of the unknown quantities; i.e. node voltages & currents through the voltage sources. It can be easily be found as

\[ x = A^{-1}b \]  

(3.56)

which has the form

\[ x = \begin{bmatrix} v \\ j \end{bmatrix} \]  

(3.57)

where

- \( v \in \mathbb{R}^{n \times 1} \): Unknowns node voltages.
- \( j \in \mathbb{R}^{m \times 1} \): Unknown currents through the voltage sources.

In general, the MNA will result in a matrix with unsymmetric sparse coefficient matrices with identical nonzero pattern, and thus matrix inversion will be computationally inefficient. In fact, for \( O(n^2) \) entries the system is highly sparse with \( O(n) \) nonzero entries. This, in fact, means that approximately 99% of the entries in \( A \) are zeros [237]. Thus, for medium matrices, one can use the sparse LU factorization whereas for large matrices one can resort to iterative scheme (e.g., conjugate gradient).

For a spintronic circuit, the rules of MNA hold, but everything has to be extended to spin space, i.e. by replacing \( n \leftarrow 4n \) and \( m \leftarrow 4m \) [48]. This implies that all the matrix entries now extend to \( 4 \times 4 \) block matrices. Table 3.1 below summarizes the dimensions of the matrices and vectors in the classical and generalized MNA.

**Table 3.1**: Dimensions of variables in the MNA. Table adapted by the author from [48].
Chapter 4

Circuit Modeling of ASL

In this chapter, we introduce all-spin logic (ASL), discuss its basic operation principles, describe the general modeling procedure, and simulate a basic ASL switch. The modeling and simulations will be based on our finite-difference model using the algorithm we developed.
4.1 Motivation

Spintronic devices [8, 9] are prime candidates for Beyond CMOS technologies to sustain the advancements of Moore’s law [1] due to their potential for low power consumption and high-density computation and storage. The success of planar CMOS has naturally triggered extensive research on spintronic structures that resembles the FET. Namely, lateral structures made up of conducting channels and at least two terminals that act as the source and drain of carriers. Fig. 4.1 shows two examples of such devices. Fig. 4.1a shows a lateral local spin valve (LLSV) that switches due to the locally injected spin currents, whereas Fig. 4.1b shows a lateral nonlocal spin valve (LNLSV) that switches due to the nonlocally injected spin currents\(^1\) [36–42]. Although both devices work on the principles of STT switching, the nonlocal device is rather preferred. This is because the LNLSV decouples charge from spin, generating pure spin currents. This is advantageous because it eliminates the spurious effects accompanying spin-polarized (and pure charge) currents [37, 43].

![Fig. 4.1: Schematics showing the difference between local and nonlocal STT in a lateral spin valve (LSV). (a) In local STT, the information is read from the input FM by translating \(V_{source}\) to \(I_S\), whereas information is written to the output FM through local STT due to the interaction with the spin-polarized current \(I_S\). (b) In nonlocal STT, information is read from the input FM by translating \(V_{source}\) to \(I_S\), whereas information is written to the output FM through nonlocal STT due to the interaction with the pure spin current \(I_S\).]

Although the device in Fig. 4.1b is certainly an attractive candidate for logic switching, there are some limitations that prevents using it in an integrated circuit. One issue is that one cannot prevent crosstalking between concatenated stages of these devices. That is, there are no isolations between the different stages to prevent diffusion of injected/back-injected currents. Fortunately, this problem can be easily solved by inserting a spacer beneath every FM such that each has isolated input and output sides (Fig. 4.2). The beauty of this solution is that both of the exposed sides of the FM are identical, and thus every FM can act as an injector/detector. The latter is one requirement for a proper logic operation.

\(^1\)Performing nonlocal STT [238–242].
Figure 4.2: Every FM can act as an injector and as a detector. The left side is the write, detect or receive side that acts as the input of the FM where information sent from the previous stage is received. This side is also referred to as the sense side since it senses the pure spin currents diffusion from the previous stage. The right side is the read, inject or transmit side that acts as the output of the FM where information to the next stage is sent. This side is also referred to as the polarize side since it polarizes the DC current injected from the energy source $V_{sourcem}$. Figure adapted by the author from [52, 55, 56]

4.2 All-Spin Logic (ASL)

Among the most promising spintronic logic switches is a device called all-spin logic (ASL) [44–46] that is based on a LNLSV structure and STT switching (Fig. 4.3). The device has recently attracted increasing interest due to its low power operation and logic-in-memory structure. In addition, the device utilizes pure spin currents throughout every stage of its operation, eliminating the need for repeated spin-to-charge conversion and thus any extra hardware [44, 46]. This is in contrast to most spintronic logic switches which uses spins internally but have logic gates with charge-based terminals [44]. Moreover, as discussed in the previous section, using pure spin currents eliminates the spurious effects accompanying charge currents, which is certainly advantageous.

Figure 4.3: A generic ASL device with its constituent elements labeled.

$^2$Less voltage operation also means less parasitic capacitance and stray charge [47]. Moreover, non-volatility ideally implies zero stand-by power.

$^3$Other examples of devices that do not require spin-to-charge conversion: Magnetic quantum cellular automata (MQCA) [243–245] and domain wall (DW) logic [246]. However, these devices use the Oersted fields generated by the passing DC currents to switch the FMs, i.e. preforming nanomagnetic logic (NML). ASL, on the other hand, utilizes spin currents directly to switch using nonlocal STT, and is thus not limited to nearest-neighbor communication like MQCA (i.e., not limited to cellular architectures) [46].
4.2.1 Device Operation

ASL utilizes two bistable FMs whereby binary information is stored (e.g., “0” = left, “1” = right) that communicate with pure spin currents through a spin-coherent NM channel. The main principle behind the operation of the device is the accumulation of spins beneath the input FM upon the passage of a charge current. This occurs due to the spin filtering process at the FM/NM interface which creates a difference in population of spin density across the NM channel, driving diffusion of up- and down-spins in both directions\(^4\). If sufficient amount of noncollinear spins reaches the output FM, enough torque can then be exerted on the nanomagnet, switching it into another stable state.

With reference to Figs. 4.5 and 4.6, we can summarize the operation of ASL shown in Fig. 4.4 as follows\(^5\) [52, 55]:

- **Positive voltage (NOT operation):** Extracts majority spins, and injects minority spins. Thus a positive \(V_{\text{source}}\) makes the input FM a sink of majority spins.
- **Negative voltage (COPY operation):** Extracts minority spins, and injects majority spins. Thus a negative \(V_{\text{source}}\) makes the input FM a source of majority spins.

![Figure 4.4: ASL inverter in operation. (a) P → AP (NOT). (b) AP → P (COPY).](image)

We note that while the operation of ASL is reciprocal in that reversing the direction of the current will cause a spin current of the opposite polarization to reach the output FM, the currents are not necessarily equal in magnitude, i.e the current required for switching P → AP and AP → P are not necessarily equal and neither are the switching times. This will be shown later in the simulations.

\(^4\)For them to bring the electrochemical potential into equilibrium. Recall the discussion in 2.1.4.

\(^5\)Here, recall that we refer to the spins that are parallel to the magnetization as *majority* spins, whereas those antiparallel are referred to as *minority* spins.
Figure 4.5: P $\rightarrow$ AP (NOT). (a) A charge current is injected from the FM to the NM. (b) Electrons are injected from the NM to the FM. Majority spins are most likely to transmit, whereas minority spins are most likely to reflect and accumulate beneath the FM. (c) The result is that the passage of a charge current from the FM to the NM accumulates minority spins beneath the FM. (d) The difference in population of spin density across the channel drives diffusion of opposite spins in both directions to bring the electrochemical potential into equilibrium. Minority spins will diffuse to the right and majority spins will diffuse to the left. (e) Majority spins diffusing to the left are equivalent to minority spins diffusing to the right. Thus, the result is that a total spin current of minority spins will diffuse to the right, switching the output FM antiparallel through STT.
Figure 4.6: AP → P (COPY). (a) A charge current is injected from the NM to the FM. (b) Electrons are injected from the FM to the NM. Majority spins are most likely to transmit, whereas minority spins are most likely to reflect and accumulate above the FM. (c) The result is that the passage of a charge current from the NM to the FM transmits majority spins to the NM. (d) The difference in population of spin density across the channel drives diffusion of opposite spins in both directions to bring the electrochemical potential into equilibrium. Majority spins will diffuse to the right and minority spins will diffuse to the left. (e) Minority spins diffusing to the left are equivalent to majority spins diffusing to the right. Thus, the result is that a total spin current of majority spins will diffuse to the right, switching the output FM parallel through STT.
4.2.2 Basic Elements of ASL

• FMs (Input/Output)
  □ Role: Used to store the information represented in the magnetizations (e.g., “0” = left, “1” = right) in a nonvolatile manner. For a single ASL device (Fig. 4.3), the left FM is the injector, whereas the right FM is the detector.
  □ Material: Usually transition metal FMs like Fe, Co, Ni, and their alloys such as Py (Ni$_{80}$Fe$_{20}$), CoFeB, CoPd, CoNi, CoPtCr, Co$_3$Pt, FePd, FePt, CoPt, Fe$_{14}$Nd$_2$B, or even MnAl$^6$.

• NM Channel (Interconnect)
  □ Role: Connects the input FM to both the output FM and to the ground, effectively creating two paths to route two types of currents in the device:
    1. The pure spin current diffusing from the injecting FM to the detecting FM;
    2. The spin-polarized current flowing from the injecting FM to the ground terminal.
  □ Material: Could be either a metal or a semiconductor. For the former, noble metals such as Cu, Ag, and Au are usually used. For the latter, degenerately doped Si and GaAs channels are possible or even the novel zero band gap semiconductor, Graphene. In general, the advantage of using semiconducting channel is the longer spin-diffusion length obtained. However, when using a semiconductor, one has to overcome the conductance mismatch problem across a FM/NM interface for the case of metallic FM and use the solution proposed by Rashba (and later by Fert and Jaffres) which suggests using a spin-dependent interface resistance; a tunnel barrier in particular.

$^6$For more possible FMs, see footnote 23.

$^7$Note that moderately doped semiconductors usually have long spin-diffusion lengths. However, highly doping a semiconductor could decrease the spin-diffusion length whereas lightly doping it have no major effect.

$^8$For an all-semiconductor structure, this is not a problem and spin injection will be efficient.

$^9$Schmidt et al. [259] provided an explanation for the conductance mismatch across a FM(metal)/NM(semiconductor) interface: For diffusive electrons, the spin polarization of the injected carriers is $\beta \left( \rho_F^{FM}/\rho_N^{NM} \right) (t_F^{FM}/t_N^{NM})$, where $\beta$ is the spin polarization of the FM. The problem in injection is the low ratio of $\rho_F^{FM}/\rho_N^{NM}$ which reduces the spin polarization in the NM drastically.

$^{10}$The enhancement of spin injection from FM(metal)/NM(semiconductor) with tunnel barriers have only been recently (experimentally) demonstrated in normal semiconductors [253, 260–262], few years after it has been demonstrated in all-metallic structures [249].
• Spacers (Isolation Layers)

  □ **Role:** Used to ensure that the communication between the two FMs is limited to the channel and no unwanted crosstalk occurs between the different stages [45, 46].

  □ **Material:** Could comprise electrostatic barriers (e.g., oppositely doped semiconductor), deposited oxides (SiO$_2$, Al$_2$O$_3$, or HfO$_2$), or physical cuts [44, 46, 52].

### 4.2.3 Viability of ASL (The Tenets of Logic)

For a proper logic operation, a solid-state device has to fulfill five indispensable requirements “tenets” [263]:

1. **Nonlinearity (SNR):** [✓]
   
   Satisfied because of the nonlinearity of the FMs which corrects any error in the magnetization direction (*self-correcting feature*) [46]. This is because the FMs are bistable with two states separated by an energy barrier (Fig. 2.43) which imply that information will inherently be digitized from any weak perturbation to one of the two binary states, correcting any error and increasing the SNR [44].

2. **Power Amplification** (*gain > 1*): [✗]

   An essential feature to ensure good signal level during logic operation over a long chain of gates [44]. This is unfortunately not satisfied with the ASL of the type shown in Fig. 4.3. The problem is that the voltage developed between the output FM and the NM channel (i.e., the nonlocal voltage) is relatively low, probably several orders of magnitude smaller than that at the input and thus insufficient to drive subsequent stages [52].$^{11}$

   The problem can be solved if the switching energy came from one unclocked $V_{source}$ and not the input FM [44, 46, 52]. That is, instead of conveying both the information (provided by the input FM) and the energy (provided by $V_{source}$) through the channel, one can employ an alternative scheme that applies $V_{source}$ to both FMs, and thus only convey the information through the channel, where the energy is provided to both FMs by $V_{source}$ as in Fig. 4.7.$^{12}$ This might be in fact an advantage since it is easier to apply the same voltage to closely spaced structures and will also minimize the associated capacitive charges [45]. However,

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$^{11}$Unless intervened with a CMOS circuitry to perform amplification and/or clocking, resulting in a CMOS-dependent logic [52].

$^{12}$This was suggested in the original paper [44] and also in [52].
these advantages come at the expense of requiring a sophisticated clocking scheme [44].

![Figure 4.7: An alternative ASL structure in which the voltage is applied to both FMs.](image)

3. **Concatenability** (*output of one device can drive another*): [✓]

   Readily ensured since the input and output information are of the same form (i.e., magnetization) [46] and the FMs are identical where each act as an injector/detector [44, 45].

4. **Feedback Prevention** (*output does not drive input*): [✓]

   The directivity of a signal in one direction (and not the other) can be achieved by various means, for example:
   
   (i) Using a tunnel barrier below the injecting side of the input FM as proposed in [44–46], which can enhance spin injection into the channel. In addition, the absence of the tunneling layer in the detecting side of the output FM will create an Ohmic contact, efficiently sinking spins and suppressing back-injection [44, 46]. The barriers can be oxides or Schottky [44].

![Figure 4.8: An ASL device with a tunnel barrier inserted beneath the injecting sides of the FMs.](image)

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13 As mentioned in the Supplementary Material of the original paper [44], the height of the Schottky barrier can be lowered by degenerately doping the channel and can also be tuned by using a low work-function metal like the rare-earth FM, Gd.
(ii) Placing the ground lead closer to one FM which then causes the side of the FM exposed to the ground to act as the injector [46]. In this way, every injecting/detecting FM has two sides (separated by the spacer) that are electrically distinguished due to the ground placement [45, 46]. This solution was already implemented in Figs. 4.3 and 4.7 introduced previously.14

(iii) Using nonidentical FMs, for example (a) fixed and free layers for the input and output FMs, respectively, or (b) FMs of different sizes where the output FM is smaller than the input FM [45]. However, these solutions are not suitable for logic implementation since every FM has to act as an injector/detector (i.e., they have to be identical).

(iv) Using nonidentical sides for the FMs, for example by using different injection polarizations for each side of the FM such that the FM injects more spin current than it can receive [55]. One way to achieve this is to employ solution (i). Other solutions are also possible; for example, using nonidentical interface areas for the input and output FMs [45].

(v) Using a clocking circuitry (e.g., Bennett clocking) [44–46].

(vi) Applying different voltages to the FMs, for example by grounding the output FM and applying the signal to the input FM [46, 47]. However, as demonstrated in [45, 46], this will not yield a stable state and the FMs will keep switching between all states (though in a well-known fashion, i.e. a deterministic oscillation, which might have some applications).

Fig. 4.9b illustrates the state diagram for an ASL with nonreciprocal operation [45].

5. **A Complete Set of Boolean operations** (*AND and NOT, or OR and NOT*: ✔)

A well-known functionally complete set of Boolean operators is AND & NOT (OR & NOT), which can be used to construct every possible logic gate. In particular, these gates can be assembled to make the universal gate, NAND (NOR). Demonstration of this property using ASL is shown in [45, 46, 52, 56].

14For the latter design, an important point has to be asserted: *There is a path from FM-out to the ground underneath FM-in, allowing charge current to flow and for spins to accumulate underneath FM-out too. However, due to the asymmetric ground placement, the spin current injected by FM-out is small compared to the one injected by FM-in, and thus the torque \( \tau_{\text{STT, in}} = (1/eN_s) m_{\text{in}} \times (I_{S, in} \times m_{\text{in}}) \) is smaller than \( \tau_{\text{STT, out}} = (1/eN_s) m_{\text{out}} \times (I_{S, out} \times m_{\text{out}}) \) [45]. Indeed, this can be roughly seen from the inequality \((R_{\text{in, ground}} \times L_{\text{in, ground}}) < (R_{\text{out, g}} \times L_{\text{out, ground}})\).
4.3 Modeling & Simulations of ASL

Previous successful attempts have been made to model ASL with circuit components, and most fall into one of two categories: (1) Self-consistently solving the magnetization dynamics (governed by the LLGS) and the spin transport model (governed by the steady-state SDDE represented in the four-component spin circuit formalism), as in [45, 47–57]; (2) Simulations solely based on circuit models of the LLGS and the time-dependent SDDE for implementation in SPICE and similar software as performed in [58]. As pointed out in [47, 52], the framework of simultaneously solving the magnetization dynamics and the steady-state transport is accurate as long as the transit time of carrier diffusion in the transport section is much shorter than the dynamics of the nanomagnets, i.e. for $\tau_t \ll \tau_{sw}$, where the transit time by diffusion can be estimated as $\tau_t = L^2/2D$, with $L$ being the section length and $D$ the diffusion coefficient. Although this condition holds sufficiently well for metals of a few 100’s of nm [59], these times might become comparable as we advance in technology where magnetization switching becomes faster and/or in the case of moderately long-channel devices. In fact, we are not restricted to all-metallic structures and might use semiconducting channels, which, in addition to modifying the diffusion coefficient, brings up the advantage of longer spin-diffusion lengths. Moreover, some parasitic capacitances will be present in the transport section due to the interaction between the thin films [264] and they must taken into account as they are the most significant contributors to the dynamic power dissipation (especially at high frequencies). In any of the previous scenarios, a dynamical description of carrier transport is necessary.
Although the second model provides the necessary tools to capture the dynamics in the transport section, it lacks the freedom provided by the first model and the ability to program in common languages since it was meant for SPICE implementation. In addition, it assumes a macrospin magnet, and thus neglects any spatial variations in magnetization. It might also be difficult to augment or modify to include other interesting phenomena like spin Hall effect (SHE) and spin-orbit torque (SOT). These considerations suggest an extension of the currently available models.

![Circuit Diagram](image)

**Figure 4.10:** Coupled magnetization dynamics/spin transport simulation framework. Figure adapted by the author from [45–47, 52, 55, 56].

Starting from the theory introduced throughout the thesis, and based on the four-component spin circuit formalism, we present our improved stochastic magnetization dynamics/time-dependent spin transport model based on new finite-difference conductance matrices, which can capture both the dissipative and dynamic behavior of spins in the channel of spintronic devices in general, and ASL in particular. The derivation of the model goes in the spirit of:

1. **Coupled Magnetization Dynamics/Carrier Transport** [45, 47, 52, 55]
2. **Circuit-Based Model** [58].

In addition, we also use some of the ideas/derivations scattered throughout [48, 60, 71].

### 4.3.1 Finite-Difference Circuit Model for a Spintronic Device

In this subsection, we derive new $4 \times 4$ finite-difference conductance matrices for a non-collinear FM/NM multilayer in a spintronic device and then apply it to ASL. To avoid ambiguities, the geometrical definitions of each section/wire are as shown below.

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15Which was based on the work of Brataas *et al*. [71, 150, 265].
4.3.1.1 FM/NM Interface

Collinear Magnetizations: FMs have spin-dependent transport properties. In the absence of strong spin-flip scattering one can use the two-current model in analyzing a collinear FM/NM multilayer similar to the one shown below.

\[ I_C = I_\uparrow + I_\downarrow \quad (4.1) \]
\[ I_S = I_\uparrow - I_\downarrow \quad (4.2) \]

Similarly, the charge and spin conductances are defined by

\[ G_C = G_\uparrow + G_\downarrow \quad (4.3) \]
\[ G_S = G_\uparrow - G_\downarrow \quad (4.4) \]

Using the two-current model for the FM/NM, one can write the following equations [71]

\[ I_C = I_\uparrow + I_\downarrow = G_\uparrow (V_C^{NM} + V_S^{NM} - V_C^{FM}) + G_\downarrow (V_C^{NM} - V_S^{NM} - V_C^{FM}) \quad (4.5) \]
\[ I_S = I_\uparrow - I_\downarrow = G_\uparrow (V_C^{NM} + V_S^{NM} - V_C^{FM}) - G_\downarrow (V_C^{NM} - V_S^{NM} - V_C^{FM}) \quad (4.6) \]
where $V_{C}^{FM}$ is the charge voltage on the FM, $V_{C}^{NM}$ the charge voltage on the NM, and $V_{S}^{NM}$ the spin voltage on the NM.\textsuperscript{16} If we introduce the polarization \[71, 106]\]

\[ P = \frac{G_{\uparrow} - G_{\downarrow}}{G_{\uparrow} + G_{\downarrow}} \tag{4.7} \]

then the two equations can be rewritten as\textsuperscript{17}

\[ I_{C} = G \left( V_{C}^{NM} - V_{C}^{FM} + PV_{S}^{NM} \right) \tag{4.8} \]
\[ I_{S} = G \left( P \left( V_{C}^{NM} - V_{C}^{FM} \right) + V_{S}^{NM} \right) \tag{4.9} \]

or in matrix form

\[ \begin{bmatrix} I_{C} \\ I_{S} \end{bmatrix} = \begin{bmatrix} G & PG \\ PG & G \end{bmatrix} \begin{bmatrix} V_{C}^{NM} - V_{C}^{FM} \\ V_{S}^{NM} \end{bmatrix} \tag{4.10} \]

or

\[ \mathbf{I} = G_{FM/NM} \mathbf{V} \tag{4.11} \]

where

\[ G_{FM/NM} = \begin{bmatrix} G & PG \\ PG & G \end{bmatrix} \tag{4.12} \]

is the FM/NM interface matrix in a collinear FM/NM/FM structure.

**Noncollinear Magnetizations:** In the noncollinear case, the two-current model is not applicable anymore and one has to take the vectorial nature of spins into account \[71, 106].

\textbf{Figure 4.13}: Noncollinear FM/NM/FM trilayer with a voltage applied across the structure.

\textsuperscript{16}Notice how the spin voltage is projected (on the spin quantization axis) for the down-spins. This will be easily seen in the noncollinear case later.

\textsuperscript{17}The equations in fact reveal that a spin current can be generated by a spin accumulation even for a zero voltage drop. It is instructive to compare these to (3.38) and (3.39).
It can be shown that a generalization of the above equations for the transport across a FM/NM interface in a noncollinear FM/NM/NM multilayer is given by [71]

\[
I_C = G \left( V_C^{NM} + V_S^{NM} \cdot m - V_{CF}^{FM} \right) + G \left( V_C^{NM} - V_S^{NM} \cdot m - V_{CF}^{FM} \right)
\]
\[
I_{S,||} = \left[ G \left( V_C^{NM} + V_S^{NM} \cdot m - V_{CF}^{FM} \right) - G \left( V_C^{NM} - V_S^{NM} \cdot m - V_{CF}^{FM} \right) \right] m
\]
\[
I_{S,\perp} = 2 \text{Re} \left\{ G_{\uparrow \downarrow} \right\} m \times \left( V_S^{NM} \times m \right) + 2 \text{Im} \left\{ G_{\uparrow \downarrow} \right\} V_S^{NM} \times m
\]

where \( I_{S,||} \) and \( I_{S,\perp} \) are the longitudinal and transverse spin currents, respectively. Using the polarization \( P \), we can rewrite (4.13)–(4.15) as\(^\text{18}\)

\[
I_C = G \left( V_C^{NM} - V_{CF}^{FM} + PV_S^{NM} \right)
\]
\[
I_{S,||} = G \left( P \left( V_C^{NM} - V_{CF}^{FM} \right) + V_S^{NM} \cdot m \right) m
\]
\[
I_{S,\perp} = 2 \text{Re} \left\{ G_{\uparrow \downarrow} \right\} m \times \left( V_S^{NM} \times m \right) + 2 \text{Im} \left\{ G_{\uparrow \downarrow} \right\} V_S^{NM} \times m
\]

Now, to obtain the interface conductance matrix, we can start by considering a simple case in which the magnetization coincides with a single axis, say \( m_0 = a_x \) (later we will generalize to any arbitrary direction). Since \( I_{S,||} = (I_S \cdot m) m \), we can write

\[
I_{S,||} = G \left( P \left( V_C^{NM} - V_{CF}^{FM} \right) + V_S^{NM} \cdot a_x \right) a_x = G \left( P \left( V_C^{NM} - V_{CF}^{FM} \right) + V_S^{NM} \right) a_x
\]
\[
I_{S,\perp} = I_S - I_{S,||} = (I_{S,x} a_x + I_{S,y} a_y + I_{S,z} a_z) - (I_{S,x} a_x) = I_{S,y} a_y + I_{S,z} a_z
\]

Moreover, the cross products in (4.20) are given by

\[
V_S^{NM} \times m = V_{S,z}^{NM} a_y - V_{S,y}^{NM} a_z
\]
\[
m \times \left( V_S^{NM} \times m \right) = V_{S,y}^{NM} a_y + V_{S,z}^{NM} a_z
\]

Therefore

\[
I_{S,\perp} = 2 \text{Re} \left\{ G_{\uparrow \downarrow} \right\} \left( V_{S,y}^{NM} a_y + V_{S,z}^{NM} a_z \right) + 2 \text{Im} \left\{ G_{\uparrow \downarrow} \right\} \left( V_{S,z}^{NM} a_y - V_{S,y}^{NM} a_z \right)
\]
\[= \left( 2 \text{Re} \left\{ G_{\uparrow \downarrow} \right\} V_{S,y}^{NM} + 2 \text{Im} \left\{ G_{\uparrow \downarrow} \right\} V_{S,z}^{NM} \right) a_y + \left( 2 \text{Re} \left\{ G_{\uparrow \downarrow} \right\} V_{S,z}^{NM} - 2 \text{Im} \left\{ G_{\uparrow \downarrow} \right\} V_{S,y}^{NM} \right) a_z
\]
\[= I_{S,y} + I_{S,z}
\]

\(^\text{18}\)Sometimes written more compactly as [71]

\[
I_C = G \left( V_{C,N} + PV_{N,S} \cdot m - V_{C,F} \right)
\]
\[
I_S = G \left( \left( V_{N,S} \cdot m + PV_{N,C,F} \right) m + \eta_R m \times \left( V_{S,N} \times m \right) + \eta_I V_{S,N} \times m \right)
\]

where \( \eta_R = 2 \text{Re} \left\{ G_{\uparrow \downarrow} \right\} / G \) and \( \eta_I = 2 \text{Im} \left\{ G_{\uparrow \downarrow} \right\} / G \) are the real and imaginary parts of reduced mixing conductance (scaled by 2), \( 2G_{\uparrow \downarrow}/G \).
where the orthogonal spin current components are given by

\[ I_{S,y} = (2 \text{Re} \{ G_{\uparrow,\downarrow} \} V_{S,y}^{NM} + 2 \text{Im} \{ G_{\uparrow,\downarrow} \} V_{S,z}^{NM}) a_y \] (4.26)

\[ I_{S,z} = (2 \text{Re} \{ G_{\uparrow,\downarrow} \} V_{S,z}^{NM} - 2 \text{Im} \{ G_{\uparrow,\downarrow} \} V_{S,y}^{NM}) a_z \] (4.27)

Hence we can write the charge and spin components as

\[ I_C = G (V_C^{NM} - V_C^{FM}) + G P V_{S,x}^{NM} \] (4.28)

\[ I_{S,x} = G P (V_C^{NM} - V_C^{FM}) + G V_{S,x}^{NM} \] (4.29)

\[ I_{S,y} = 2 \text{Re} \{ G_{\uparrow,\downarrow} \} V_{S,y}^{NM} + 2 \text{Im} \{ G_{\uparrow,\downarrow} \} V_{S,z}^{NM} \] (4.30)

\[ I_{S,z} = -2 \text{Im} \{ G_{\uparrow,\downarrow} \} V_{S,y}^{NM} + 2 \text{Re} \{ G_{\uparrow,\downarrow} \} V_{S,z}^{NM} \] (4.31)

and then cast the previous equations in matrix form

\[
\begin{pmatrix}
    I_C \\
    I_{S,x} \\
    I_{S,y} \\
    I_{S,z}
\end{pmatrix}
= \begin{pmatrix}
    G & PG & 0 & 0 \\
    PG & G & 0 & 0 \\
    0 & 0 & 2 \text{Re} \{ G_{\uparrow,\downarrow} \} & 2 \text{Im} \{ G_{\uparrow,\downarrow} \} \\
    0 & 0 & -2 \text{Im} \{ G_{\uparrow,\downarrow} \} & 2 \text{Re} \{ G_{\uparrow,\downarrow} \}
\end{pmatrix}
\begin{pmatrix}
    V_C^{NM} - V_C^{FM} \\
    V_{S,x}^{NM} \\
    V_{S,y}^{NM} \\
    V_{S,z}^{NM}
\end{pmatrix}
\] (4.32)

or equivalently

\[ \mathbf{I} = G_{FM/NM} (\mathbf{m}_0) \mathbf{V} \] (4.33)

where

\[ G_{FM/NM} (\mathbf{m}_0) = \begin{pmatrix}
    G & PG & 0 & 0 \\
    PG & G & 0 & 0 \\
    0 & 0 & 2 \text{Re} \{ G_{\uparrow,\downarrow} \} & 2 \text{Im} \{ G_{\uparrow,\downarrow} \} \\
    0 & 0 & -2 \text{Im} \{ G_{\uparrow,\downarrow} \} & 2 \text{Re} \{ G_{\uparrow,\downarrow} \}
\end{pmatrix} \] (4.34)

is the FM/NM interface matrix for a noncollinear FM/NM/FM structure. The upper-left $2 \times 2$ matrix is equivalent to (4.10). The lower-right $2 \times 2$ matrix, on the other hand, is related to the noncollinear components, and is related to the action of STT, where, in this context, the diagonal and off-diagonal terms are related to the Slonczewski and field-like torques, respectively. For a metallic structure (i.e., Ohmic contacts) the field-like terms can be neglected [71, 148–150]. In addition, if the interface is clean, one can assume the interface conductance to be close to the ballistic limit [52]. For non-Ohmic interfaces (e.g., tunnel), more complex treatment is needed [150].

The conductance matrix above was obtained for a fixed magnetization orientation. Although this would not matter for a single magnet, when working with multiple non-collinear magnets one has to write all the matrices in a single uniform basis. In general,
the matrix above can be transformed to any arbitrary basis by a unitary rotation operation using an extended rotation matrix belonging to SO(3)—the group of all rotation matrices—under the constraint of keeping the charge component invariant.

Let us assume we have a unitary rotation matrix $R$ that relates the vectors in the new (primed) and old (unprimed) coordinates as

$$I' = RI$$  \hspace{1cm} (4.35)  

$$V' = RV$$  \hspace{1cm} (4.36)  

Using these relations, we can write Ohm’s law in the new coordinate frame

$$R^{-1}I' = G_{FM/NM}(m_0) R^{-1}V'$$  \hspace{1cm} (4.37)  

or

$$I' = G_{FM/NM}(m)V'$$  \hspace{1cm} (4.38)  

where the rotated matrix is given by the quaternion formula $G_{FM/NM}(m) = RG_{FM/NM}(m_0) R^{-1}$.

Since the matrix is unitary, we can equivalently write $G_{FM/NM}(m) = RG_{FM/NM}(m_0) R^T$.

The rotation matrix of interest to us, in general, belongs to the subgroup of SO(4) consisting of matrices of the form

$$R = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & r^{11} & r^{12} & r^{13} \\
0 & r^{21} & r^{22} & r^{23} \\
0 & r^{31} & r^{32} & r^{33}
\end{bmatrix}$$  \hspace{1cm} (4.39)  

which leaves one component invariant under rotation (e.g. charge in our case). The components of the block $3 \times 3$ matrix $R'$ in $R$ can found by using Rodrigues’ rotation formula, which efficiently computes a rotation matrix in SO(3) of $\mathbb{R}^3$ corresponding to a rotation by an angle $\theta$ (anticlockwise) about a fixed axis specified by the unit vector $m_0 = (m_x, m_y, m_z)$. The formula is given as the exponential map

$$R' = e^{M_0 \theta} = I + \sin \theta M_0 + (1 - \cos \theta) M_0^2$$  \hspace{1cm} (4.40)  

where $M_0$ is the skew-symmetric matrix of the Lie algebra $\mathfrak{so}(3)$ of SO(3) given by

$$M_0 = \begin{bmatrix}
0 & -m_z & m_y \\
m_z & 0 & -m_x \\
-m_y & m_x & 0
\end{bmatrix}$$  \hspace{1cm} (4.41)
Using Rodrigues’ formula, we find
\[
R' = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix} + \sin \theta \begin{bmatrix}
0 & -m_{x0} & m_{y0} \\
m_{x0} & 0 & -m_{x0} \\
-m_{y0} & m_{x0} & 0
\end{bmatrix} + (1 - \cos \theta) \begin{bmatrix}
-m_{y0}^2 & m_{x0} m_{y0} & m_{x0} m_{z0} \\
m_{x0} m_{y0} & -m_{x0}^2 - m_{z0}^2 & m_{y0} m_{z0} \\
m_{x0} m_{z0} & m_{y0} m_{z0} & -m_{z0}^2 - m_{x0}^2
\end{bmatrix}
\]

or
\[
R' = \begin{bmatrix}
1 - (1 - \cos \theta) (m_{x0}^2 + m_{y0}^2) & (1 - \cos \theta) m_{x0} m_{y0} - m_{z0} \sin \theta & (1 - \cos \theta) m_{x0} m_{z0} + m_{y0} \sin \theta \\
(1 - \cos \theta) m_{x0} m_{y0} + m_{z0} \sin \theta & 1 - (1 - \cos \theta) (m_{x0}^2 + m_{y0}^2) & (1 - \cos \theta) m_{y0} m_{z0} - m_{x0} \sin \theta \\
(1 - \cos \theta) m_{x0} m_{z0} - m_{y0} \sin \theta & (1 - \cos \theta) m_{y0} m_{z0} + m_{x0} \sin \theta & 1 - (1 - \cos \theta) (m_{y0}^2 + m_{z0}^2)
\end{bmatrix}
\]

which is equivalent to
\[
R' = \begin{bmatrix}
1 - m_{x0}^2 - m_{y0}^2 & (1 - \cos \theta) m_{x0} m_{y0} - m_{z0} \sin \theta & (1 - \cos \theta) m_{x0} m_{z0} + m_{y0} \sin \theta \\
(1 - \cos \theta) m_{x0} m_{y0} + m_{z0} \sin \theta & 1 - m_{x0}^2 - m_{y0}^2 & (1 - \cos \theta) m_{y0} m_{z0} - m_{x0} \sin \theta \\
(1 - \cos \theta) m_{x0} m_{z0} - m_{y0} \sin \theta & (1 - \cos \theta) m_{y0} m_{z0} + m_{x0} \sin \theta & 1 - m_{y0}^2 - m_{z0}^2
\end{bmatrix}
\]

Now, from the micromagnetic constraint (2.110) we know that \( m_{x0}^2 + m_{y0}^2 + m_{z0}^2 = 1 \).

Therefore
\[
R' = \begin{bmatrix}
m_{x0}^2 + (1 - m_{z0}^2) \cos \theta & (1 - \cos \theta) m_{x0} m_{y0} - m_{z0} \sin \theta & (1 - \cos \theta) m_{x0} m_{z0} + m_{y0} \sin \theta \\
(1 - \cos \theta) m_{x0} m_{y0} + m_{z0} \sin \theta & m_{y0}^2 + (1 - m_{z0}^2) \cos \theta & (1 - \cos \theta) m_{y0} m_{z0} - m_{x0} \sin \theta \\
(1 - \cos \theta) m_{x0} m_{z0} - m_{y0} \sin \theta & (1 - \cos \theta) m_{y0} m_{z0} + m_{x0} \sin \theta & m_{z0}^2 + (1 - m_{y0}^2) \cos \theta
\end{bmatrix}
\]

Hence \( R \) becomes
\[
R = \begin{bmatrix}
1 & 0 & 0 \\
0 & m_{x0}^2 + (1 - m_{z0}^2) \cos \theta & m_{x0} m_{y0} (1 - \cos \theta) - m_{z0} \sin \theta \\
0 & m_{x0} m_{y0} (1 - \cos \theta) + m_{z0} \sin \theta & m_{y0}^2 + (1 - m_{z0}^2) \cos \theta \\
0 & m_{x0} m_{z0} (1 - \cos \theta) - m_{y0} \sin \theta & m_{y0} m_{z0} (1 - \cos \theta) + m_{z0} \sin \theta
\end{bmatrix}
\]

4.3.1.2 NM

Here, we derive the conductance matrices that models the 1D transport of charge and spin in a NM section.

![Figure 4.14: A NM element with voltage applied across it.](image)
Charge Transport: In a 1D diffusive wire, the continuity and current density equations are given by

\[
\frac{\partial n}{\partial t} - \frac{1}{e} \frac{\partial J_C}{\partial z} = 0 \tag{4.47}
\]

\[
J_C = eD \frac{\partial n}{\partial z} + \sigma E \tag{4.48}
\]

Ignoring diffusion current and using the relation \( \rho_v = -en \), we can write

\[
\frac{\partial J_C}{\partial z} = -\frac{\partial \rho_v}{\partial t} \tag{4.49}
\]

\[
J_C = \sigma E \tag{4.50}
\]

For a uniform cross-section \( A \) we have \( I_C = J_C A \) and \( \rho_l = \rho_v A \). Also, \( E = -\partial V_C / \partial z \).

Thus

\[
\frac{\partial I_C}{\partial z} = -\frac{\partial \rho_l}{\partial t} \tag{4.51}
\]

\[
I_C = -\sigma A \frac{\partial V_C}{\partial z} \tag{4.52}
\]

In addition, the relation \( Q = CV_C \) on a per length basis is given by \( \rho_l = C_l V_C \), where \( C_l \) is the capacitance per unit length. This yields

\[
\frac{\partial I_C}{\partial z} = -C_l \frac{\partial V_C}{\partial t} \tag{4.53}
\]

\[
I_C = -\sigma A \frac{\partial V_C}{\partial z} \tag{4.54}
\]

Now, employing a first-order finite-difference for a finite section \( \Delta z \), we obtain

\[
I_C(z) - I_C(z + \Delta z) = C_l \Delta z \frac{\partial V_C}{\partial t} \tag{4.55}
\]

\[
I_C = \frac{\sigma A}{\Delta z} [V_C(z) - V_C(z + \Delta z)] \tag{4.56}
\]

which yields the typical RC network with \( G = \sigma A / \Delta z \) and \( C = C_l \Delta z \). The \( \pi \)- and \( T \)-model networks are shown in 4.15.

![Figure 4.15](image-url)
Spin Transport: As with the charge transport, the transport of spins starts from the 1D continuity and current density equations. Taking the fact that spins can, in general, be noncollinear, one has \[ \frac{\partial s}{\partial t} - \frac{1}{e} \nabla \cdot \mathbf{J}_S = \frac{\delta s}{\tau_{sf}} \] (4.57)

\[ \mathbf{J}_S = eD \frac{\partial \delta s}{\partial z} + e\bar{\mu}E_s \] (4.58)

Following [58], we use the relation \( s_k = \bar{\mu}_{s,k} \frac{\partial n_0}{\partial \mu} \) for each spin component to obtain

\[ \frac{\partial n_0}{\partial \mu} \frac{\partial \bar{\mu}_{s,k}}{\partial t} = \frac{1}{e} \frac{\partial J_{S,k}}{\partial z} - \frac{\partial n_0}{\partial \mu} \frac{\bar{\mu}_{s,k}}{\tau_{sf}} \] (4.59)

\[ J_{S,k} = e \frac{\partial n_0}{\partial \mu} D \frac{\partial \bar{\mu}_{s,k}}{\partial z} + e \frac{\partial n_0}{\partial \mu} \bar{\mu} E_{S,k} \] (4.60)

Then using the relation between the spin quasi-chemical potential and the spin voltage, \( \bar{\mu}_{s,k} = eV_{S,k} \), we obtain

\[ e \frac{\partial n_0}{\partial \mu} \frac{\partial V_{S,k}}{\partial t} = \frac{1}{e} \frac{\partial J_{S,k}}{\partial z} - e \frac{\partial n_0}{\partial \mu} V_{S,k} \] (4.61)

\[ J_{S,k} = e^2 \frac{\partial n_0}{\partial \mu} D \frac{\partial V_{S,k}}{\partial z} + e^2 \frac{\partial n_0}{\partial \mu} \bar{\mu} E V_{S,k} \] (4.62)

Now we recognize that \( e^2 \frac{\partial n_0}{\partial \mu} \) is the quantum capacitance per unit volume. Indeed \( C_q = \frac{e_{sk}}{V_{S,k}} = e^2 \frac{\partial n_0}{\partial \mu} = \frac{\varepsilon}{D} \), where the last equality results from Einstein’s relation. The quantum capacitance can be used along with \( I_{S,k} = J_{S,k} A \) to write

\[ C_q A \frac{\partial V_{S,k}}{\partial t} = \frac{\partial I_{S,k}}{\partial z} - C_q A \frac{V_{S,k}}{\tau_{sf}} \] (4.63)

\[ I_{S,k} = C_q D A \frac{\partial V_{S,k}}{\partial z} + C_q \bar{\mu} E A V_{S,k} \] (4.64)

Now, we notice that \( C_q E A = \sigma EA/D = J_{CA}/D = I_{CA}/D \) and \( C_q DA = \sigma A \). Therefore

\[ C_q A \frac{\partial V_{S,k}}{\partial t} = \frac{\partial I_{S,k}}{\partial z} - C_q A \frac{V_{S,k}}{\tau_{sf}} \] (4.67)

\[ I_{S,k} = \sigma A \frac{\partial V_{S,k}}{\partial z} + \bar{\mu}_C \frac{\partial I_{S,k}}{D} V_{S,k} \] (4.68)

\[ ^{19} \text{In vector notation} \]

\[ C_q A \frac{\partial \mathbf{V}_s}{\partial t} = \frac{\partial \mathbf{I}_s}{\partial z} - C_q A \frac{\mathbf{V}_s}{\tau_{sf}} \] (4.65)

\[ \mathbf{I}_s = \sigma A \frac{\partial \mathbf{V}_s}{\partial z} + \bar{\mu}_C \frac{\partial \mathbf{I}_s}{D} \mathbf{V}_s \] (4.66)
Employing finite-differences for each component of spin, we obtain

\[ I_{S,k}(z) - I_{S,k}(z + \Delta z) = C_q A \Delta z \frac{V_{S,k}}{\tau_{sf}} = C_q A \Delta z \frac{\partial V_{S,k}}{\partial t} \]  

\[ I_{S,k} = \frac{\sigma A}{\Delta z} [V_{S,k}(z) - V_{S,k}(z + \Delta z)] + \frac{\mu I_c}{D} V_{S,k} \]  

which result in the equivalent circuit shown in Fig. 4.16. In the figure, \( G = \sigma A/\Delta z \), \( G_S = C_q A \Delta z / \tau_{sf} \), \( C_S = C_q A \Delta z \), and \( I(V_{S,k}) = \mu I_c V_{S,k}/D \). The last term would vanish in the ASL channel.

![Figure 4.16: Distributed circuit model for 1D spin transport through \( \Delta z \).](image)

Now that we found the circuit representations of charge and spin transport in the NM, we employ finite-differences again, but for the time derivatives. In particular, using finite-differences in the relation \( I = C \frac{\partial V}{\partial t} \), we obtain, using:

- **Backward Euler (BE):**

\[ \begin{align*}
I^{n+1} &= \frac{C}{\Delta t} (V^{n+1} - V^n) \\
&= \frac{C}{\Delta t} V^{n+1} - \frac{C}{\Delta t} V^n \\
&= G_0 V^{n+1} + I_0
\end{align*} \]

- **Trapezoidal Rule (TR):**

\[ \begin{align*}
I^{n+1} &= \frac{2C}{\Delta t} (V^{n+1} - V^n) - I^n_C \\
&= \frac{2C}{\Delta t} V^{n+1} - \frac{2C}{\Delta t} V^n - I^n_C \\
&= G_0 V^{n+1} + I_0
\end{align*} \]

both suggesting the finite-difference capacitor model shown below.
Figure 4.17: Finite-difference model of a capacitor.

Now we use the finite-difference model above for (4.55) and (4.69). Using BE

\[
I_{C}^{n+1} (z) - I_{C}^{n+1} (z + \Delta z) = C_{t} \frac{\Delta z}{\Delta t} (V_{C}^{n+1} - V_{C}^{n})
\]
\[
= C_{t} \frac{\Delta z}{\Delta t} V_{C}^{n+1} - C_{t} \frac{\Delta z}{\Delta t} V_{C}^{n}
\]  
\( (4.77) \)

\[
I_{S,k}^{n+1} (z) - I_{S,k}^{n+1} (z + \Delta z) = C_{q} A \frac{\Delta z}{\Delta t} \left( V_{S,k}^{n+1} - V_{S,k}^{n} \right) + \frac{C_{q} A \frac{\Delta z}{\tau_{sf}}}{\Delta t} V_{S,k}^{n+1}
\]
\[
= C_{q} A \frac{\Delta z}{\Delta t} \left( \frac{1}{\Delta t} + \frac{1}{\tau_{sf}} \right) V_{S,k}^{n+1} - \frac{C_{q} A \frac{\Delta z}{\Delta t}}{\Delta t} V_{S,k}^{n}
\]  
\( (4.78) \)

Similarly, one can use the TR

\[
I_{C}^{n+1} (z) - I_{C}^{n+1} (z + \Delta z) = \frac{2C_{t} \Delta z}{\Delta t} \left( V_{C}^{n+1} - V_{C}^{n} \right) - \left[ I_{C}^{n} (z) - I_{C}^{n} (z + \Delta z) \right]
\]
\[
= 2C_{t} \frac{\Delta z}{\Delta t} V_{C}^{n+1} - 2C_{t} \frac{\Delta z}{\Delta t} V_{C}^{n} - \left[ I_{C}^{n} (z) - I_{C}^{n} (z + \Delta z) \right]
\]

\[
I_{S,k}^{n+1} (z) - I_{S,k}^{n+1} (z + \Delta z) = \frac{2C_{q} A \frac{\Delta z}{\Delta t}}{\Delta t} \left( V_{S,k}^{n+1} - V_{S,k}^{n} \right) + \frac{C_{q} A \frac{\Delta z}{\tau_{sf}}}{\Delta t} \left( V_{S,k}^{n+1} + V_{S,k}^{n} \right)
\]
\[
- \left[ I_{S,k}^{n} (z) - I_{S,k}^{n} (z + \Delta z) \right]
\]
\[
= C_{q} A \frac{\Delta z}{\Delta t} \left( \frac{2}{\Delta t} + \frac{1}{\tau_{sf}} \right) V_{S,k}^{n+1} - C_{q} A \frac{\Delta z}{\Delta t} \left( \frac{2}{\Delta t} - \frac{1}{\tau_{sf}} \right) V_{S,k}^{n}
\]  
\( (4.79) \)

Both obviously result in relations of the form

\[
I_{C}^{n+1} (z) - I_{C}^{n+1} (z + \Delta z) = G_{C,0} V_{C}^{n+1} + I_{C,0} (V_{C}^{n})
\]  
\( (4.80) \)

\[
I_{S,k}^{n+1} (z) - I_{S,k}^{n+1} (z + \Delta z) = G_{S,0} V_{S}^{n+1} + I_{S,0} (V_{S,k}^{n})
\]  
\( (4.81) \)

implying that we can approximate the capacitors in Figs. 4.15 and 4.16 with the one in Fig. 4.17.
As with the FM/NM interface, we can now represent every T-model\textsuperscript{20} with the following series and shunt finite-difference conductance matrices

\[
G_{NM,se} = \begin{bmatrix}
G_{C,se} & 0 & 0 & 0 \\
0 & G_{S,se} & 0 & 0 \\
0 & 0 & G_{S,se} & 0 \\
0 & 0 & 0 & G_{S,se}
\end{bmatrix}
\] (4.84)

\[
G_{NM,sh} = \begin{bmatrix}
G_{C,sh} & 0 & 0 & 0 \\
0 & G_{S,sh} & 0 & 0 \\
0 & 0 & G_{S,sh} & 0 \\
0 & 0 & 0 & G_{S,sh}
\end{bmatrix}
\] (4.85)

along with the vector current

\[
I_{NM,0}(V^n) = \begin{bmatrix}
I_{C,0}(V^n_C) \\
I_{S,x,0}(V^n_{S,x}) \\
I_{S,y,0}(V^n_{S,y}) \\
I_{S,z,0}(V^n_{S,z})
\end{bmatrix}
\] (4.86)

where the components are given by:-

- For BE:

\[
G_{C,se} = G_{S,se} = \frac{2\sigma A}{\Delta z}
\] (4.87)

\[
G_{C,sh} = \frac{C_q \Delta z}{\Delta t}
\] (4.88)

\[
G_{S,sh} = C_q A \Delta z \left( \frac{1}{\Delta t} + \frac{1}{\tau_{sf}} \right)
\] (4.89)

\[
I_{C,0}(V^n_C) = \frac{-C_q A \Delta z}{\Delta t} V^n_C
\] (4.90)

\[
I_{S,k}(V^n_{S,k}) = -\frac{C_q A \Delta z}{\Delta t} V^n_{S,k}
\] (4.91)

\textsuperscript{20}The π- and T-networks are related by the following transformations \cite{48}

\[
G_{se,T} = 2G_{se,\pi} + G_{sh,\pi}
\] (4.82)

\[
G_{sh,T} = G_{sh,\pi} G_{se,\pi}^{-1} G_{sh,\pi} + 2G_{sh,\pi}
\] (4.83)
4.3.2 Resulting ASL Model

Consider the ASL device shown below. As mentioned in \([47, 52]\), modeling ASL involves coupling the magnetization dynamics of the FMs (described by the sLLGS equation) with a spin transport model (described by the SDDE equation). Below we show how each of these models apply to the device below.

**4.3.2.1 Stochastic Magnetization Dynamics**

Here, we assume single domain, identical FMs in the macrospin limit. The FMs are assumed to be rectangular prisms lying in the \(xz\) plane with an easy-axis along the \(z\)-axis. In the presence of STT and thermal effects, the dynamics of each FM are governed
by the sLLGS equation
\[
\frac{d\mathbf{m}_1}{dt} = -\frac{\gamma G}{1 + \alpha^2} [\mathbf{m}_1 \times (\mathbf{H}_{eff,1} + \mathbf{H}_{T,1})] - \frac{\gamma G}{1 + \alpha^2} \alpha \{ \mathbf{m}_1 \times [\mathbf{m}_1 \times (\mathbf{H}_{eff,1} + \mathbf{H}_{T,1})] \}
+ \frac{1}{1 + \alpha^2} \alpha \mathbf{m}_1 \times \tau_{STT,1} + \frac{1}{1 + \alpha^2} \tau_{STT,1}, \quad \mathbf{m}_1 (r,0) = \mathbf{m}_{0,1}
\]
\[
\frac{d\mathbf{m}_2}{dt} = -\frac{\gamma G}{1 + \alpha^2} [\mathbf{m}_2 \times (\mathbf{H}_{eff,2} + \mathbf{H}_{T,2})] - \frac{\gamma G}{1 + \alpha^2} \alpha \{ \mathbf{m}_2 \times [\mathbf{m}_2 \times (\mathbf{H}_{eff,2} + \mathbf{H}_{T,2})] \}
+ \frac{1}{1 + \alpha^2} \alpha \mathbf{m}_2 \times \tau_{STT,2} + \frac{1}{1 + \alpha^2} \tau_{STT,2}, \quad \mathbf{m}_2 (r,0) = \mathbf{m}_{0,2}
\]

where \( \tau_{STT,1} = (1/eN_s) \mathbf{m}_1 \times (I_{S,1} \times \mathbf{m}_1), \mathbf{m}_1 \times \tau_{STT,1} = (1/eN_s) \mathbf{m}_1 \times I_{S,1}, \tau_{STT,2} = (1/eN_s) \mathbf{m}_2 \times (I_{S,2} \times \mathbf{m}_2), \) and \( \mathbf{m}_2 \times \tau_{STT,2} = (1/eN_s) \mathbf{m}_2 \times I_{S,2}. \) Here, it is assumed that the STT term does not contain a fluctuating field, which is a good assumption considering the fact that the transport properties of the conduction electrons are less affected by the thermal field since they have much higher Fermi level than the thermal energy [225]. The thermal field of each FM is an uncorrelated and independent Gaussian white noise, formally defined as the derivative of a Wiener process, i.e. \( \mathbf{H}_{T,1} = \sigma_1 \dot{\mathbf{W}}_1, \mathbf{H}_{T,2} = \sigma_1 \dot{\mathbf{W}}_2. \) Each white noise is characterized by the following two moments
\[
\left\langle \dot{W}_i (t) \right\rangle = 0
\]
\[
\left\langle \dot{W}_i (t) \dot{W}_j (t + \tau) \right\rangle = 2D\delta_{ij}\delta (\tau)
\]
for \( i \in \{x, y, z\}, \) where the measure of the fluctuating fields is given by \( D_1 = D_2 = \alpha k_B T/\gamma G \mu_0 V M_S. \) Since every component of the white noise vector follows a Gaussian distribution, i.e. \( \dot{\mathbf{W}}_i \sim \mathcal{N} (1, 0), \) then for numerical simulations one has to generate Gaussian random numbers (and not uniformly distributed ones). An efficient and easy algorithm to generate such numbers is the Box-Muller transform (see Appendix C).

Now, the effective fields for uniformly magnetized specimens with uniaxial anisotropy (in the absence of external fields) are given by
\[
\mathbf{H}_{eff,1} = H_K (\mathbf{e}_{an} \cdot \mathbf{m}_1) \mathbf{e}_{an} - M_s N \mathbf{m}_1
\]
\[
\mathbf{H}_{eff,2} = H_K (\mathbf{e}_{an} \cdot \mathbf{m}_2) \mathbf{e}_{an} - M_s N \mathbf{m}_2
\]
where \( H_{K,1} = H_{K,2} = 2K_1/\mu_0 M_s \) is the anisotropy field and \( N \) is the demagnetization tensor for a thin film. The latter in our case is written as
\[
N = \begin{bmatrix} 0 & 0 & 0 \\ 0 & N_y & 0 \\ 0 & 0 & 0 \end{bmatrix}
\]
For an infinite thin film, \( N_y = 1. \) However, for a finite size thin film, \( N_y < 1 \) and \( N_x \neq 0, \)
$N_z \neq 0$, as expected. Fortunately, $N_y$ can be computed analytically using the result derived by Aharoni [266]

\[
N_y = \frac{b^2 - c^2}{2bc} \ln \left( \frac{\sqrt{a^2 + b^2 + c^2} - a}{\sqrt{a^2 + b^2 + c^2} + a} \right) + \frac{b^2 - c^2}{2ac} \ln \left( \frac{\sqrt{a^2 + b^2 + c^2} - b}{\sqrt{a^2 + b^2 + c^2} + b} \right) + \frac{b}{2c} \ln \left( \frac{\sqrt{a^2 + b^2} + a}{\sqrt{a^2 + b^2} - a} \right)
\]

\[+ \frac{a}{2c} \ln \left( \frac{\sqrt{a^2 + b^2} + b}{\sqrt{a^2 + b^2} - b} \right) + \frac{c}{2a} \ln \left( \frac{\sqrt{b^2 + c^2} - b}{\sqrt{b^2 + c^2} + b} \right) + \frac{c}{2b} \ln \left( \frac{\sqrt{a^2 + c^2} - a}{\sqrt{a^2 + c^2} + a} \right)
\]

\[+ 2\tan^{-1} \left( \frac{ab}{c\sqrt{a^2 + b^2 + c^2}} \right) + \frac{a^3 + b^3 - 2c^3}{3abc} + \frac{a^2 + b^2 - 2c^2}{3abc} \sqrt{a^2 + b^2 + c^2}
\]

\[+ \frac{c}{ab} \left( \sqrt{a^2 + b^2} + \sqrt{b^2 + c^2} - \left( \sqrt{a^2 + b^2} \right)^3 + \left( \sqrt{b^2 + c^2} \right)^3 + \left( \sqrt{a^2 + c^2} \right)^3 \right)
\]

(4.104)

where, in terms of our geometrical definition: $a = 2L$, $b = 2t$, and $c = 2W$. The other components can be found from the same equation by applying twice the cyclic permutation $c \to a \to b \to c$, and it can be readily shown that $N_x + N_y + N_z = 1$.

Owing to thermal agitation, the initial angle is also thermally distributed, and for consistency one has to randomize it with the most probable angle. Using the equipartition theorem from statistical mechanics, one can use the average value

\[
\langle \theta_0 \rangle = \sqrt{\frac{k_B T}{2K_{eff}}} V
\]

(4.105)

where $K_{eff} = K_1 + K_d = K_1 + \mu_0 M_s^2 \left( N_\perp - N_\parallel \right) / 2$ is the effective anisotropy constant which takes both magnetocrystalline and shape anisotropy into account.

To obtain the stochastic magnetization trajectories, one can use a generalized form of Heun’s predictor-corrector scheme. By casting the SDE into a system of Langevin equations

\[dm_i = a_i(t, m) dt + b_{ik}(t, m) \circ H_{T,k}(t) dt, \quad m_i(t_0) = m_{i,0}\]

for $i \in \{x, y, z\}$, Heun’s predictor-corrector scheme is given by

\[
\tilde{m}_i^{n+1} = m_i^n + a_i(t^n, m^n) \Delta t + b_{ik}(t^n, m^n) \Delta W_k^n
\]

\[
m_i^{n+1} = m_i^n + \frac{\Delta t}{2} \left[ a_i(t^n, m^n) + a_i(t^{n+1}, \tilde{m}^{n+1}) \right]
\]

\[+ \frac{\Delta W_k^n}{2} \left[ b_{ik}(t^n, m^n) + b_{ik}(t^{n+1}, \tilde{m}^{n+1}) \right]
\]

where $n = 1, 2, \ldots, N$ and $N = (t_{final} - t_0) / \Delta t$. The $i$-th component of the deterministic and stochastic terms can be found by using Levi-Civita symbol.
4.3.2.2 Spin Circuit

Using the spatially (and temporally) finite-difference model derived in 4.3.1, we can represent an ASL with the equivalent circuit shown in Fig. 4.19 below.

To analyze the circuit, we invoke the MNA algorithm, extended to spin space. Since we have \( n = 5 \) nodes (excluding ground), we labeled the node voltages with the vectors \( \mathbf{V}_1, \mathbf{V}_2, \ldots, \mathbf{V}_5 \). Moreover, we have \( m = 1 \) independent voltage source and have labeled the charge current through it with \( \mathbf{I}_{\text{source}} \). Node 5 was introduced to facilitate computations since \( G_{FM/NM} \) has in general non-zero off-diagonal entries and thus any conductance in series with it does not make use of the simple rule \( (G_{NM1,se}^{-1} + G_{FM2/NM1}^{-1})^{-1} \).

The generalized MNA algorithm generates the linear system

\[
A \mathbf{x} = \mathbf{b} \tag{4.106}
\]

where \( A \in \mathbb{R}^{24 \times 24}, \mathbf{x} \in \mathbb{R}^{24 \times 1}, \mathbf{b} \in \mathbb{R}^{24 \times 1} \). The linear system can be decomposed as

\[
\begin{bmatrix} G & B \\ C & D \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ \mathbf{j} \end{bmatrix} = \begin{bmatrix} \mathbf{i} \\ \mathbf{e} \end{bmatrix} \tag{4.107}
\]

where \( \mathbf{v} \in \mathbb{R}^{20 \times 1}, \mathbf{j} \in \mathbb{R}^{4 \times 1}, G \in \mathbb{R}^{20 \times 20}, B \in \mathbb{R}^{20 \times 4}, C \in \mathbb{R}^{4 \times 20}, D \in \mathbb{R}^{4 \times 4}, \mathbf{i} \in \mathbb{R}^{20 \times 1}, \) and \( \mathbf{e} \in \mathbb{R}^{4 \times 1} \). Using the rules of MNA, one can easily find the entries of each matrix. The resulting system is shown on the next page.
\[ A = \begin{bmatrix}
G_{FM1/NM1} + G_{FM2/NM1} & -G_{FM1/NM1} & O & -G_{FM2/NM1} & 0 & 0 & I \\
-G_{FM1/NM1} & G_{FM1/NM1} + G_{NM1,se} + G_{NM2,se} & -G_{NM1,se} & O & -G_{NM2,se} & 0 & 0 \\
O & -G_{NM1,se} & 2G_{NM1,se} + G_{NM1,sh} & -G_{NM1,se} & O & O & O \\
-G_{FM2,NM1} & O & -G_{NM1,se} & G_{FM2/NM1} + G_{NM1,se} & O & O & O \\
O & O & O & O & O & O & O \\
O & O & O & O & O & O & O \\
1 & \end{bmatrix} \]

\[ x = \begin{bmatrix}
V_1 \\
V_2 \\
V_3 \\
V_4 \\
V_5 \\
I_{source} \\
\end{bmatrix} \]

\[ b = \begin{bmatrix}
0 \\
0 \\
-I_{NM1,0} \\
0 \\
-I_{NM2,0} \\
V_{source} \\
\end{bmatrix} \]
4.3.3 Simulations

With the model introduced above, namely the stochastic magnetization dynamics and the spin circuit matrix, one can start simulating the circuit and obtain the magnetization trajectories. For algorithm implementation, we have made 9 scripts on MATLAB® that can also be easily translated to other programming languages. A simplified flow chart of the algorithm is also shown. The simulation has been performed with a time-step $\Delta t = 1$ ps with the parameters shown in Table 4.1 on the next page.

---

![Flowchart](image)

**Figure 4.20:** Simplified flowchart of the algorithm developed to simulate ASL on MATLAB®.

---

21 For questions/suggestions about the algorithm and MATLAB® scripts, please contact the author on meshal.alawein@kaust.edu.sa.
Table 4.1: ASL simulation parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t_{FM} )</td>
<td>Thickness</td>
<td>3</td>
<td>nm</td>
</tr>
<tr>
<td>( W_{FM} )</td>
<td>Width</td>
<td>50</td>
<td>nm</td>
</tr>
<tr>
<td>( L_{FM} )</td>
<td>Length</td>
<td>100</td>
<td>nm</td>
</tr>
<tr>
<td>( \rho_{FM} )</td>
<td>Resistivity</td>
<td>56</td>
<td>nΩ·m</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>Damping factor</td>
<td>0.01</td>
<td>-</td>
</tr>
<tr>
<td>( M_s )</td>
<td>Saturation magnetization</td>
<td>1.414\times10^6</td>
<td>A/m</td>
</tr>
<tr>
<td>( K_1 )</td>
<td>First uniaxial anisotropy constant</td>
<td>10\times10^4</td>
<td>J/m^3</td>
</tr>
<tr>
<td>( H_K )</td>
<td>Anisotropy Field</td>
<td>1.126\times10^5</td>
<td>A/m</td>
</tr>
<tr>
<td>( N_x, N_y, N_z )</td>
<td>Demagnetization factors</td>
<td>0.055, 0.89, 0.055</td>
<td>-</td>
</tr>
</tbody>
</table>

**FM/NM Interface**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P )</td>
<td>Polarization</td>
<td>0.5</td>
<td>-</td>
</tr>
<tr>
<td>( g_{\uparrow} )</td>
<td>Spin-up conductance</td>
<td>0.42\times10^{15}</td>
<td>S/m^2</td>
</tr>
<tr>
<td>( g_{\downarrow} )</td>
<td>Spin-down conductance</td>
<td>0.38\times10^{15}</td>
<td>S/m^2</td>
</tr>
<tr>
<td>( \text{Re}{g_{\downarrow}} )</td>
<td>Real-part of the mixing conductance</td>
<td>0.546\times10^{15}</td>
<td>S/m^2</td>
</tr>
<tr>
<td>( \text{Im}{g_{\downarrow}} )</td>
<td>Imaginary-part of the mixing conductance</td>
<td>0.015\times10^{15}</td>
<td>S/m^2</td>
</tr>
</tbody>
</table>

**NM_1 (Cu)**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t_{NM1} )</td>
<td>Thickness</td>
<td>200</td>
<td>nm</td>
</tr>
<tr>
<td>( W_{NM1} )</td>
<td>Width</td>
<td>50</td>
<td>nm</td>
</tr>
<tr>
<td>( L_{NM1} )</td>
<td>Length</td>
<td>100</td>
<td>nm</td>
</tr>
<tr>
<td>( l_{sf,NM1} )</td>
<td>Spin-diffusion length</td>
<td>450</td>
<td>nm</td>
</tr>
<tr>
<td>( \rho_{NM1} )</td>
<td>Resistivity</td>
<td>16.7</td>
<td>nΩ·m</td>
</tr>
</tbody>
</table>

**NM_2 (Al)**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t_{NM2} )</td>
<td>Thickness</td>
<td>200</td>
<td>nm</td>
</tr>
<tr>
<td>( W_{NM2} )</td>
<td>Width</td>
<td>50</td>
<td>nm</td>
</tr>
<tr>
<td>( L_{NM2} )</td>
<td>Length</td>
<td>100</td>
<td>nm</td>
</tr>
<tr>
<td>( l_{sf,NM2} )</td>
<td>Spin-diffusion length</td>
<td>600</td>
<td>nm</td>
</tr>
<tr>
<td>( \rho_{NM2} )</td>
<td>Resistivity</td>
<td>26.3</td>
<td>nΩ·m</td>
</tr>
</tbody>
</table>
4.3.4 Results and Discussion

The simulations were performed with the following in mind: (i) To show that our model works, we first simulated ASL assuming no dynamics in the transport section. Figs. 4.22 & 4.23, 4.24, and 4.25 shows the transient simulations of magnetization, spin current, and injected power, respectively. Fig. 4.21, on the other hand, shows the 3D trajectory of the magnetization tip on the unit sphere. (ii) We introduced some dynamics in the transport section to check if our model is able to capture it and also study the dependency on capacitance. Such dynamics can occur due to the presence of, say, some parasitics or loading effect. By varying the capacitance between 0.1 pF and 100 pF (which are reasonable values [264]), we generated Figs. 4.26 and 4.27, the transient spin currents and magnetizations, respectively.

First, we discuss Fig. 4.23, which shows the switching character of ASL. The device was driven by a 5 mV pulse with a frequency 0.25 x 10^9 GHz. It is apparent that the device functions as NOT for positive voltages, and as COPY for negative voltages. The device roughly switches P → AP after 0.7 – 0.8 ns, and AP → P after 1.3 – 1.4 ns. In addition, from Fig. 4.24 one can see that the spin currents flow only when switching occurs, as also pointed out in [46, 47]. This is also the case with the injected power shown in 4.25. The transient response above is expected and conforms with the results in literature (e.g., in [48, 60]), and thus our model correctly reduces to the steady-state case and recovers the expected results.

Second, from 4.21, we see that FM1 is effectively fixed in its position, though it fluctuates around its easy-axis. The fluctuations occur due to the different interactions present such as thermal perturbations or torques exerted by the spin current injected from the passage of I_C from FM2 to the ground terminal. FM2, on the other hand, switches between the two stable states due to the pulsed current injected.

Finally, we introduce some parasitics in the transport section to see if our model captures the dynamics and responds to the effects of energy storage elements. Figs. 4.26 and 4.27 show the transients spin currents and magnetizations, respectively. Although there is apparently some overshoot “spiking” due to the increase in the parasitic, one might wonder why is not there a notable charging/discharging character on time scales G/C. We recall that we are using an all-metallic structure for which voltage swings on the capacitors are on the order of Δμ_s = 1 μeV, which would imply a very large capacitor to be used for the transient current C (∂Δμ_s/∂t) to be significantly altered

22 Or a Schottky contact in the case of semiconductors.
23 In general, a 100 pF is very large and the parasitics will probably be much less, say something in the range 0.1 – 10 pF, as we learned from CMOS. However, for the sake of observing the dependency on the capacitance we chose an upper bound of 100 pF rather than 10 pF as was also done in [264].
with significant finite rise and fall times [59]. In fact, by deliberately adding a large parasitic capacitance $C = 100 \text{ pF}$, the currents are clearly affected by the energy storage element. Now regarding the magnetization, we can immediately see that there is no major effect on the switching event $P \rightarrow AP$, but a strong one on $AP \rightarrow P$. In fact, for $C = 1 \text{ pF}$ (a moderate capacitance), the magnetization does not keep up with the pulse and yields improper switching behavior. However, it is interesting that for even larger values, the switching behavior is recovered. This might be an oscillatory dependence of the switching character on capacitance which one can use to find an optimal value to reduce the switching time. Further discussions about this peculiar dependency can be found in [264].
Figure 4.21: Magnetization trajectories on the unit sphere $S^2$. (a) $\mathbf{m}_1$. (b) $\mathbf{m}_2$. 
Figure 4.22: Time evolution of magnetization showing ASL inverter switching characteristics. (a) $m_1$ vs $t$. (b) $m_2$ vs $t$. 
Figure 4.23: Time evolution of $m_1$ & $m_2$ showing ASL inverter switching characteristics.

Figure 4.24: Time evolution of $I_{S,1}$ & $I_{S,2}$. 
Figure 4.25: Time evolution of $P_1$ & $P_2$. 
Figure 4.26: Time evolution of spin currents with varying parasitic capacitance. (a) $C = 0.1$ pF. (b) $C = 1$ pF. (c) $C = 10$ pF. (d) $C = 50$ pF. (e) $C = 100$ pF.
Figure 4.27: Time evolution of magnetization with varying parasitic capacitance. (a) $C = 0.1$ pF. (b) $C = 1$ pF. (c) $C = 10$ pF. (d) $C = 50$ pF. (e) $C = 100$ pF.
Chapter 5

Summary and Outlook

With CMOS miniaturization and energy-efficiency rapidly approaching an inevitable physical limit, a search for an alternative technology is accelerating. Spintronic devices are one of the prime candidates for Beyond CMOS technologies due to their low-power operation, nonvolatile nature, and high density computation and storage. In the category of promising spintronic switches is a device called all-spin logic (ASL) that has recently attracted increasing interest due to its low-power operation and built-in memory structure. In addition, the device utilizes pure spin currents throughout every stage, eliminating the need for repeated spin-to-charge conversion and any spurious effects accompanying charge currents. To assess the feasibility of spintronic devices in general and ASL in particular to function as logic and memory elements, we presented in this thesis a dynamic circuit model for rapid computer-aided design and verification.

In chapters 2 and 3, we reviewed some of the essential concepts in nanomagnetism and spintronics. Following that, we discussed the statics and dynamics of a nanomagnet and presented an algorithm to compute the trajectories from the stochastically perturbed dynamic equations in the presence of spin-polarized currents. We then discussed the basics of spin circuit theory and magnetoelectronics. In particular, the four-component circuit variables; a novel circuit framework to analyze spintronic devices in a way analogue to the well-known circuit theory.

In chapter 4, we invoked the well-known physics of nanomagnetism and spin, in particular, the stochastic Landau-Lifshitz-Gilbert-Slonczewski (sLLGS) and spin drift-diffusion equation (SDDE) as bases formalisms for our ASL model. Using the recently proposed four-component spin circuit theory and a finite-difference scheme for both the spatial and temporal derivatives, we modeled ASL with new finite-difference conductance matrices. By applying a self-consistent algorithm that passes the solution back-and-forth between...
the “spin circuit” and the “stochastic nanomagnet dynamics”, we simulated an ASL inverter. While in the steady-state limit, the results match the ones in literature, for a finite channel parasitic capacitance, the transient currents exhibit finite charging/discharging time which is captured by our model.

Although the model adequately captures any introduced dynamics in the transport channel, there are still limitations and challenges that one must be aware of. For example, the model neglects spin dissipation associated with spin-flipping events occurring in the FM. In other words, we modeled the spin transport in the NM and the scattering at the FM/NM interface, but neglected spin relaxation inside the FM. For a more accurate model, one has to invoke the SDDE in the FM and apply the same spatial- and temporal-discretization to obtain a dynamic circuit model. Despite the minor limitation, the model generally encompasses a discretization framework that we believe can be used for improved dynamic circuit modeling for ASL and other emerging spintronic devices.
Appendix A

Mathematical Review

Many excellent graduate-level texts provide detailed and thorough treatment of the material in this appendix. The aim here is not to discuss the concepts in detail or proof every statement, but rather introduce the notation used in the thesis and provide a reference for some of the results used in proofs and derivations. Readers who are interested in more rigor and in-depth discussions are referred to [267–270].

A.1 Tensor Calculus in Curvilinear Coordinates

In a differentiable manifold such as $\mathbb{E}^n$, the Cartesian coordinates are arguably the most intuitive and easy handle, but by no means the only possible option. Physical problems are generally approached by choosing an appropriate coordinate system that fits the given problem symmetry, which in some cases can be non-Cartesian or even global, common examples being the famous cylindrical and spherical coordinates. The previous three coordinates are just a subset of the so-called curvilinear coordinates.

For the sake of generality, a brief glimpse through tensor analysis is introduced in arbitrary curvilinear coordinates. The formalism provides a unified and general description of the standard coordinate systems. Throughout the discussion, we assume all coordinate frames to be right-handed trihedrals.

\footnote{A differentiable manifold is a topological Hausdorff space locally homeomorphic to $\mathbb{E}^n$.}
A.1.1 Some Preliminary Notions

A.1.1.1 Suffixes and Einstein’s Convention

We start by introducing the very useful index notation for tensor algebra. Let \( \mathbf{v} \in V \) be a vector, where \( V \) is a vector space over the reals with dimension \( n \). Moreover, let \( S = \{ \mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n \} \) be a basis for \( V \). We can then uniquely write the vector \( \mathbf{v} \) as a linear combination of the the basis vectors

\[
\mathbf{v} = v_1 \mathbf{e}_1 + v_2 \mathbf{e}_2 + \cdots + v_n \mathbf{e}_n \quad \text{(A.1)}
\]

where \( (v_1, v_2, \ldots, v_n) \) are the coordinates of \( \mathbf{v} \) relative to the basis \( S \). Assume we were given a transformation matrix \( A \) associated with the linear map \( T : \mathbb{R}^n \to \mathbb{R}^n \), and would like to find the coordinates in terms of a new basis \( S' = \{ \mathbf{e}'_1, \mathbf{e}'_2, \ldots, \mathbf{e}'_n \} \). For example

\[
\begin{bmatrix}
v_1' \\
v_2' \\
\vdots \\
v_n'
\end{bmatrix} =
\begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{1n} \\
a_{21} & a_{22} & \cdots & a_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
a_{n1} & a_{n2} & \cdots & a_{nn}
\end{bmatrix}
\begin{bmatrix}
v_1 \\
v_2 \\
\vdots \\
v_n
\end{bmatrix} \quad \text{(A.2)}
\]

Using suffixes, we can refer to the \( i \)-th component of the vector \( \mathbf{v}' \) as \( v'_i \). Similarly, the \( (i, j) \)-th entry of the matrix \( A \) is written as \( a_{ij} \). According to the rules of matrix multiplication, one can write the \( i \)-th component of the transformed vector as

\[
v'_i = \sum_{j} a_{ij} v_j, \quad i = 1, 2, \ldots, n
\]

In such formulae, we call the suffix \( i \) (that appears once) the \textit{running index} (also known as the \textit{free index}), and the suffix \( j \) (that appears twice) the \textit{dummy index}. A way to avoid the tedium of writing summation signs, especially for matrix products and complex equations, is to use a short-cut notation given by the rules of \textit{Einstein summation convention}, which we summarize below:

1. Omit summation signs;
2. A suffix appearing twice (i.e., dummy index) implies summation;
3. A suffix appearing once (i.e., free index) can take any value in a specified subset of integers and is not summed over;
4. A suffix cannot appear more than twice.
Example A.1. Let \( v, u, w, x, y \in V, \alpha \in \mathbb{R}, \) and \( A \) the transformation matrix given above. Then according to the convention presented we can write the following operations as

\[
\alpha = v \cdot u \leftrightarrow \alpha = v_i u_i \\
y = Av \leftrightarrow y_i = a_{ij} v_j \\
y = (v \cdot u)w \leftrightarrow y_i = v_j u_j w_i \\
y = x + |v|^2|u|^2 w \leftrightarrow y_i = x_i + v_j u_j u_k w_i
\]

where we notice that the free index \( i \) appears only once in each term.

\[\square\]

A.1.1.2 Delta and Epsilon

The suffix notation can be made easier by introducing two important functions. The first is the Kronecker delta

\[
\delta_{ij} = \begin{cases} 
1, & i = j \\
0, & i \neq j 
\end{cases}
\]  

(A.3)

The delta function is symmetric \( \delta_{ij} = \delta_{ji} \), and has the sifting property

\[
\delta_{ij} v_j = v_i
\]  

(A.4)

The second is the three-dimensional Levi-Civita symbol\(^2\)

\[
\varepsilon_{ijk} = \begin{cases} 
1, & \text{if } (i, j, k) \text{ is } (1, 2, 3), (2, 3, 1), (3, 1, 2) \\
-1, & \text{if } (i, j, k) \text{ is } (3, 2, 1), (2, 1, 3), (1, 3, 2) \\
0, & \text{if } i = j, j = k, k = i
\end{cases}
\]  

(A.5)

Example A.2. Let \( v, u \in V, \alpha \in \mathbb{R}, \) and \( A \) the transformation matrix given above. Then we can use the functions introduced to write the following operations using suffixes

\[
y = u \times b \leftrightarrow y_i = \varepsilon_{ijk} u_j v_k \\
\alpha = \det (A) \leftrightarrow \alpha = \varepsilon_{ijk} A_{1i} A_{2j} A_{3k}
\]

\[\square\]

\(^2\)Also known as the permutation, antisymmetric or alternating symbol.
A.1.2 General Considerations

A.1.2.1 Coordinate Transformation

Two different coordinate systems are related by a coordinate transformation. Consider the open domain \( X \subset \mathbb{R}^n \) endowed with the Cartesian coordinates \( x^1, x^2, \ldots, x^n \). Assigning each point \( p \in X \) a set of \( n \) real numbers, we define \( n \) scalar-valued functions \( f_1(p), f_2(p), \ldots, f_n(p) \) on the region \( X \), which we shall use to define the curvilinear coordinates patch. Thus we consider another open subset \( U \subset \mathbb{R}^n \) that represents the curvilinear coordinates \( u^1, u^2, \ldots, u^n \). This allows us to define a continuous coordinate system in a region \( X \subset \mathbb{R}^n \) as the \( n \)-tuple of continuous functions \((u^1, u^2, \ldots, u^n)\) given by

\[
\begin{align*}
  u^1 &= f_1(x^1, x^2, \ldots, x^n) \\
  u^2 &= f_2(x^1, x^2, \ldots, x^n) \\
  \vdots \\
  u^n &= f_n(x^1, x^2, \ldots, x^n)
\end{align*}
\]

where each \( u^i = f_i(x^1, x^2, \ldots, x^n) \) maps \( X \) both bijectively and continuously in both directions into some domain \( U \subset \mathbb{R}^n \). In other words, the function is a bi-continuous bijection and we say that for each point \( p \), the map \( f(p) = (f_1(p), f_2(p), \ldots, f_n(p)) \) is a homeomorphism of \( X \) onto \( U \), and the spaces are said to be homeomorphic. Fig. A.1 shows a rough sketch of the map action.

The values \( f_1(p), f_2(p), \ldots, f_n(p) \) are called the coordinates of \( p \) relative to the coordinate map \( f : X \to U \), and the scalar-valued functions (the components) themselves \( f_1, f_2, \ldots, f_n \) are called the coordinate functions. In the category of continuous maps, we are merely interested in smooth ones, namely those for which the component functions (and their inverses) are continuously differentiable of all orders; that is, functions belonging to the class \( C^\infty \).

---

3. A set \( X \subset \mathbb{R}^n \) is open if \( \forall x \in X \), there is an open \( \varepsilon \)-neighborhood entirely contained in \( X \). That is, \( \exists \varepsilon > 0 \) such that \( X_\varepsilon(x) \subset X \), where \( X_\varepsilon(x) = \{ y \in \mathbb{R}^n | |x - y| < \varepsilon \} \). In other words, \( X_\varepsilon(x) \) is in open ball of radius \( \varepsilon \) with center \( x \).

4. Note how we use superscripts for coordinates, which are the contravariant components of vectors (more about this later). We stick to this policy (borrowed from differential geometry) for nonorthogonal coordinate systems, which will prove useful. Later for orthogonal systems we drop superscripts and use subscripts all the way.

5. \( \mathbb{R}^n \) here is another copy of the Euclidean space.

6. Not to be confused with homomorphism, which is not a topological term but an algebraic one.
Viewing the map as a vector of $n$ variables, we write the direct transformation as the vector-valued function $f : X \subset \mathbb{R}^n \to U \subset \mathbb{R}^n$, or as the column vector

$$f(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_n(x) \end{bmatrix} \quad (A.6)$$

where the components $f_1, f_2, \ldots, f_n$ are scalar-valued functions and $x \in X$. The best affine approximation of $f$ at $p \in X$ is given by

$$f(x) = f(p) + J_f(p)(x - p) + o(\|x - p\|) \quad (A.7)$$

in the limit as $x \to p$.\(^7\) Here, $J_f(p)$ is the functional matrix

$$J_f(p) = \frac{df(p)}{dx} = \begin{bmatrix} \frac{\partial f_1}{\partial x^1} & \frac{\partial f_1}{\partial x^2} & \cdots & \frac{\partial f_1}{\partial x^n} \\ \frac{\partial f_2}{\partial x^1} & \frac{\partial f_2}{\partial x^2} & \cdots & \frac{\partial f_2}{\partial x^n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x^1} & \frac{\partial f_n}{\partial x^2} & \cdots & \frac{\partial f_n}{\partial x^n} \end{bmatrix} = \begin{bmatrix} \nabla f_1 \\ \nabla f_2 \\ \vdots \\ \nabla f_n \end{bmatrix} \quad (A.8)$$

known as the *Jacobi matrix* of the transformation $f : X \to U$, typically written as $J^i_j = \frac{\partial u^i}{\partial x^j}$.\(^8\) The determinant of that matrix, $\det(J_f(p))$, is known as the *Jacobian*. The Jacobi matrix gives the best affine approximation of $f$ near $p$, and the Jacobian gives an indication about the local behavior of $f$. In particular, if the Jacobian is nonzero (matrix nonsingular), then $f$ possess a differentiable inverse function in a neighborhood of $p$ (i.e., it is locally invertible)—this is the *inverse function theorem*, which ensures that the

\(^7\)A natural extension of the differential of a smooth function of a single variable, where in that case, the equation of the tangent line is the best affine approximation

$$f(x) = f(p) + f'(p)(x - p) + o(|x - p|)$$

in the limit as $x \to p$.

\(^8\)Notice how it generalizes the notion of the gradient.
The inverse map \( g : U \to X \) is also smooth with the Jacobi matrix

\[
J_g(p) = J_f(p)^{-1}
\]

and thus \( \det(J_f(p)) \det(J_g(p)) = 1 \). A vanishing Jacobian implies that \( f_1, f_2, \cdots, f_n \) are not independent functions, but rather connected by a relationship \( F(f_1, f_2, \cdots, f_n) = 0 \).

The Jacobi matrix locally describes the amount by which \( f \) imposes stretching, compressing, rotating, etc. If \( \det(J_f(p)) > 0 \), then \( f \) preserves the orientation near \( p \), and otherwise if \( \det(J_f(p)) < 0 \). The absolute value of the Jacobian \( |\det(J_f(p))| \) indicates the amount by which \( f \) shrinks or expands a volume. The Jacobi matrix also maps tangent vectors from one frame to the other. To see this, consider the direct transformation \( f : X \to U \). For \( p \in X \), the map gives the \( n \)-tuple \( u = f(p) \). Taking the temporal derivative

\[
\frac{du}{dt} = \frac{df(p)}{dt}
\]

and applying the chain rule and using (A.8), one finds

\[
\frac{df(p)}{dt} = \frac{df(p)}{dx} \cdot \frac{dx}{dt} = J_f(p) \frac{dx}{dt},
\]

or

\[
\frac{du}{dt} = J_f(p) \frac{dx}{dt}
\]

Similarly, for the inverse transformation \( g : U \to X \), one can show

\[
\frac{dx}{dt} = J_g(p) \frac{du}{dt}
\]

Under the conditions stated above, we call our curvilinear system regular, and we say the regular curvilinear coordinates are generated by a diffeomorphism.\(^9\) The system of curvilinear coordinates determines a family of \( n \) coordinate lines at each point in the region (Fig. A.2).

\[\text{Figure A.2: The smooth trajectory from point } P \text{ to } P_0 \text{ on an arbitrary coordinate line generated by varying one curvilinear coordinate while fixing the rest.}\]

\(^9\) A diffeomorphism is a one-to-one onto map which is smooth and has a smooth inverse.
Definition A.1 (Regular Smooth Coordinate System). In a region $X$, a regular smooth coordinate system is a family of smooth functions $f_i(x_1, x_2, \cdots, x_n)$ determining a bijection map from $X \subset \mathbb{R}^n$ onto a region $U \subset \mathbb{R}^n$, and such that the Jacobian of the map $f : X \to U$ is nonzero at all points of the region.

Lemma A.2. Suppose the Jacobian of a family of smooth functions $f_1(p), f_2(p), \cdots, f_n(p)$ is nonzero at all points of the region. Then for each point there exists an open neighborhood in which these functions determine a regular (local) coordinate system. At the same time, this family of functions may fail to determine the global curvilinear coordinates in the entire region.

A.1.2.2 Contravariant and Covariant Vectors

Although we typically would like to perform our computations on an orthogonal three-dimensional curvilinear coordinate system, physical laws and quantities should be independent of any particular coordinate system. A point on a map should remain invariant under a change of coordinates; we should get the same point whether we use Cartesian or spherical coordinates, for example. Tensors introduce invariant (i.e., coordinate independent) formulation. A good tensor transformation leaves the quantities invariant in either a covariant or contravariant manner (more about this later). Assume we were given a multi-component object with coefficients $v_i, i = 1, 2, \cdots, n$, representing the components in some coordinate system. The coefficients by themselves have no meaning; they only acquire it upon relating them to a certain basis (which spans the coordinate space). Moreover, under a change of coordinate frame, such as rotation or dilation, we must be able to describe the vector in the other coordinate frame. For the vector to properly represent an object, it must remain unchanged under transformation. This means that the components of the vector will transform in a certain way when we apply a coordinate transformation. The concepts of contravariance and covariance essentially describes how would a physical entity change with a change of basis.

Consider an $n$-dimensional manifold with two different frames given by the coordinates $x^1, x^2, \cdots, x^n$ and $u^1, u^2, \cdots, u^n$. Under a change of coordinates, the coordinates are governed by the transformation $f : X \to U$

$$u^i = f_i(x^1, x^2, \cdots, x^n) \quad (A.12)$$

Depending on the transformation, we will have two kind of vectors (i.e., tensor objects of rank-1):-

\[10\] Also called a curvilinear coordinate system.
1. **Contravariant vectors**: Quantities that transform like the coordinate differentials

\[ du^i = \frac{\partial u^i}{\partial x^j} du^j \]  

(A.13)

which we can write by letting \( du^i = v'^i \) and \( du^j = v^j \) as

\[ v'^i = \frac{\partial u^i}{\partial x^j} v^j \]  

(A.14)

or with the use of \( J_j^i = \frac{\partial u^i}{\partial x^j} \) as

\[ v'^i = J_j^i v^j \]  

(A.15)

In general, most of the vectors we deal with are contravariant, with common examples being the displacement vector and any quantity involving its temporal derivative (e.g., velocity, acceleration, force, momentum, etc.) From the transformation rule (A.14), the contravariant components “transform inversely to the old coordinates”. That is, for the contravariant vectors to be independent of the coordinate system, the components of the vector *contra-vary*, and we say the vector components are *contravariant components*. In linear algebra, we represent such vectors by column vectors. The contravariant components are distinguished with superscripts, and using Einstein’s notation, we write

\[ \mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} \leftrightarrow \mathbf{v} = v^i \mathbf{e}_i \]  

(A.16)

where \( \mathbf{e}_i \)'s are the bases vectors.

2. **Covariant vectors**: Quantities that transform like the derivatives of a scalar \( \phi \)

\[ \frac{\partial \phi}{\partial u^i} = \frac{\partial x^j}{\partial u^i} \frac{\partial \phi}{\partial x^j} \]  

(A.17)

which we can write by letting \( v'_i = \frac{\partial \phi}{\partial u^i} \) and \( v_i = \frac{\partial \phi}{\partial x^j} \) as

\[ v'_i = \frac{\partial x^j}{\partial u^i} v^j \]  

(A.18)

---

11. Also called tensors of order (1,0).
12. Assuming no danger of confusion with exponents.
13. Also known as a covectors, dual vectors, tensors of order (0,1), or 1-forms.
14. An object characterized by the identical transformation

\[ \phi'(\mathbf{u}) = \phi(\mathbf{x}) \]

is called a scalar, or a tensor of rank-0, which is invariant with respect to coordinate transformation.
or with the use of \((J^{-1})^j_i = \frac{\partial x^j}{\partial u^i}\) as

\[
v'_i = (J^{-1})^j_i v_j
\]  

(A.19)

An example of a covariant vector is the gradient operator. From the transformation rule (A.18), the covariant components “transform as the old coordinates do”. That is, for the covariant vector to be independent of the coordinate system, the components of the vector \(co-vary\), and we say the vector components are \(co-\)variant components. In linear algebra, we represent such vectors by row vectors. The covariant components are distinguished with subscripts, and using Einstein’s notation, we write

\[
v = \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} \leftrightarrow v = v_i e^i
\]  

(A.20)

where \(e^i\)’s are the dual bases, which is the reciprocal set of standard bases,\(^{15}\) and are only important for nonorthogonal coordinate systems.

When a vector space \(V\) is equipped with an inner product, then for vectors \(v, u \in V\), the dot product is given by\(^{16}\)

\[
v \cdot v = \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = v^j v_i
\]  

(A.22)

Moreover, on this inner product space (also called metric in this context), one can convert a covariant vector into a contravariant vector, and vice versa. Such operations can be accomplished through the use of the so-called metric tensor and one of the fundamental operations for tensors, called contraction.\(^{17}\) The metric tensor can be either contravariant or covariant. For example, multiplying a covariant metric tensor by a contravariant vector

\[^{15}\text{Given three noncoplanar (i.e., not linearly dependent) vectors } A, B \text{ and } C, \text{ the vectors } A’, B’ \text{ and } C’ \text{ given by} \]

\[
A’ = \frac{B \times C}{A \cdot (B \times C)}, \quad B’ = \frac{C \times A}{A \cdot (B \times C)}, \quad C’ = \frac{A \times B}{A \cdot (B \times C)}
\]  

(A.21)

are called the reciprocal set of vectors. The sets satisfy

\[
A’ \cdot A = B’ \cdot B = C’ \cdot C = 1
\]

\[
A’ \cdot B = A’ \cdot C = 0, \quad B’ \cdot A = B’ \cdot C = 0, \quad C’ \cdot A = C’ \cdot B = 0
\]

\[^{16}\text{Those who are familiar with the language of quantum mechanics will notice that contravariant vectors } v^i \text{ are associated with kets } |v\rangle, \text{ while covariant vectors } v_i \text{ are associated with bras } \langle v|. \text{ As such, the dot product is given by } \langle v|v\rangle = v_i v^i. \]

\[^{17}\text{Contraction simply means setting one free index equal to another so that we can perform the sum. For example, the contraction of } v_{ij} \text{ is } v_{i}, \text{ which is just equivalent to multiplying by a Kronecker delta since } v_{ij} \delta_{ij} = v_{i}.\]
and contracting results in a covariant vector

\[ v_i = g_{ij} v^j \]  

(A.23)

Similarly, multiplying a contravariant metric tensor by a covariant vector and contracting results in a contravariant vector

\[ v^i = g^{ij} v_j \]  

(A.24)

The above can be thought as mere operations for “lowering” or “raising” the index. Thus one might suspect that raising and then lowering the index (or the converse) are inverse operations, and it is indeed the case. In fact

\[ g^{ij} g_{jk} = \delta_i^k \]  

(A.25)

\[ g_{kj} g^{ji} = \delta_k^i \]  

(A.26)

where \( \delta_i^k = \delta_k^i \) is the mixed Kronecker delta, a mixed tensor of rank-2.

The concepts introduced above for rank-1 tensors can be easily generalized to tensors of rank \( \geq 2 \). For example, a rank-2 covariant tensor (or two-form) results from the product of two covariant vectors

\[ G'_{ij} = \frac{\partial x^k}{\partial u^i} \frac{\partial x^\ell}{\partial u^j} G_{k\ell} \]

whereas a rank-2 contravariant tensor results from the product of two contravariant vectors

\[ G''_{ij} = \frac{\partial u^i}{\partial x^k} \frac{\partial u^j}{\partial x^\ell} G^{k\ell} \]

Also, in this case we have a mixed tensor

\[ G_j^i = \frac{\partial u^i}{\partial x^k} \frac{\partial x^\ell}{\partial u^j} G_{k\ell}^i \]

From now on, and in addition to Einstein’s summation convention, we conform to the notation of tensor calculus in differentiating between vectors and covectors by using superscripts and subscripts for their components, respectively (with the only exception in denoting coordinates). This distinction is especially important if one is dealing with nonorthogonal coordinate systems or coordinate transformation and mixed tensor analysis.\(^{18}\)

---

\(^{18}\)That is, when dealing with orthogonal coordinates or when there is a fixed coordinate basis, one may omit the distinction of index position and use subscripts for all components.
A.1.3 Skew (Oblique) Curvilinear Coordinates in $\mathbb{R}^3$

Consider the three-dimensional Euclidean space, $\mathbb{R}^3$. The curvilinear coordinates may be derived from a set of Cartesian coordinates by using a locally invertible transformation. Let $f : X \to U$ be a $C^1$ bijective mapping between the open connected regions $X \subset \mathbb{R}^3$ and $U \subset \mathbb{R}^3$ on which we respectively prescribe the Cartesian $(x^1, x^2, x^3)$ and curvilinear $(u^1, u^2, u^3)$ coordinates to a point $P$. A general point $P$ is referred in the two coordinate systems through the bijection

$$u^i = f_i(x^1, x^2, x^3) \leftrightarrow x^i = g_i(u^1, u^2, u^3)$$  \hspace{1cm} (A.27)

where $i = 1, 2, 3$. Automatically, the Jacobi matrix is invertible and the Jacobian is nonvanishing. For the transformation $f : X \to U$, the Jacobi and its inverse are given by

$$J_f(p) = \begin{bmatrix} \frac{\partial f_1}{\partial x^1} & \frac{\partial f_1}{\partial x^2} & \frac{\partial f_1}{\partial x^3} \\ \frac{\partial f_2}{\partial x^1} & \frac{\partial f_2}{\partial x^2} & \frac{\partial f_2}{\partial x^3} \\ \frac{\partial f_3}{\partial x^1} & \frac{\partial f_3}{\partial x^2} & \frac{\partial f_3}{\partial x^3} \end{bmatrix} \leftrightarrow J_f^{-1}(p) = \begin{bmatrix} \frac{\partial x^1}{\partial f_1} & \frac{\partial x^1}{\partial f_2} & \frac{\partial x^1}{\partial f_3} \\ \frac{\partial x^2}{\partial f_1} & \frac{\partial x^2}{\partial f_2} & \frac{\partial x^2}{\partial f_3} \\ \frac{\partial x^3}{\partial f_1} & \frac{\partial x^3}{\partial f_2} & \frac{\partial x^3}{\partial f_3} \end{bmatrix}$$  \hspace{1cm} (A.28)

which is equivalent if someone started from $g : U \to X$\footnote{Equivalent in the sense of (A.9), equipped with (A.27)}.

$$J_g(p) = \begin{bmatrix} \frac{\partial g_1}{\partial u^1} & \frac{\partial g_1}{\partial u^2} & \frac{\partial g_1}{\partial u^3} \\ \frac{\partial g_2}{\partial u^1} & \frac{\partial g_2}{\partial u^2} & \frac{\partial g_2}{\partial u^3} \\ \frac{\partial g_3}{\partial u^1} & \frac{\partial g_3}{\partial u^2} & \frac{\partial g_3}{\partial u^3} \end{bmatrix} \leftrightarrow J_g^{-1}(p) = \begin{bmatrix} \frac{\partial u^1}{\partial g_1} & \frac{\partial u^1}{\partial g_2} & \frac{\partial u^1}{\partial g_3} \\ \frac{\partial u^2}{\partial g_1} & \frac{\partial u^2}{\partial g_2} & \frac{\partial u^2}{\partial g_3} \\ \frac{\partial u^3}{\partial g_1} & \frac{\partial u^3}{\partial g_2} & \frac{\partial u^3}{\partial g_3} \end{bmatrix}$$  \hspace{1cm} (A.29)

Fig. A.3 shows a general three-dimensional curvilinear coordinate system where a point $P$ in a region $U$ is determined by the 3-tuple $(u^1, u^2, u^3)$. The three family of surfaces $u^1 = c_1$, $u^2 = c_2$, and $u^3 = c_3$ are called the coordinate surfaces. Each coordinate surface can be generated by fixing one coordinate and varying the other two. To define a coordinate system, the three surfaces must obviously be noncoplanar. When the surfaces meet at right-angles, the resulting coordinate system is orthogonal, otherwise it is called skew (or oblique). The intersection each pair of these surfaces generates a coordinate line, which is now curved. When the three surfaces intersect, the tangents along the coordinate lines at the point of intersection generates the coordinate axes, which are generally allowed to vary in direction from point to point.\footnote{The exact function expressions can be written only when we know expressions for coordinate surfaces.}
A.1.3.1 Base Vectors

With any coordinate system, one associates coordinate bases for vectors at each point of the space. As mentioned previously, the tangents to the coordinate lines at the point of intersection generally varies in direction from point to point, and thus is a function of position \( \mathbf{r} \). A basis whose vectors vary in magnitude and/or direction from point to point is called a \textbf{local basis}. Basis vectors that are the same at all point are known as \textbf{global bases}, with the obvious example being the standard basis vectors in Cartesian coordinates. All bases associated with a curvilinear coordinate system are necessarily local. Global bases, on the other hand, can be associated only with affine or linear coordinates. In the following, we will consider arbitrary bases where the basis vectors are not necessarily orthogonal nor of unit length (and thus not necessarily global).

With our knowledge of standard bases \( \{\mathbf{e}_i\}_{i=1}^{3} \) in Cartesian coordinates, we would like to define a similar set of basis vectors in the curvilinear coordinate system. In general, a curvilinear coordinate system has two sets of local basis vectors at every point \( P \). The first is the \textbf{covariant basis} (also known as \textbf{tangent basis}) \( \{\mathbf{g}_i\}_{i=1}^{3} \), and is made up by those vectors locally \textit{tangent} to the coordinate curves at the point \( P \). Using this set, we write the position vector in the curvilinear frame as the contravariant vector

\[
\mathbf{r} = u^i \mathbf{g}_i
\]

where \( u^i \)'s are the contravariant components. The second set is the \textbf{contravariant basis} (also known as \textbf{dual basis}, \textbf{covector basis}, or \textbf{cobasis}) \( \{\mathbf{g}^i\}_{i=1}^{3} \), and is made up those vectors locally \textit{normal} to the isosurfaces at a point \( P \). Using this set, we write the
position vector in the curvilinear frame as the covariant vector

$$\mathbf{r} = u_i \mathbf{g}^i$$  \hspace{1cm} (A.31)

where $u_i$'s are the covariant components. The two sets constitutes reciprocal (also known as dual) systems of vectors and have reciprocal units. They become identical in the case of orthogonal coordinates (which is of special interest to us). As stated above, unlike in Cartesian coordinates, in which the standard bases are of fixed direction, it is generally not the case for curvilinear bases. Moreover, the curvilinear bases are generally not of unit length and thus not unit base vectors (they are called unitary base vectors).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figureA.4}
\caption{Curvilinear coordinate system with the associated tangent (covariant) and normal (contravariant) bases.}
\end{figure}

- **Covariant Basis Vectors $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$**

If $\mathbf{r} = x^i \mathbf{e}_i$ is the position vector of a point $P$ in the Cartesian frame, then the standard basis $\{\mathbf{e}_i\}_{i=1}^3$ can be found by taking the derivative of $\mathbf{r} = x^i \mathbf{e}_i$ at the point $P$ with respect to the local coordinates $x^i$

$$\mathbf{e}_i = \frac{\partial \mathbf{r}}{\partial x^i}, \quad i = 1, 2, 3$$  \hspace{1cm} (A.32)

In the curvilinear coordinates frame, the same point $P$ is given by the position vector $\mathbf{r} = u^i \mathbf{g}_i$. Applying the same definition we used for $\{\mathbf{e}_i\}_{i=1}^3$ locally at the point $P$, we
obtain the triple of vectors\(^{21}\)

\[
g_i = \frac{\partial r}{\partial u^i} = \frac{\partial x^j}{\partial u^i} e_j, \quad i = 1, 2, 3
\]  
(A.34)

having the direction of the tangents to the coordinate lines (Fig. A.4). The basis vectors may not be of unit length and may not also be orthogonal.

To gain more insight into the construction of the covariant basis, consider the position vector in the Cartesian coordinates frame, \(r = g_1 (u^1, u^2, u^3) e_1 + g_2 (u^1, u^2, u^3) e_2 + g_3 (u^1, u^2, u^3) e_3\). Let us rewrite the system (A.34) explicitly

\[
g_1 = \frac{\partial g_1}{\partial u^1} e_1 + \frac{\partial g_2}{\partial u^1} e_2 + \frac{\partial g_3}{\partial u^1} e_3
\]  
(A.35)

\[
g_2 = \frac{\partial g_1}{\partial u^2} e_1 + \frac{\partial g_2}{\partial u^2} e_2 + \frac{\partial g_3}{\partial u^2} e_3
\]  
(A.36)

\[
g_3 = \frac{\partial g_1}{\partial u^3} e_1 + \frac{\partial g_2}{\partial u^3} e_2 + \frac{\partial g_3}{\partial u^3} e_3
\]  
(A.37)

Similarly, from (A.32)

\[
e_1 = \frac{\partial u^1}{\partial g_1} b_1 + \frac{\partial u^2}{\partial g_2} b_2 + \frac{\partial u^3}{\partial g_3} b_3
\]

\[
e_2 = \frac{\partial u^1}{\partial g_1} b_1 + \frac{\partial u^2}{\partial g_2} b_2 + \frac{\partial u^3}{\partial g_3} b_3
\]

\[
e_3 = \frac{\partial u^1}{\partial g_1} b_1 + \frac{\partial u^2}{\partial g_2} b_2 + \frac{\partial u^3}{\partial g_3} b_3
\]

The coefficient matrix of the first and second systems are just the transpose of (A.29), the Jacobi of the transformation \(g\), and its inverse, respectively. For the basis to be well-defined at every point \(P\), there must exists one and only one set of basis vectors. This condition is ensured if the system has a unique nontrivial solution, which is equivalent to ensuring that the system is nonsingular (i.e., Jacobian is nonvanishing). Note that we could have derived this directly from the scalar triple product

\[
g_1 \cdot (g_2 \times g_3) = \begin{vmatrix}
  (g_1)_1 & (g_1)_2 & (g_1)_3 \\
  (g_2)_1 & (g_2)_2 & (g_2)_3 \\
  (g_3)_1 & (g_3)_2 & (g_3)_3
\end{vmatrix} = \begin{vmatrix}
  \frac{\partial x^1}{\partial u^1} & \frac{\partial x^2}{\partial u^1} & \frac{\partial x^3}{\partial u^1} \\
  \frac{\partial x^1}{\partial u^2} & \frac{\partial x^2}{\partial u^2} & \frac{\partial x^3}{\partial u^2} \\
  \frac{\partial x^1}{\partial u^3} & \frac{\partial x^2}{\partial u^3} & \frac{\partial x^3}{\partial u^3}
\end{vmatrix} = \det (J_g (p))
\]  
(A.38)

and a nonvanishing Jacobian then ensures that the set of vectors is linearly independent and thus can form a basis.

\(^{21}\)This can also be seen as follows: Just like we related the position vector in both frames through \(r = u^i g_i = x^i e_i\), we can relate the increment of the position vector \(dr\) in both frames by using the definition of total differential to obtain

\[
dr = \frac{\partial r}{\partial u^i} du^i = \frac{\partial r}{\partial x^i} dx^i
\]  
(A.33)
Finally, we assert that unlike the case in Cartesian coordinate in which the standard basis form an orthonormal set
\[ \mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \] (A.39)
it is not necessarily the case for the covariant basis. That is, \( \mathbf{g}_i \cdot \mathbf{g}_j \neq \delta_{ij} \). This is in fact the main motivation for introducing the other contravariant basis vectors, which we discuss next.

- **Contravariant Basis Vectors \( \{\mathbf{g}^1, \mathbf{g}^2, \mathbf{g}^3\} \)**

As mentioned in the introduction, the contravariant basis vectors are normal to the level surfaces (see also A.4), and we thus can define them by using the gradient operator as follows
\[ \mathbf{g}^i = \nabla u^i = \frac{\partial u^i}{\partial x^j} \mathbf{e}_j, \quad i = 1, 2, 3 \] (A.40)

Using the triple scalar product, we find
\[ \mathbf{g}^1 \cdot (\mathbf{g}^2 \times \mathbf{g}^3) = \begin{vmatrix} (\mathbf{g}^1)_1 & (\mathbf{g}^1)_2 & (\mathbf{g}^1)_3 \\ (\mathbf{g}^2)_1 & (\mathbf{g}^2)_2 & (\mathbf{g}^2)_3 \\ (\mathbf{g}^3)_1 & (\mathbf{g}^3)_2 & (\mathbf{g}^3)_3 \end{vmatrix} = \begin{vmatrix} \frac{\partial u^1}{\partial x^1} & \frac{\partial u^1}{\partial x^2} & \frac{\partial u^1}{\partial x^3} \\ \frac{\partial u^2}{\partial x^1} & \frac{\partial u^2}{\partial x^2} & \frac{\partial u^2}{\partial x^3} \\ \frac{\partial u^3}{\partial x^1} & \frac{\partial u^3}{\partial x^2} & \frac{\partial u^3}{\partial x^3} \end{vmatrix} = \det \left( J_{\mathbf{g}}(\mathbf{p})^{-1} \right) = \det \left( J_{\mathbf{f}}(\mathbf{p}) \right) \] (A.41)
which again implies that for the set of vector to be linearly independent (and hence form a basis), the determinant has to be nonzero.

### A.1.3.2 Metric Tensor

From the definition of the covariant (A.34) and contravariant (A.40) bases and the orthonormality condition of the standard basis and its dual (A.20), one can show
\[ \mathbf{g}^i \cdot \mathbf{g}_j = \delta^i_j = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \] (A.42)
where \( \delta^i_j \) is now appropriately called the *mixed Kronecker delta*. The last relation essentially states that each contravariant vector \( \mathbf{g}^i \) is orthogonal to the other two covariant vectors \( \mathbf{g}_j \) (see Fig. A.4); this is the main reason for introducing the contravariant basis.
Just as with the covariant bases, the contravariant bases do not form an orthonormal set, and thus the dot product between the different pairs is nonzero.\(^{22}\) In fact

\[
g_{ij} = g_i \cdot g_j = \frac{\partial x^k}{\partial u^i} \frac{\partial x^k}{\partial u^j} \tag{A.43}
\]

\[
g^{ij} = g^i \cdot g^j = \frac{\partial u^i}{\partial x^k} \frac{\partial u^j}{\partial x^k} \tag{A.44}
\]

are defined as the **metric coefficients**. Since the dot product is commutative, the metric coefficients are symmetric \(g_{ij} = g_{ji}, \ g^{ij} = g^{ji}\). Using the previously developed relations, one can easily show the following properties

\[
g_i = g_{ij} g^j \tag{A.45}
\]

\[
g^i = g^{ij} g_j \tag{A.46}
\]

and

\[
g^{ij} g_{kj} = \delta^i_k = \begin{cases} 1, & i = k \\ 0, & i \neq k \end{cases} \tag{A.47}
\]

The metric coefficients constitute the **metric tensors**\(^{23}\)

\[
G_{ij} = \begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix} \tag{A.48}
\]

\[
G^{ij} = \begin{bmatrix} g^{11} & g^{12} & g^{13} \\ g^{21} & g^{22} & g^{23} \\ g^{31} & g^{32} & g^{33} \end{bmatrix} \tag{A.49}
\]

which we can rewrite by using (A.43) and (A.44) as

\[
G_{ij} = \begin{bmatrix} \frac{\partial x^k}{\partial u^i} \frac{\partial x^k}{\partial u^j} & \frac{\partial x^k}{\partial u^i} \frac{\partial x^k}{\partial x^j} & \frac{\partial x^k}{\partial u^i} \frac{\partial x^k}{\partial x^j} \\ \frac{\partial x^k}{\partial x^i} \frac{\partial x^k}{\partial u^j} & \frac{\partial x^k}{\partial x^i} \frac{\partial x^k}{\partial x^j} & \frac{\partial x^k}{\partial x^i} \frac{\partial x^k}{\partial x^j} \\ \frac{\partial x^k}{\partial x^i} \frac{\partial x^k}{\partial x^j} & \frac{\partial x^k}{\partial x^i} \frac{\partial x^k}{\partial x^j} & \frac{\partial x^k}{\partial x^i} \frac{\partial x^k}{\partial x^j} \end{bmatrix} = \begin{bmatrix} \frac{\partial x^1}{\partial u^1} & \frac{\partial x^1}{\partial u^2} & \frac{\partial x^1}{\partial u^3} \\ \frac{\partial x^2}{\partial u^1} & \frac{\partial x^2}{\partial u^2} & \frac{\partial x^2}{\partial u^3} \\ \frac{\partial x^3}{\partial u^1} & \frac{\partial x^3}{\partial u^2} & \frac{\partial x^3}{\partial u^3} \end{bmatrix}^T \tag{A.50}
\]

\[
G^{ij} = \begin{bmatrix} \frac{\partial u^1}{\partial x^1} \frac{\partial u^1}{\partial x^j} & \frac{\partial u^1}{\partial x^1} \frac{\partial u^2}{\partial x^j} & \frac{\partial u^1}{\partial x^1} \frac{\partial u^3}{\partial x^j} \\ \frac{\partial u^2}{\partial x^1} \frac{\partial u^1}{\partial x^j} & \frac{\partial u^2}{\partial x^1} \frac{\partial u^2}{\partial x^j} & \frac{\partial u^2}{\partial x^1} \frac{\partial u^3}{\partial x^j} \\ \frac{\partial u^3}{\partial x^1} \frac{\partial u^1}{\partial x^j} & \frac{\partial u^3}{\partial x^1} \frac{\partial u^2}{\partial x^j} & \frac{\partial u^3}{\partial x^1} \frac{\partial u^3}{\partial x^j} \end{bmatrix} = \begin{bmatrix} \frac{\partial u^1}{\partial x^1} & \frac{\partial u^1}{\partial x^2} & \frac{\partial u^1}{\partial x^3} \\ \frac{\partial u^2}{\partial x^1} & \frac{\partial u^2}{\partial x^2} & \frac{\partial u^2}{\partial x^3} \\ \frac{\partial u^3}{\partial x^1} & \frac{\partial u^3}{\partial x^2} & \frac{\partial u^3}{\partial x^3} \end{bmatrix} \tag{A.51}
\]

\(^{22}\)Unless in orthogonal coordinate system, which we discuss later.

\(^{23}\)Called *metric* because it determines the square of the length, as will be shown later.
which are nothing but Jacobi’s matrices. Therefore we can compactly define the metric tensors as

\[ G_{ij} = J_g(p)^T J_g(p) \]  

(A.52)

\[ G^{ij} = J_g(p)^{-1} \left( J_g(p)^{-1} \right)^T \]  

(A.53)

which has the determinants

\[ \det(G_{ij}) = \det \left( J_g(p)^T J_g(p) \right) = \det(J_g(p))^2 = G \]  

(A.54)

\[ \det(G^{ij}) = \det \left( J_g(p)^{-1} \left( J_g(p)^{-1} \right)^T \right) = \det \left( J_g(p)^{-1} \right)^2 = \frac{1}{\det(J_g(p))^2} = \frac{1}{G} \]  

(A.55)

that are related by \( G = \det(G_{ij}) = \frac{1}{\det(G^{ij})} \).

### A.1.3.3 Scale Factors

Since the covariant and contravariant base vectors are not of unit length, we can normalize them to obtain the unit bases

\[ \hat{g}_i = \frac{g_i}{|g_i|} = \frac{g_i}{\sqrt{g_{ii}}} \]

\[ \hat{g}^i = \frac{g^i}{|g^i|} = \frac{g^i}{\sqrt{g^{ii}}} \]

The normalizing factors are given special names: The **covariant scale factor** (or just **scale factor**)

\[ h_i = |g_i| = \sqrt{g_{ii}} \quad \text{(no sum)} \]  

(A.56)

and the **contravariant scale factor**

\[ h^i = |g^i| = \sqrt{g^{ii}} \quad \text{(no sum)} \]  

(A.57)

### A.1.3.4 Components of a Vector

Having introduced the two sets of bases, we can write the position vector in two ways; either as a covariant vector

\[ \mathbf{r} = u_i \hat{g}^i = u_i h^i \hat{g}^i = u_i \sqrt{g^{ii}} \hat{g}^i = u_0 \hat{g}^i \]  

(A.58)
that is composed of a covariant component and contravariant basis, or as a contravariant vector

$$\mathbf{r} = u^i \mathbf{g}_i = u^i h_{il} \tilde{\mathbf{g}}_l = u^i \sqrt{g} h_{il} \tilde{\mathbf{g}}_l = u^{(i)} \tilde{\mathbf{g}}_i$$ (A.59)

made up of a contravariant component and a covariant basis. Most importantly, we call $u^{(i)}$ and $u_{(i)}$ the **physical components** of the vector.

The contravariant and covariant components can be related through the metric coefficients

$$u^i = g^{ij} u_j$$ (A.60)
$$u_i = g_{ij} u^j$$ (A.61)

### A.1.3.5 Scalar and Vector Products

Given two vectors $\mathbf{u}$ and $\mathbf{v}$, their dot product can be found as

$$\mathbf{u} \cdot \mathbf{v} = u_i v^i = u^i v_i$$ (A.62)

From the determinant relation (A.54) and the scalar triple products (A.38) and (A.41), we can find

$$G = (g_1 \cdot g_2 \times g_3)^2 = \frac{1}{(g_1 \cdot g_2 \times g_3)^2}$$ (A.63)

Now, with the help of the Levi-Civita permutation symbol (A.5), we can write the triple scalar product as

$$g_i \cdot g_j \times g_k = \varepsilon_{ijk} \sqrt{G}$$ (A.64)

$$g^i \cdot g^j \times g^k = \varepsilon^{ijk} \frac{1}{\sqrt{G}}$$ (A.65)

Moreover, we can show that the cross product of the basis vectors is given by

$$g_i \times g_j = \varepsilon_{ijk} \sqrt{G} g^k$$ (A.66)

$$g^i \times g^j = \varepsilon^{ijk} \frac{1}{\sqrt{G}} g_k$$ (A.67)

which we can use to find the cross product of two vectors as

$$\mathbf{u} \times \mathbf{v} = \sqrt{G} \begin{vmatrix} g^1 & g^2 & g^3 \\ u^1 & u^2 & u^3 \\ v^1 & v^2 & v^3 \end{vmatrix} = \frac{1}{\sqrt{G}} \begin{vmatrix} g_1 & g_2 & g_3 \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix}$$ (A.68)
A.1.3.6 Differential Length, Surface, and Volume Elements

In the curvilinear frame, the position vector \( \mathbf{r} = u^i \mathbf{g}_i \) has the differential displacement \( d\mathbf{r} = du^i \mathbf{g}_i \). We use this incremental displacement to find the square of the differential length element (also known as the metric or fundamental quadratic form of the space), which is the distance between two infinitesimally close points

\[
(d\ell)^2 = d\mathbf{r} \cdot d\mathbf{r} = (du^i \mathbf{g}_i) \cdot (du^j \mathbf{g}_j) = (g_i \cdot g_j) du^i du^j = g_{ij} du^i du^j \tag{A.69}
\]

or

\[
d\ell_i = \sqrt{g_{ij} du^i du^j} \mathbf{g}_i \tag{A.70}
\]

Now consider an infinitesimal surface element. Using the geometrical interpretation of the cross product of the tangent vectors (which are normal to that small surface), we can write

\[
dS_i = |d\mathbf{r}_j \times d\mathbf{r}_k| \tag{A.71}
\]

\[
= |(du^i \mathbf{g}_j) \times (du^k \mathbf{g}_k)| \tag{A.72}
\]

\[
= |\mathbf{g}_j \times \mathbf{g}_k| du^i du^j du^k \tag{A.73}
\]

\[
= \sqrt{(\mathbf{g}_j \times \mathbf{g}_k) \cdot (\mathbf{g}_j \times \mathbf{g}_k)} du^i du^j du^k \tag{A.74}
\]

\[
= \sqrt{(g_j \cdot g_j) (g_k \cdot g_k) - (g_j \cdot g_k) (g_j \cdot g_k)} du^i du^j du^k \tag{A.75}
\]

\[
= \sqrt{G} du^i du^j du^k \tag{A.76}
\]

Hence we obtain

\[
dS_i = \sqrt{G} g^{ij} du^i du^k \mathbf{g}_i \quad \text{(no sum)} \tag{A.77}
\]

where \( i \neq j \neq k \).

Finally, it is well-known that the scalar triple product of three vectors gives the volume of the parallelepiped formed by the three vectors as its sides. Taking the vector components of the differential vector \( d\mathbf{r} \) as the three sides of the skew-angled parallelepiped, we obtain the differential volume

\[
dV = d\mathbf{r}_i \cdot (d\mathbf{r}_j \times d\mathbf{r}_k) \tag{A.78}
\]

\[
= g_i \cdot (\mathbf{g}_j \times \mathbf{g}_k) du^i du^j du^k \tag{A.79}
\]

\[
= \varepsilon_{ijk} \sqrt{G} du^i du^j du^k \tag{A.80}
\]
Hence\textsuperscript{24}
\[dV = \sqrt{G} du^i du^j du^k \quad \text{(no sum)} \quad (A.81)\]
where \(i \neq j \neq k\).

### A.1.4 Orthogonal Curvilinear System in \(\mathbb{R}^3\)

In the case of an orthogonal trihedron of basis vectors, the contravariant and covariant bases become collinear, and we obtain

\[\hat{g}_i = \hat{g}^i \quad (A.82)\]

Thus from now on for orthogonal coordinates we drop all superscripts and use subscripts instead. The unit vectors, though have fixed magnitudes, do not have a fixed direction and can point in different directions from point to point (in contrast to the Cartesian standard basis). Moreover, since the coordinate lines are everywhere orthogonal, the orthogonal trihedron of the unit base vectors satisfy

\[\hat{g}_i \cdot \hat{g}_j = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \quad (A.83)\]

and are always normal to the coordinate surfaces. The last result can be easily used to show that \(h_i = \frac{1}{h_i}, \forall i\). In the orthogonal case, the scale factors \(h_i\) are sometimes called \textbf{Lame’s coefficients}. The fact that \(h_i = \frac{1}{h_i}\) implies that the vectors themselves (not the unit base vectors) are not identical but rather of different magnitudes

\[g_i = h_i \hat{g}_i \quad (A.84)\]
\[g^i = \frac{1}{h_i} \hat{g}^i \quad (A.85)\]

and thus we represent the unit vector as

\[\hat{g}_i = \frac{g_i}{h_i} = h_i g^i \quad (A.86)\]

Then we can use (A.58) or (A.59) (which are now identical) to express the contravariant and covariant components of a vector \(\mathbf{r} = u^i g_i = u_ig^i\) in terms of the physical components

\textsuperscript{24}Notice how the permutation is irrelevant here and thus ignored.
and Lame’s coefficients

\[
\begin{align*}
    u^i &= \frac{u_{(i)}}{h_i} \quad (A.87) \\
    u_i &= h_i u_{(i)} \quad (A.88)
\end{align*}
\]

Using the last results, we obtain the metric coefficients

\[
\begin{align*}
    g_{ij} &= g_i \cdot g_j = h_i h_j (\hat{g}_i \cdot \hat{g}_j) = h_i h_j \delta_{ij} = \begin{cases} 
        h_i^2, & i = i \\
        0, & i \neq j
    \end{cases} \quad (A.89) \\
    g^{ij} &= g^i \cdot g^j = \frac{1}{h_i h_j} (\hat{g}_i \cdot \hat{g}_j) = \frac{1}{h_i h_j} \delta_{ij} = \begin{cases} 
        \frac{1}{h_i^2}, & i = i \\
        0, & i \neq j
    \end{cases} \quad (A.90)
\end{align*}
\]

where the metric tensors \( G_{ij} \) and \( G^{ij} \) become diagonal

\[
G_{ij} = \begin{bmatrix}
    h_1^2 & 0 & 0 \\
    0 & h_2^2 & 0 \\
    0 & 0 & h_3^2
\end{bmatrix} \quad (A.91)
\]

\[
G^{ij} = \begin{bmatrix}
    \frac{1}{h_1^2} & 0 & 0 \\
    0 & \frac{1}{h_2^2} & 0 \\
    0 & 0 & \frac{1}{h_3^2}
\end{bmatrix} \quad (A.92)
\]

and has the determinants

\[
\begin{align*}
    \det (G_{ij}) &= (h_i h_j h_k)^2 = G \quad (A.93) \\
    \det (G^{ij}) &= \frac{1}{(h_i h_j h_k)^2} = \frac{1}{G} \quad (A.94)
\end{align*}
\]

where \( i \neq j \neq k \). Finally, the differential elements become

\[
\begin{align*}
    d\ell &= h_i du_i \hat{g}_i \quad (A.95) \\
    dS_i &= h_j h_k du_j du_k \hat{g}^i \quad \text{(no sum)} \quad (A.96) \\
    dV &= h_i h_j h_k du_i du_j du_k \quad \text{(no sum)} \quad (A.97)
\end{align*}
\]

where again \( i \neq j \neq k \).

### A.1.4.1 The Del-Operator \( \nabla \)

To be able to use vector calculus on a general curvilinear system, one must represent the del (also called nabla) operator in the local basis. The form taken by the operator \( \nabla \)
can be found by defining the gradient $\nabla V$, where $V(u_1, u_2, u_3)$ is a $C^1$ scalar field as the quantity relating the total differentials

$$dV = \nabla V \cdot dr$$  \hspace{1cm} (A.98)

where $dr$ is an arbitrary displacement and $V$ is a scalar. Using the chain rule from multivariable calculus along with both (A.34) and (A.86), we can write

$$\frac{\partial V}{\partial u_i} du_i = \nabla V \cdot (h_i \hat{g}_i du_i)$$  \hspace{1cm} (A.99)

since $u_i$’s are independent. From the orthogonality of basis vectors, one can write

$$\nabla V = \frac{1}{h_i} \frac{\partial V}{\partial u_i} \hat{g}_i$$  \hspace{1cm} (A.100)

allowing us to define the vector differential operator $\nabla$ as

$$\nabla = \frac{1}{h_1} \frac{\partial}{\partial u_1} \hat{g}_1 + \frac{1}{h_2} \frac{\partial}{\partial u_2} \hat{g}_2 + \frac{1}{h_3} \frac{\partial}{\partial u_3} \hat{g}_3$$  \hspace{1cm} (A.101)

or explicitly

$$\nabla = \frac{1}{h_1} \frac{\partial}{\partial u_1} \hat{g}_1 + \frac{1}{h_2} \frac{\partial}{\partial u_2} \hat{g}_2 + \frac{1}{h_3} \frac{\partial}{\partial u_3} \hat{g}_3$$  \hspace{1cm} (A.102)

Now consider a scalar field $V : U \subset \mathbb{R}^3 \to \mathbb{R}$ and a vector field $A : U \subset \mathbb{R}^3 \to \mathbb{R}^3$, both at least $C^1$. Below we find the expressions of typical operations in vector calculus for a general orthogonal curvilinear system.

**Gradient: $\nabla V$**

Expanding the expression of the gradient (A.100), one finds

$$\nabla V = \frac{1}{h_1} \frac{\partial V}{\partial u_1} \hat{g}_1 + \frac{1}{h_2} \frac{\partial V}{\partial u_2} \hat{g}_2 + \frac{1}{h_3} \frac{\partial V}{\partial u_3} \hat{g}_3$$  \hspace{1cm} (A.103)

**Divergence: $\nabla \cdot A$**

Taking the divergence of the vector field $A = A_i \hat{g}_i$

$$\nabla \cdot A = \nabla \cdot (A_i \hat{g}_i) = \nabla \cdot \left( h_j h_k A_i \frac{\hat{g}_i}{h_j h_k} \right)$$  \hspace{1cm} (A.104)

Using the vector identity $\nabla \cdot (V A) = V \nabla \cdot A + A \cdot \nabla V$, we find

$$\nabla \cdot \left( h_j h_k A_i \frac{\hat{g}_i}{h_j h_k} \right) = h_j h_k A_i \nabla \cdot \left( \frac{\hat{g}_i}{h_j h_k} \right) + \frac{\hat{g}_i}{h_j h_k} \cdot \nabla (h_j h_k A_i)$$  \hspace{1cm} (A.105)
But for a right-handed trihedron \( \varepsilon_{ijk} \hat{g}_i = \hat{g}_j \times \hat{g}_k \) and from (A.40), we can rewrite \( \nabla \cdot \left( \frac{\hat{g}_i}{h_j h_k} \right) \) as
\[
\nabla \cdot \left( \frac{\hat{g}_i}{h_j h_k} \right) = \nabla \cdot (\nabla u_j \times \nabla u_k) = 0
\]
where we used the identities \( \nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B}) \) and \( \nabla \times (\nabla V) = 0 \). Thus (A.105) equipped with the definition (A.102) yields
\[
\nabla \cdot \left( h_j h_k A_i \frac{\hat{g}_i}{h_j h_k} \right) = \frac{\hat{g}_i}{h_j h_k} \nabla \left( h_j h_k A_i \right) = \frac{1}{h_i h_j h_k} \frac{\partial}{\partial u_i} (h_j h_k A_i) \frac{\hat{g}_i}{h_j h_k} = \frac{1}{h_i h_j h_k} \frac{\partial}{\partial u_i} (h_j h_k A_i)
\]
(A.106)
where \( i \neq j \neq k \). By explicitly summing the coefficients, we obtain (A.104) in the form
\[
\nabla \cdot \mathbf{A} = \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial}{\partial u_1} (h_2 h_3 A_1) + \frac{\partial}{\partial u_2} (h_3 h_1 A_2) + \frac{\partial}{\partial u_3} (h_1 h_2 A_3) \right]
\]
(A.107)

• **Curl:** \( \nabla \times \mathbf{A} \)

Taking the curl of the vector field \( \mathbf{A} = A_k \hat{g}_k \)
\[
\nabla \times \mathbf{A} = \nabla \times (A_i \hat{g}_k) = \nabla \times \left( h_k A_k \frac{\hat{g}_k}{h_k} \right)
\]
(A.108)
and using the identity \( \nabla \times (\nabla \mathbf{A}) = \nabla \mathbf{V} \times \mathbf{A} + \mathbf{V} \cdot (\nabla \times \mathbf{A}) \), we obtain
\[
\nabla \times \left( h_k A_k \frac{\hat{g}_k}{h_k} \right) = \nabla (h_k A_k) \times \left( \frac{\hat{g}_k}{h_k} \right) + (h_k A_k) \nabla \times \left( \frac{\hat{g}_k}{h_k} \right) = \frac{1}{h_k} \nabla \left( h_k A_k \right) \times \hat{g}_k
\]
(A.109)
where we used the fact that \( \nabla \times \left( \frac{\hat{g}_k}{h_k} \right) = \nabla \times (\nabla u_k) = 0 \). Using the definition of the del operator and the fact that for a right-handed coordinate system \( \varepsilon_{ijk} \hat{g}_i = \hat{g}_j \times \hat{g}_k \), we get
\[
\frac{1}{h_k} \nabla (h_k A_k) \times \hat{g}_k = \frac{1}{h_k} \frac{1}{h_j} \frac{\partial}{\partial u_k} (h_k A_k) (\hat{g}_j \times \hat{g}_k) = \frac{1}{h_k} \frac{1}{h_j} \frac{\partial}{\partial u_k} (h_k A_k) \varepsilon_{ijk} \hat{g}_i = \varepsilon_{ijk} \frac{1}{h_i h_j h_k} \frac{\partial}{\partial u_k} (h_k A_k) \hat{g}_i
\]
(A.110)
which can be casted in a matrix form and thus (A.108) can be written as
\[
\nabla \times \mathbf{A} = \frac{1}{h_1 h_2 h_3} \begin{vmatrix} h_1 \hat{g}_1 & h_2 \hat{g}_2 & h_3 \hat{g}_3 \\ \frac{\partial}{\partial u_1} & \frac{\partial}{\partial u_2} & \frac{\partial}{\partial u_3} \\ h_1 A_1 & h_2 A_2 & h_3 A_3 \end{vmatrix}
\]
(A.111)
• Laplacian: $\nabla^2 V$

By definition, the Laplacian is given by $\nabla^2 V = \nabla \cdot \nabla V$. Thus we can directly make use of the divergence formula (A.107) to obtain the Laplacian, merely by writing $A = A_i \hat{g}_i = \left( \frac{1}{h_i} \frac{\partial V}{\partial u_i} \right) \hat{g}_i$ to obtain

$$\nabla^2 V = \frac{1}{h_1 h_2 h_3} \left[ \frac{\partial}{\partial u_1} \left( \frac{h_2 h_3 \partial V}{h_1} \right) + \frac{\partial}{\partial u_2} \left( \frac{h_3 h_1 \partial V}{h_2} \right) + \frac{\partial}{\partial u_3} \left( \frac{h_1 h_2 \partial V}{h_3} \right) \right]$$

(A.112)

### A.1.4.2 Special Orthogonal Curvilinear Coordinates

We now consider two examples of orthogonal curvilinear coordinate systems. From now on, we denote the unit bases vectors ($\hat{g}_i$ and $\hat{g}^i$) with the symbol $a_{u^i}$, where $u^i$ is the $i$-th curvilinear coordinate.

**Example A.3 (Cylindrical Coordinates).** With reference to Fig. A.5, the cylindrical coordinates $(u^1, u^2, u^3) = (\rho, \phi, z)$ maps a point $P$ to the Cartesian coordinates $(x^1, x^2, x^3) = (x, y, z)$ through the transformation $g : \mathbb{R}^+ \times [0, 2\pi) \times \mathbb{R} \to \mathbb{R}^3$ and its inverse

$$\begin{align*}
\rho &= \sqrt{x^2 + y^2} & x &= \rho \cos \phi \\
\phi &= \tan^{-1} \left( \frac{y}{x} \right) & y &= \rho \sin \phi \\
z &= z & z &= z
\end{align*}$$

(A.113) - (A.115)

![Figure A.5: Cylindrical coordinates system.](image-url)
The Jacobian is given by (A.29)

\[
\det (J_g) = \begin{vmatrix}
\frac{\partial x}{\partial x} & \frac{\partial x}{\partial \phi} & \frac{\partial x}{\partial z} \\
\frac{\partial y}{\partial x} & \frac{\partial y}{\partial \phi} & \frac{\partial y}{\partial z} \\
\frac{\partial z}{\partial x} & \frac{\partial z}{\partial \phi} & \frac{\partial z}{\partial z}
\end{vmatrix} = \frac{1}{\rho} \quad \det (J_g^{-1}) = \begin{vmatrix}
\frac{\partial x}{\partial \phi} & \frac{\partial y}{\partial \phi} & \frac{\partial z}{\partial \phi} \\
\frac{\partial x}{\partial z} & \frac{\partial y}{\partial z} & \frac{\partial z}{\partial z}
\end{vmatrix} = \rho \quad (A.116)
\]

which shows that \( \rho = 0 \) is a singular point of the transformation and this is why we excluded it from the domain of definition above.

The metrics \( g_{11}, g_{22} \) and \( g_{33} \), can be found from (A.43)

\[
g_{11} = (\frac{\partial x}{\partial \rho})^2 + (\frac{\partial y}{\partial \rho})^2 + (\frac{\partial z}{\partial \rho})^2 = 1 \quad (A.117)
\]

\[
g_{22} = (\frac{\partial x}{\partial \phi})^2 + (\frac{\partial y}{\partial \phi})^2 + (\frac{\partial z}{\partial \phi})^2 = \rho^2 \quad (A.118)
\]

\[
g_{33} = (\frac{\partial x}{\partial z})^2 + (\frac{\partial y}{\partial z})^2 + (\frac{\partial z}{\partial z})^2 = 1 \quad (A.119)
\]

and thus from (A.56) we find the following scale factors

\[
h_1 = \sqrt{g_{11}} = 1 \quad (A.120)
\]

\[
h_2 = \sqrt{g_{22}} = \rho \quad (A.121)
\]

\[
h_3 = \sqrt{g_{33}} = 1 \quad (A.122)
\]

The line, surface, and volume elements are given respectively by (A.95), (A.96), and (A.97) as

\[
d\ell = h_1 d\rho a_\rho + h_2 d\phi a_\phi + h_3 d\phi a_z = d\rho a_\rho + \rho d\phi a_\phi + d\phi a_z \quad (A.123)
\]

\[
dS = h_2 h_3 d\phi dz a_\rho = \rho d\phi dz a_\rho \quad (A.124)
\]

\[
h_1 h_3 dp dz a_\phi = dp dz a_\phi
\]

\[
h_1 h_2 dp dz a_z = \rho dp dz a_z
\]

\[
dV = h_1 h_2 h_3 dp \phi dz = \rho dp \phi dz \quad (A.125)
\]
Example A.4 (Spherical Coordinates). With reference to Fig. A.6, the spherical coordinates \((u^1, u^2, u^3) = (r, \theta, \phi)\) maps a point \(P\) to the Cartesian coordinates \((x^1, x^2, x^3) = (x, y, z)\) through the transformation \(g : \mathbb{R}^+ \times [0, \pi] \times [0, 2\pi) \to \mathbb{R}^3\) and its inverse

\[
\begin{align*}
  r &= \sqrt{x^2 + y^2 + z^2} \quad x = r \sin \theta \cos \phi \quad \text{(A.126)} \\
  \theta &= \tan^{-1}\left(\frac{\sqrt{x^2 + y^2}}{z}\right) \quad y = r \sin \theta \sin \phi \quad \text{(A.127)} \\
  \varphi &= \tan^{-1}\left(\frac{y}{x}\right) \quad z = r \cos \theta \quad \text{(A.128)}
\end{align*}
\]

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig_a6.png}
\caption{Spherical coordinates system.}
\end{figure}

The Jacobian is given by (A.29)

\[
\det (J_g) = \begin{vmatrix}
  \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\
  \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\
  \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi}
\end{vmatrix} = \frac{1}{r^2 \sin \theta} \quad \det (J_g^{-1}) = \begin{vmatrix}
  \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} & \frac{\partial z}{\partial r} \\
  \frac{\partial x}{\partial \theta} & \frac{\partial y}{\partial \theta} & \frac{\partial z}{\partial \theta} \\
  \frac{\partial x}{\partial \phi} & \frac{\partial y}{\partial \phi} & \frac{\partial z}{\partial \phi}
\end{vmatrix} = r^2 \sin \theta
\]

which shows that \(r = 0\) is a singular point of the transformation and this is why we excluded it from the domain of definition above.

The metrics \(g_{11}, g_{22}\) and \(g_{33}\) can be found from (A.43)

\[
\begin{align*}
  g_{11} &= \frac{\partial x}{\partial r}^2 + \frac{\partial y}{\partial r}^2 + \frac{\partial z}{\partial r}^2 = 1 \quad \text{(A.129)} \\
  g_{22} &= \frac{\partial x}{\partial \theta}^2 + \frac{\partial y}{\partial \theta}^2 + \frac{\partial z}{\partial \theta}^2 = r^2 \\
  g_{33} &= \frac{\partial x}{\partial \phi}^2 + \frac{\partial y}{\partial \phi}^2 + \frac{\partial z}{\partial \phi}^2 = r^2 \sin^2 \theta \quad \text{(A.131)}
\end{align*}
\]
and thus from (A.56) we find the following scale factors

\[ h_1 = \sqrt{g_{11}} = 1 \]  \hspace{1cm} (A.132)
\[ h_2 = \sqrt{g_{22}} = r \]  \hspace{1cm} (A.133)
\[ h_3 = \sqrt{g_{33}} = r \sin \theta \]  \hspace{1cm} (A.134)

The line, surface, and volume elements are given respectively by (A.95), (A.96), and (A.97) as

\[ d\ell = h_1 dr + h_2 d\theta a_\phi + h_3 d\phi a_\phi = dr a_r + r d\theta a_\theta + r \sin \theta d\phi a_\phi \]  \hspace{1cm} (A.135)
\[ dS = h_2 h_3 dr d\phi a_r = r^2 \sin \theta d\theta d\phi a_r \]  \hspace{1cm} (A.136)
\[ h_1 h_3dr d\phi a_\theta = r \sin \theta dr d\phi a_\theta \]
\[ h_1 h_2 dr d\theta a_\phi = rdr d\theta a_\phi \]
\[ dV = h_1 h_2 h_3 dr d\theta d\phi = r^2 \sin \theta dr d\theta d\phi \]  \hspace{1cm} (A.137)

### A.1.5 Mathematical Theorems and Identities

#### A.1.5.1 Definitions and Theorems

**Theorem A.3** (Stokes’ (or curl) Theorem). Consider a smooth vector field \( \mathbf{A} : X \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3 \) that is \( C^1 \) on a domain \( X \) such that the piecewise smooth surface \( \Sigma \) with boundary \( L \) is completely contained in \( X \). Then we find

\[ \oint_L \mathbf{A} \cdot d\ell = \iint_\Sigma \nabla \times \mathbf{A} \cdot dS \]  \hspace{1cm} (A.138)

where \( dS \) points in the direction of the outward normal to the closed boundary \( \Sigma \) of \( \Omega \).

**Theorem A.4** (Gauss’ (or divergence) Theorem). Consider a vector field \( \mathbf{A} : X \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3 \) that is \( C^1 \) on a domain \( X \) such that the volume \( \Omega \) with piecewise smooth closed boundary \( \Sigma \) is completely contained in \( X \). Then we find

\[ \iiint_\Sigma \mathbf{A} \cdot dS = \iiint_\Omega \nabla \cdot \mathbf{A} dV \]  \hspace{1cm} (A.139)

where \( dS \) points in the direction of the outward normal to the closed boundary \( \Sigma \) of \( \Omega \).

**Theorem A.5** (Gauss’ 1st and 2nd Theorems). Consider the scalar fields \( \phi, \psi : X \subset \mathbb{R}^3 \rightarrow \mathbb{R} \) defined on a domain \( X \) such that the volume \( \Omega \) with piecewise smooth closed boundary \( \Sigma \) is completely contained in \( X \). Then Gauss’ 1st and 2nd theorems are given
respectively by

\[
\iiint_{\Omega} (\phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi) \, dV = \iint_{\Sigma} \phi \nabla \psi \cdot dS \tag{A.140}
\]

\[
\iiint_{\Omega} (\phi \nabla^2 \psi - \psi \nabla^2 \phi) \, dV = \iint_{\Sigma} (\phi \nabla \psi - \psi \nabla \phi) \cdot dS \tag{A.141}
\]

where \(dS\) points in the direction of the outward normal to the closed boundary \(\Sigma\) of \(\Omega\).

**Definition A.6** (Irrotational Field). A vector field \(\mathbf{A} : X \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3\) with \(X\) open is called *irrotational* (or *curl-free*) if

\[
\nabla \times \mathbf{A} = 0 \tag{A.142}
\]

Under this condition, one can express \(\mathbf{A}\) in terms of a scalar field \(V : X \subset \mathbb{R}^3 \rightarrow \mathbb{R}\) as \(\mathbf{A} = -\nabla V\).

**Definition A.7** (Solenoidal Field). A vector field \(\mathbf{A} : X \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3\) with \(X\) open is called *solenoidal* (or *divergence-free*) if

\[
\nabla \cdot \mathbf{A} = 0 \tag{A.143}
\]

Under this condition, one can express \(\mathbf{A}\) in terms of a vector field \(\mathbf{B} : X \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3\) as \(\mathbf{A} = \nabla \times \mathbf{B}\).

### A.1.5.2 List of Vector Identities

For the following, let the vector fields \(\mathbf{A}\) and \(\mathbf{B}\) and the scalar fields \(U\) and \(V\) be sufficiently smooth. For more properties and details, see [66, 166].

**General:**

\[
\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) = \begin{vmatrix} A_x & A_y & A_z \\ B_x & B_y & B_z \\ C_x & C_y & C_z \end{vmatrix} \tag{A.144}
\]

\[
\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) = \mathbf{B} \cdot (\mathbf{C} \times \mathbf{A}) = \mathbf{C} \cdot (\mathbf{A} \times \mathbf{B}) \tag{A.145}
\]

\[
\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B} \cdot (\mathbf{C} \times \mathbf{A}) - \mathbf{C} \cdot (\mathbf{A} \times \mathbf{B}) \tag{A.146}
\]

\[
\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) + \mathbf{B} \times (\mathbf{C} \times \mathbf{A}) + \mathbf{C} \times (\mathbf{A} \times \mathbf{B}) = 0 \tag{A.147}
\]
Gradient:

\[ \nabla (U + V) = \nabla U + \nabla V \]  
(A.148)

\[ \nabla (UV) = U \nabla V + V \nabla U \]  
(A.149)

\[ \nabla \left[ \frac{U}{V} \right] = \frac{V \nabla U - U \nabla V}{V^2} \]  
(A.150)

\[ \nabla V^n = n V^{n-1} \nabla V, \quad n \in \mathbb{Z} \]  
(A.151)

\[ \nabla (A \cdot B) = (A \cdot \nabla) B + (B \cdot \nabla) A + A \times (\nabla \times B) + B \times (\nabla \times A) \]  
(A.152)

Divergence:

\[ \nabla \cdot (A + B) = \nabla \cdot A + \nabla \cdot B \]  
(A.153)

\[ \nabla \cdot (A \times B) = B \cdot (\nabla \times A) - A \cdot (\nabla \times B) \]  
(A.154)

\[ \nabla \cdot (VA) = V \nabla \cdot A + A \cdot \nabla V \]  
(A.155)

\[ \nabla \cdot (\nabla V) = \nabla^2 V \]  
(A.156)

\[ \nabla \cdot (\nabla \times A) = 0 \]  
(A.157)

Curl:

\[ \nabla \times (A + B) = \nabla \times A + \nabla \times B \]  
(A.158)

\[ \nabla \times (A \times B) = A (\nabla \cdot B) - B (\nabla \cdot A) + (B \cdot \nabla) A - (A \cdot \nabla) B \]  
(A.159)

\[ \nabla \times (VA) = \nabla V \times A + V (\nabla \times A) \]  
(A.160)

\[ \nabla \times (\nabla V) = 0 \]  
(A.161)

\[ \nabla \times (\nabla \times A) = \nabla (\nabla \cdot A) - \nabla^2 A \]  
(A.162)

Integral:

\[ \oint_L V d\ell = - \int \oint_{\Sigma} \nabla V \times dS \]  
(A.163)

\[ \int \int_{\Sigma} V dS = \int \int_{\Omega} \nabla V dV \]  
(A.164)

\[ \int \int_{\Sigma} A \times dS = - \int \int_{\Omega} \nabla \times A dV \]  
(A.165)
A.2 Stochastic Differential Equations (SDEs)

Stochastic differential equations (SDEs) can be heuristically defined as those differential equations where the exogenous driving term is a stochastic process, producing solutions that are also stochastic processes. Below, we briefly introduce SDEs. We will typically represent SDEs as first-order differential equations since higher-order equations can almost always be reduced into a system of first-order differential equations by introducing new unknowns. For more in-depth discussion, the reader is referred to [196, 214, 216, 220, 271, 272].

A.2.1 Gaussian Process

Definition A.8 (Gaussian Process). A stochastic process \( X_t \) is a Gaussian process if \((X_{t_1}, X_{t_2}, \ldots, X_{t_n})\) is jointly normally distributed for all \( n \) and every \( 0 \leq t_1 \leq t_2 \leq \ldots \leq t_n \).

If \( X_t \) is a Gaussian process, then it is represented by its mean and variance

\[
\mu = E[X_t] \tag{A.166}
\]
\[
\sigma^2 = E[X_t^2] - E[X_t]^2 \tag{A.167}
\]

A.2.2 Brownian Motion

Brownian motion refers to the mathematical model of the random movement of particles immersed in a fluid (or gas). Such motion was first observed by the biologist Robert Brown in 1828, and later treated statistically in 1905 in the fundamental work of Einstein and Smoluchowski. In 1923, Norbert Wiener rigorously described the stochastic processes of Brownian motion and thus such processes are interchangeably called Wiener process. Wiener process is a Gaussian process, and thus can be completely characterized by the first two moments.

Definition A.9 (Wiener Process as a Gaussian Process). The Wiener process is a Gaussian process with the following mean and covariance

\[
\mu = E[W_t] = 0 \tag{A.168}
\]
\[
\sigma^2 = E[W_t^2] - E[W_t]^2 = t \tag{A.169}
\]
Figure A.7: Sample random walk (or Brownian motion) trajectories in two dimensions.

for all $t \geq 0$. This also implies that the Wiener process has the covariance

$$C(t, s) = E[(W_t - \mu)(W_s - \mu)] = \min(t, s)$$

(A.170)

for all $t, s \geq 0$.

One can formally define a Wiener process as that process possessing the following properties.

**Definition A.10 (Wiener Process).** A stochastic process $W_t : \mathbb{R}^+ \to \mathbb{R}$ is a Wiener process if

1. $W_0 = 0$;

2. With probability 1, it has continuous sample paths $t \to W_t$ for $t \geq 0$ that are nowhere differentiable;

3. The increments $W_t - W_s$ are normally distributed with the following mean and variance

   $$\mu = E[W_t - W_s] = 0$$

   (A.171)

   $$\sigma^2 = E[(W_t - W_s)^2] = t - s$$

   (A.172)

   on $0 \leq s < t$. That is, $W_t - W_s \sim \mathcal{N}(0, t - s)$ for $0 \leq s < t$.

4. The increments are uncorrelated\footnote{Because it is a martingale.} That is

   $$E[(W_{t_1} - W_{s_1})(W_{t_2} - W_{s_2})] = E[W_{t_1} - W_{s_1}] E[W_{t_2} - W_{s_2}] = 0$$

   (A.173)

   when $0 \leq s_2 \leq t_2 \leq s_1 < t_1$. 
Notice that by using property 2. (Gaussian character of the Wiener process) along with property 4., we can restate 4. by saying that the increments are independent. The nondifferentiability of the trajectory paths follows directly from property 3. by noting that

\[
\lim_{t \to s} E \left[ \left( \frac{W_t - W_s}{t - s} \right)^2 \right] = \lim_{t \to s} \frac{1}{(t - s)^2} E \left[ (W_t - W_s)^2 \right] = \infty \quad (A.174)
\]

In fact, as opposed to differentiable functions of time (which are first-order in \( dt \)), for Wiener process

\[
E \left[ dW_t^2 \right] = dt \quad (A.175)
\]

**Definition A.11** (n-dimensional Wiener Process). The vector \( W_t : \mathbb{R}^+ \to \mathbb{R}^n \) is an n-dimensional Wiener process if

1. \( W_t^i \) is a Wiener process, for all \( i = 1, 2, \ldots, n \).
2. \( W_t^i \) are independent Wiener processes, for all \( i = 1, 2, \ldots, n \).

Using the last definition, we can extend (A.175) to an isotropic Wiener process vector

\[
E \left[ dW_t^i dW_t^j \right] = \delta_{ij} dt \quad (A.176)
\]

The reason Wiener process is introduced is that typically SDEs contain a driving Gaussian white noise term that is calculated as the formal derivative of a Wiener process. That is

\[
\eta_t = \frac{dW_t}{dt} \leftrightarrow W_t = \int_0^t \eta_s ds \quad (A.177)
\]

where \( W_t \) is a Wiener process, and \( \eta_t \) is a Gaussian white noise process. Using definition (A.177) along with the properties of a Wiener process and (A.175), one can find

\[
E \left[ \eta_t^2 \right] = 0 \quad (A.178)
\]
\[
E \left[ \eta_t \eta_s \right] = \delta (t - s) \quad (A.179)
\]

or more generally for an isotropic vector white noise \( \eta_t \) by utilizing (A.176)

\[
E \left[ \eta_t^2 \right] = 0 \quad (A.180)
\]
\[
E \left[ \eta_t^i \eta_t^j \right] = \delta_{ij} \delta (t_1 - t_2) \quad (A.181)
\]

Notice from the above definition that the white noise process is stationary.
From a SDE point of view, it is well-known fact that any diffusion process can be expressed in terms of a Wiener process. For example, consider the following SDE

\[
\frac{dX_t}{dt} = a(t, X_t) + b(t, X_t) dW_t
\]  

(A.182)

where the white noise appears as a driving term on the right-hand side. The equation has the obvious problem that the Wiener process is nowhere differentiable (resulting in irregularity in time of the white noise) and thus solving it requires its own rules of calculus.

### A.2.3 A Heuristic Introduction to SDEs

SDEs are usually interpreted in two ways, depending on which calculus on uses; Itô or Stratonovich. Before discussing the two calculi, let us first motivate their introduction by introducing the concept of a stochastic integral. Consider the n-dimensional SDE in the differential form

\[
dX_t = a(t, X_t) dt + B(t, X_t) \eta dt
\]  

(A.183)

where \( X_t \in \mathbb{R}^n \) is the vector of unknowns and \( \eta \in \mathbb{R}^m \) is a delta correlated Gaussian white noise with zero mean. Here, the vector \( a(t, X_t) \in \mathbb{R}^n \) and matrix \( B(t, X_t) \in \mathbb{R}^{n \times m} \) have arbitrary functions as components. The term \( a(t, a_t) dt \) is called the “drift” term, whereas the term \( B(t, X_t) \eta dt \) is called the “noise” term. If the second term is zero, \( X_t \) will be a martingale. In other words, any change in \( E[X_t] \) is actually due to the drift term. That is

\[
\frac{dE[X_t]}{dt} = E[a(t, X_t)]
\]  

(A.184)

The SDE above is not a differential equation in the normal sense since in the classical theory of differential equations one cannot permit discontinuous functions such as \( \eta \).\textsuperscript{26} In fact, the differential form is actually just a pointer, and the equation acquires its meaning when one expresses it in the integral form. Thus the differential form (A.183) is an informal way of representing

\[
X_t - X_{t_0} = \int_{t_0}^{t} a(s, X_s) ds + \int_{t_0}^{t} B(s, X_s) \eta_s ds
\]  

(A.185)

The first integral on the right-hand side is just an ordinary integral, and can be, for example, a Riemann integral, or a Lebesgue integral with respect to the Lebesgue measure (if more generality is desired). The second integral is a stochastic integral, and thus

\footnote{In fact, \( \eta \) cannot even be considered a function in the strictest sense, but rather a generalized function.}
problematic. It is not Riemann integrable since \( \eta \) is unbounded and discontinuous, viz.

\[
\int_{t_0}^{t} B(s, X_s) \eta_s ds = \lim_{n \to \infty} \sum_{k} B(t_k^*, X_{t_k^*}) \eta_{t_k^*} (t_{k+1} - t_k) \quad (A.186)
\]

where \( t_0 < t_1 < \ldots < t_n = t \) and \( t_k^* \in [t_k, t_{k+1}] \), is not convergent. One could also attempt to generalize the Riemann integral by using the Stieltjes integral (by first absorbing \( \eta_s dt \) in \( dW_t \)) so that we can write (A.185) as

\[
X_t - X_{t_0} = \int_{t_0}^{t} a(s, X_s) ds + \int_{t_0}^{t} B(s, X_s) dW_s \quad (A.187)
\]

which in fact motivates our introduction of Wiener processes above (with \( dW/dt = \eta_t \); i.e. the white noise is formally interpreted as the derivative of a Wiener process).\(^{27}\) However, the problem is not solved even after the introduction of Brownian increments since \( W_t \) is no where differentiable and in fact the white noise it represents fluctuates infinitely with infinite variance. That is, the sum in the definition of the Stieltjes (or Lebesgue) integral

\[
\int_{t_0}^{t} B(s, X_s) dW_s = \lim_{n \to \infty} \sum_{k} B(t^*_k, X_{t^*_k}) [W_{t_{k+1}} - W_{t_k}] \quad (A.189)
\]

where \( t_0 < t_1 < \ldots < t_n = t \) and \( t_k^* \in [t_k, t_{k+1}] \), diverges. The problem here is that the limit should be independent of the position of \( t_k^* \) in the interval \([t_k, t_{k+1}]\). The choice of the evaluation point is actually the crux of the so-called “Itô-Stratonovich dilemma” which originated from the second integral on the right-hand side of (A.187) (i.e., the integral of the Wiener process).

Before presenting the calculi needed to solve this issue, we point out that the process \( X_t \) appearing in equation (A.187) has a special name.

**Definition A.12 (Itô Process).** A process \( X_t \) represented as

\[
X_t - X_{t_0} = \int_{t_0}^{t} a(s, X_s) ds + \int_{t_0}^{t} B(s, X_s) dW_s \quad (A.190)
\]

where \( X_t \in \mathbb{R}^n, a(t, X_t) \in \mathbb{R}^n, B(t, X_t) \in \mathbb{R}^{n \times m}, \) and \( W \in \mathbb{R}^m \) is a vector of Wiener processes, is said to be an **Itô process**.

\(^{27}\)Wiener first introduced integrals of the form

\[
\int_{t_0}^{t} b(s) dW_s \quad (A.188)
\]

where \( b(t) \) is a deterministic function and \( W_s \) is a Brownian process. Such integrals are called Wiener integrals. Itô later generalized this to the case where \( b(t) \) is also a random function, giving rise to the so-called stochastic integrals.
A.2.3.1 Itô Calculus

Itô stochastic integral solves the previous problem by choosing the evaluation point as \( t_k^* = t_k \). This choice maintains the Martingale property in that the expectation value of a future event is equivalent to that of the present value in the sub-interval \([t_k, t_{k+1}]\).

With this choice, the Itô integral is defined as the limit

\[
\int_{t_0}^t B(s, X_s) \, dW_s = \lim_{n \to \infty} \sum_k B(t_k, X_{t_k}) \left[ W_{t_{k+1}} - W_{t_k} \right]
\]

which allows us to define the SDE with the following Itô integral equation

\[
X_t - X_{t_0} = \int_{t_0}^t a(s, X_s) \, ds + \int_{t_0}^t B(s, X_s) \, dW_s
\]

Now, if we change the limits to \( t \leftarrow t + dt, t_0 \leftarrow t \) and allow \( dt \) to be small, we can write the integral equation in the differential form

\[
dX_t = a(t, X_t) \, dt + B(t, X_t) \, dW_t
\]

which after dividing by \( dt \) yields the differential equation

\[
\frac{dX_t}{dt} = a(t, X_t) + B(t, X_t) \frac{dW_t}{dt}
\]

in which we can also interpret the white noise as the derivative \( \eta_t = \frac{dW_t}{dt} \).

Now, we present Itô’s Lemma, the cornerstone of the theory of stochastic calculus.

**Theorem A.13 (Itô’s Lemma).** Let \( X_t \) be an \( n \)-dimensional Itô process satisfying the SDE

\[
dX_t = a(t, X_t) \, dt + B(t, X_t) \, dW_t
\]

where \( X_t \in \mathbb{R}^n, a(t, X_t) \in \mathbb{R}^n, B(t, X_t) \in \mathbb{R}^{n \times m}, \) and \( W \in \mathbb{R}^m \) is a vector of Wiener processes. If \( f(t, X_t) : [0, \infty) \times \mathbb{R}^n \to \mathbb{R} \) is an arbitrary \( C^{1,2} \) scalar function and \( Y_t := f(t, X_t) \) then

\[
dF_t = \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial x_j} dX_t^j + \frac{1}{2} \frac{\partial^2 f}{\partial x_i \partial x_j} dX_t^i dX_t^j
\]

\[
= \frac{\partial f}{\partial t} dt + (\nabla f)^T dX_t + \frac{1}{2} \text{tr} \left\{ (\nabla \nabla^T f) \, dX_t dX_t^T \right\}
\]
where the mixed differentials are combined according to the rules

$$dX_t dt = 0 \quad (A.198)$$
$$dt dW_t = 0 \quad (A.199)$$

Itô’s is in essence the Taylor series

$$f(t + dt, X_t + dX_t) = f(t, X_t) + \frac{\partial f(t, X_t)}{\partial t} dt + \frac{\partial f(t, X_t)}{\partial X_i} dX_t^i + \frac{1}{2} \frac{\partial^2 f}{\partial x_i \partial x_j} dX_t^i dX_t^j + \cdots$$

$$f(t + dt, X_t + dX_t) \approx f(t, X_t) + \frac{\partial f(t, X_t)}{\partial t} dt + \frac{\partial f(t, X_t)}{\partial X_i} dX_t^i + \frac{1}{2} \frac{\partial^2 f}{\partial x_i \partial x_j} dX_t^i dX_t^j \quad (A.200)$$

where we retained terms up to first-order in $dt$ and second-order in $dX_t$. Then if we define $dY_t := f(t + dt, X_t + dX_t) - f(t, X_t)$, we obtain

$$dY_t \approx \frac{\partial f(t, X_t)}{\partial t} dt + \frac{\partial f(t, X_t)}{\partial X_i} dX_t^i + \frac{1}{2} \frac{\partial^2 f}{\partial x_i \partial x_j} dX_t^i dX_t^j \quad (A.201)$$

Now, in the deterministic case (ordinary calculus), the second-order terms are zero since $dX_t dX_T$ would be of order $dt^2$ (whereas they would be of order $dt$ in the stochastic case).

The fact that the processes have nonzero quadratic variation and thus do not go away is one main character of stochastic calculus.

As in the classical theory of differential equations, existence and uniqueness are central topics and are usually related to the coefficients appearing in the equation.

**Theorem A.14.** Consider the SDE

$$X_t - X_{t_0} = \int_{t_0}^t a(s, X_s) \, ds + \int_{t_0}^t B(s, X_s) \, dW_s \quad (A.202)$$

If $a_i(t, X_t)$ and $b_{ij}(t, X_t)$ are locally Lipschitz continuous in $X_t$, that is, if $\forall \alpha \in \mathbb{Z}, \exists C_{\alpha}$ and $|t| \leq |\alpha|$,

$$|a_i(t, X_t) - a_i(t, Y_t)| \leq C_{\alpha} |X_t - Y_t|, \forall t \in \mathbb{R}, \forall X_t, Y_t \in \mathbb{R}^n \quad (A.203)$$

$$|b_{ij}(t, X_t) - b_{ij}(t, Y_t)| \leq C_{\alpha} |X_t - Y_t|, \forall t \in \mathbb{R}, \forall X_t, Y_t \in \mathbb{R}^n \quad (A.204)$$

Then $\forall X_{t_0} \in \mathbb{R}^n$, there is at most one solution.

The previous theorem does not guarantee the existence of the solution for all $t$. However, the next theorem gives sufficient conditions.
Theorem A.15. Consider the SDE
\[ X_t - X_{t_0} = \int_{t_0}^{t} a(s, X_s) \, ds + \int_{t_0}^{t} B(s, X_s) \, dW_s \] (A.205)

If \( a_i(t, X_t) \) and \( b_{ij}(t, X_t) \) satisfy the following global Lipschitz continuity and growth conditions for \( C < \infty \)
\[ |a_i(t, X_t) - a_i(t, Y_t)| \leq C |X_t - Y_t|, \quad \forall t \in \mathbb{R}, \forall X_t, Y_t \in \mathbb{R}^n \] (A.206)
\[ |b_{ij}(t, X_t) - b_{ij}(t, Y_t)| \leq C |X_t - Y_t|, \quad \forall t \in \mathbb{R}, \forall X_t, Y_t \in \mathbb{R}^n |t| \leq |\alpha| \] (A.207)
\[ |a_i(t, X_t)| \leq C |X_t|, \quad \forall t \in \mathbb{R}, \forall X_t \in \mathbb{R}^n \] (A.208)
\[ |b_{ij}(t, X_t)| \leq C |X_t|, \quad \forall t \in \mathbb{R}, \forall X_t \in \mathbb{R}^n \] (A.209)

Then \( \forall X_{t_0} \in \mathbb{R}^n \), there is a unique solution.

A.2.3.2 Stratonovich Calculus

In contrast to Itô’s integral, Stratonovich’s integral uses the evaluation point \( t_k^* = \frac{t_k + t_{k+1}}{2} \) (midpoint), which abandons the Martingale property. With this choice, the Stratonovich integral is defined as the limit
\[ \int_{t_0}^{t} B(s, X_s) \circ dW_s = \lim_{n \to \infty} \sum_k B \left( t_k^*, X_{t_k} \right) \left[ W_{t_{k+1}} - dW_{t_k} \right] \] (A.210)

The special choice for the evaluation point makes the chain rule of ordinary calculus valid [220]. The Stratonovich SDE is similar to the Itô SDE but with integrals interpreted in the Stratonovich sense. In general, we distinguish the Stratonovich interpretation with the circle symbol “\( \circ \)” before the Wiener process. The Stratonovich SDE is then written as
\[ dX_t = a(t, X_t) \, dt + B(t, X_t) \circ dW_t \] (A.211)

The disadvantage of Stratonovich’s integral over Itô’s integral is that it is not a martingale (i.e., integrand not independent of integrator) and thus its analysis is harder. The advantage, however, is that Stratonovich’s calculus do not require changing the rules of standard calculus. In general, one can convert between Stratonovich SDE and Itô SDE by using the following theorems.

Theorem A.16 (Conversion from Stratonovich SDE to Itô SDE). If one has the Stratonovich SDE
\[ dX_t = a(t, X_t) \, dt + B(t, X_t) \circ dW_t \] (A.212)
then the Itô SDE is given by

$$dX_t = \tilde{a}(t, X_t) \, dt + B(t, X_t) \, dW_t$$  \hfill (A.213)

where

$$\tilde{a}(t, X_t) = \tilde{a}(t, X_t) + \frac{1}{2} \frac{\partial b_{ij}(t, X_t)}{\partial x_k} b_{kj}(t, X_t)$$  \hfill (A.214)

**Theorem A.17** (Conversion from Itô SDE to Stratonovich SDE). If one has the Itô SDE

$$dX_t = a(t, X_t) \, dt + B(t, X_t) \circ dW_t$$  \hfill (A.215)

then the Stratonovich SDE is given by

$$dX_t = \tilde{a}(t, X_t) \, dt + B(t, X_t) \, dW_t$$  \hfill (A.216)

where

$$\tilde{a}(t, X_t) = \tilde{a}(t, X_t) - \frac{1}{2} \frac{\partial b_{ij}(t, X_t)}{\partial x_k} b_{kj}(t, X_t)$$  \hfill (A.217)

### A.2.4 Langevin Equation

There are many different ways to deal with stochastic processes. SDEs such as Langevin equations are one of the most popular approaches in which the right-hand term of the differential equation is the sum of a deterministic and a random white noise term. A Langevin equation describes the motion of a diffusive particle. A system of Langevin equations is written as

$$\frac{dX_i(t)}{dt} = a_i(t, X_t(t)) + b_{ik}(t, X_t(t)) W^k_t$$  \hfill (A.218)

where the “Langevin” sources $W^k_t$ are independent Gaussian processes satisfying

$$\langle W^i_t \rangle = 0$$  \hfill (A.219)

$$\langle W^i_t W^j_s \rangle = 2D \delta_{ij} \delta(t-s)$$  \hfill (A.220)

where $2D$ is the variance with $D$ being a measure of the noise fluctuation. The noise above is multiplicative, since $b_{ik}$ is a function of $X_t$. If $\partial b_{ik}/\partial X_j = 0$ (i.e., $b_{ik}$’s are constants), the noise is additive and in this case the Itô and Stratonovich calculi coincide and in fact one can use ordinary calculus to treat the problem. Otherwise (i.e., for the multiplicative noise case) one has to interpret the equation in either calculus.
A.2.5 Fokker-Planck Equation

Another equivalent formalism for SDEs is the Fokker-Planck equation. The equation represents the time evolution of the nonequilibrium probability distribution \( p(t, X_t) \) of an Itô process \( X_t \). In the Stratonovich sense the equation is given by

\[
\frac{\partial p}{\partial t} = \frac{\partial}{\partial x_i} \left[ \left( a_i + D b_{jk} \frac{\partial b_{ik}}{\partial x_j} \right) p \right] + \frac{\partial^2}{\partial x_i \partial x_j} \left[ (D b_{ik} b_{jk}) p \right] \tag{A.221}
\]

In the Itô sense, the noise-induced drift coefficient \( D b_{jk} \frac{\partial b_{ik}}{\partial x_j} \) is omitted and one obtains

\[
\frac{\partial p}{\partial t} = - \frac{\partial}{\partial x_i} \left( a_i p \right) + \frac{\partial^2}{\partial x_i \partial x_j} \left[ (D b_{ik} b_{jk}) p \right] \tag{A.222}
\]

By taking the \( x_j \) derivatives on the right-hand side, one can cast the Fokker-Planck equation in the form of continuity equation for the probability distribution

\[
\frac{\partial p}{\partial t} = \frac{\partial}{\partial x_i} \left[ \left( a_i - D b_{ik} \frac{\partial b_{jk}}{\partial x_j} - D b_{ik} b_{jk} \frac{\partial}{\partial x_j} \right) p \right] \tag{A.223}
\]
Appendix B

Multipole Expansion

Current Loop Model
The result (2.81) is merely a special case for planar loops (of any arbitrary shape) carrying uniform stationary currents [166]. To gain more insight and understand the reason behind the assumption of a 'small' current loop, we derive the result for a general current source and deduce (2.81). Moreover, we will derive expressions for the fields produced by the dipoles.

Let us assume we were given an arbitrary current distribution. Then we can use (2.72) to find the magnetic vector potential from which we can find the magnetic field using (2.65). However, most of the time calculations of the vector potential can be complex, and one is usually more interested in the 'dominant' feature of the magnetic field produced by the current distribution and not so much about high-order approximations and fine details. This is especially the case for evaluations at points far away from the source. It is thus instructive to find the fields produced in the far-field approximation.

Consider the localized current distribution in Fig. B.1, with the origin of space coordinates set at some point inside the distribution volume $\Omega$. Let us denote the source position vector by $r'$ and the evaluation point position vector by $r$, and define the separation vector as $R = r - r'$. We can write (2.72c) as [169]

$$A(r) = \frac{\mu_0}{4\pi} \iiint_{\Omega} \frac{J(r') dV'}{|r - r'|} \quad (B.1)$$

To find an approximate expression for far fields $r \gg r'$, we find the multipole expansion of $1/|r - r'|$ and truncate the series. We start by rewriting the term $1/|r - r'|$ as [166]

$$\frac{1}{|r - r'|} = \frac{1}{\sqrt{r'^2 + r'^2 - 2r \cdot r'}} = \frac{1}{r} \frac{1}{\sqrt{1 + (\frac{r'}{r})^2 - \frac{2r'r'}{r^2}}} = \frac{1}{r} \frac{1}{\sqrt{1 + x}} \quad (B.2)$$
where we have set \( x = \left( \frac{r'}{r} \right)^2 - \frac{2rr'}{r^2} = a - b \), with \( a = \left( \frac{r'}{r} \right)^2 \) and \( b = \frac{2rr'}{r^2} = \frac{2r'\cos\theta}{r} \).

Now we expand \( \frac{1}{\sqrt{1 + x}} \) in a Taylor series [166]

\[
\frac{1}{\sqrt{1 + x}} = 1 - \frac{x}{2} + \frac{3x^2}{8} - \frac{5x^3}{16} + \cdots
\]

\[
= 1 - \frac{a - b}{2} + \frac{3(a^2 - 2ab + b^2)}{8} - \frac{5(a^3 - 3a^2b + 3ab^2 - b^3)}{16} + \cdots
\]

\[
\simeq 1 - \frac{a - b}{2} + \frac{3(-2ab + b^2)}{8} - \frac{5(-b^3)}{16} + O \left( \left( \frac{r}{r'} \right)^4 \right)
\]

where we kept terms up to \((r/r')^3\) (octapole order). Dividing by \( r \) and collecting terms of the same order, we obtain [61, 166]

\[
\frac{1}{|r - r'|} \simeq \frac{1}{r} \left[ 1 + \frac{b}{2} + \left( \frac{3b^2}{8} - \frac{a}{2} \right) + \left( \frac{5b^3}{16} - \frac{3ab}{4} \right) + O \left( \left( \frac{r}{r'} \right)^4 \right) \right]
\]

\[
= \frac{1}{r} \left[ 1 + \frac{r \cdot r'}{r'^2} + \left( \frac{3}{2} \frac{r \cdot r'}{r'^2} - \frac{1}{2} \right) \left( \frac{r'}{r} \right)^2 + \frac{5b^3}{16} - \frac{3ab}{4} + O \left( \left( \frac{r}{r'} \right)^4 \right) \right]
\]

\[
= \frac{1}{r} \left[ 1 + \left( \frac{r'}{r} \right) (\cos\theta) + \left( \frac{r'}{r} \right)^2 \left( \frac{3}{2} \cos^2\theta - \frac{1}{2} \right) + \left( \frac{r'}{r} \right)^3 \left( \frac{5}{2} \cos^3\theta - \frac{3}{2} \cos\theta \right) \right] + O \left( \left( \frac{r}{r'} \right)^4 \right)
\]

Recalling Bonnet’s recursion formula for Legendre polynomials

\[
(n + 1) P_{n+1} (u) = (2n + 1) u P_n (u) - n P_{n-1} (u)
\]

with \( P_0 = 1, P_1 = u, P_2 = (3u^2 - 1)/2, P_3 = (5u^3 - 3u)/2 \) where \( u = \cos\theta \), we can, in general, write [166]

\[
\frac{1}{|r - r'|} = \frac{1}{r} \sum_{n=0}^{\infty} \left( \frac{r'}{r} \right)^n P_n (\cos\theta)
\]

Plugging the last relation in (B.1), we obtain [169]
For points far away from the source, we have \( B \). Assume that vectors \( \mathbf{r} \) are small compared to the system size \( \ell \), which is the desired result.

\[
\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \left[ \frac{1}{r} \iiint_{\Omega} \mathbf{J}(\mathbf{r}') \, dV' + \frac{1}{r^2} \iiint_{\Omega} r' \cos \theta \mathbf{J}(\mathbf{r}') \, dV' + \frac{1}{r^3} \iiint_{\Omega} r'^2 \left( \frac{3}{2} \cos^2 \theta - \frac{1}{2} \right) \mathbf{J}(\mathbf{r}') \, dV' + \cdots \right]
\]

\[
= \mathbf{A}(\mathbf{r})_{\text{Monopole}} + \mathbf{A}(\mathbf{r})_{\text{Dipole}} + \mathbf{A}(\mathbf{r})_{\text{Quadrupole}} + \cdots \tag{B.7}
\]

Now, since \( \mathbf{J} \) is solenoidal (i.e., divergenceless) for static conditions and is confined to \( \Omega \), the monopole term vanishes.\(^1\)\(^2\) For points far away from the source, we have \( r'/r \ll 1 \) and thus we can approximate the potential as\(^3\)

\[
\mathbf{A}(\mathbf{r}) \simeq \mathbf{A}(\mathbf{r})_{\text{Dipole}} = \frac{\mu_0}{4\pi} \frac{1}{r^2} \iiint_{\Omega} r' \cos \theta \mathbf{J}(\mathbf{r}') \, dV' = \frac{\mu_0}{4\pi} \frac{1}{r^3} \iiint_{\Omega} (\mathbf{r} \cdot \mathbf{r}') \mathbf{J}(\mathbf{r}') \, dV' \tag{B.8}
\]

However, from the vector identity (A.146), we can write \((\mathbf{r} \cdot \mathbf{r}') \mathbf{J}(\mathbf{r}') = (\mathbf{r} \cdot \mathbf{J}(\mathbf{r}')) \mathbf{r}' - \mathbf{r} \times (\mathbf{r}' \times \mathbf{J}(\mathbf{r}'))\), and thus (B.8) becomes

\[
\mathbf{A}(\mathbf{r}) \simeq \frac{\mu_0}{4\pi} \frac{1}{r^3} \left[ \iiint_{\Omega} (\mathbf{r} \cdot \mathbf{J}(\mathbf{r}')) \mathbf{r}' \, dV' - \mathbf{r} \times \iiint_{\Omega} (\mathbf{r}' \times \mathbf{J}(\mathbf{r}')) \, dV' \right] \tag{B.9}
\]

Consider the \( i \)-th component of the first integral

\[
\iiint_{\Omega} (\mathbf{r} \cdot \mathbf{J}(\mathbf{r}')) \mathbf{r}_i' \, dV' = \sum_{j=1}^{3} \iiint_{\Omega} r_j J_j(\mathbf{r}') \mathbf{r}_i' \, dV' = \sum_{j=1}^{3} r_j \iiint_{\Omega} (\nabla' r_j' \cdot \mathbf{J}(\mathbf{r}')) \mathbf{r}_i' \, dV' \tag{B.10}
\]

where we used the fact that \( \nabla' r_j' = \hat{\mathbf{r}}_j' \). Using the vector identity (A.155), we find 
\( \nabla' \cdot (r_j' \mathbf{J}(\mathbf{r}')) = r_j' \left( \nabla' \cdot \mathbf{J}(\mathbf{r}') \right) + \mathbf{J}(\mathbf{r}') \cdot (\nabla' r_j') \), where we used the fact that \( \mathbf{J} \) is solenoidal under stationary conditions. This allows us to write

\[
\sum_{j=1}^{3} r_j \iiint_{\Omega} \nabla' \cdot (r_j' \mathbf{J}(\mathbf{r}')) \mathbf{r}_i' \, dV' = - \sum_{j=1}^{3} r_j \iiint_{\Omega} r_j' \mathbf{J}(\mathbf{r}') \cdot (\nabla' \mathbf{r}_i') \, dV' = - \iiint_{\Omega} (\mathbf{r} \cdot \mathbf{r}') J_i(\mathbf{r}') \, dV'
\]

\(\text{This is not surprising giving the fact that there are (apparently) no isolated magnetic monopoles. See footnote 52.}\)

\(\text{If this is not obvious, consider the } i \text{-th component of the following integral}\)

\[
0 = \iiint_{\Omega} \mathbf{r} \cdot \nabla \cdot \mathbf{J} \, dV = \iiint_{\Omega} \left[ \nabla \cdot (\mathbf{r} \cdot \mathbf{J}) - \mathbf{J} \cdot \nabla \mathbf{r} \right] \, dV = \iiint_{\Omega} \nabla \cdot (\mathbf{r} \cdot \mathbf{J}) \, dV - \iiint_{\Omega} \mathbf{J} \cdot \nabla \mathbf{r} \, dV
\]

Then from the divergence theorem (A.139) and \( \nabla \mathbf{r}_i = \hat{\mathbf{r}}_i \), we find

\[
\iiint_{\Sigma} (\mathbf{r} \cdot \mathbf{J}) \cdot d\mathbf{S} - \iiint_{\Omega} \mathbf{J} \cdot dV = 0
\]

Since the current is localized (i.e., confined to a finite volume), we can take the surface of integration outside this volume. Taking the surface to infinity (where there are no current densities), we obtain \( \iiint_{\Omega} \mathbf{J} \cdot dV = 0 \) [166]. Generalizing to all three components yields

\[
\iiint_{\Omega} \mathbf{J} \cdot dV = 0
\]

which is the desired result.

\(\text{In condensed matter, this assumption is generally valid whenever } r \gg \ell_s, \text{ where } \ell_s \text{ is the characteristic system size [160].} \)
Generalizing to all three components

\[
\iiint_{\Omega} (\mathbf{r} \cdot \mathbf{J} (\mathbf{r}')) \mathbf{r}' dV' = - \iiint_{\Omega} (\mathbf{r} \cdot \mathbf{r}') \mathbf{J} (\mathbf{r}') dV' \tag{B.11}
\]

Plugging the last expression in (B.9), we finally get

\[
\mathbf{A} (\mathbf{r}) \simeq \frac{\mu_0}{4 \pi} \frac{1}{r^3} \left[ \frac{1}{2} \iiint_{\Omega} (\mathbf{r}' \times \mathbf{J} (\mathbf{r}')) dV' \right] \times \mathbf{r} \equiv \frac{\mu_0}{4 \pi} \frac{\mathbf{m} \times \mathbf{r}}{r^3} \tag{B.12}
\]

where \([61]\)

\[
\mathbf{m} = \frac{1}{2} \iiint_{\Omega} \mathbf{r}' \times \mathbf{J} (\mathbf{r}') dV' \tag{B.13}
\]

is defined as the magnetic dipole of the current distribution. Notice that just like the total charge of a localized electric charge distribution, the magnetic dipole has no spatial dependence.

One may wonder about our choice for the magnetic moment in (B.12). Here is a brief justification. As mentioned at the beginning of 2.2.2.7, the magnetic dipole is typically defined through a torque relation. In the presence of an external field \(\mathbf{B}_{\text{ext}}\), a current element \(\mathbf{J} dV'\) experiences a magnetic force given by (2.78c). Taking the differential of that equation, we obtain \(d \mathbf{F}_m = \mathbf{J} dV' \times \mathbf{B}_{\text{ext}}\). Then the differential magnetic torque is given by \(d \mathbf{\tau}_m = \mathbf{r}' \times d \mathbf{F}_m = \mathbf{r}' \times (\mathbf{J} dV' \times \mathbf{B}_{\text{ext}})\), from which we obtain the total magnetic torque as \(\mathbf{\tau}_m = \iiint_{\Omega} \mathbf{r}' \times (\mathbf{J} \times \mathbf{B}_{\text{ext}}) dV'\), which can be written in the equivalent form

\[
\mathbf{\tau}_m = \frac{1}{2} \iiint_{\Omega} \left[ \mathbf{r}' \times (\mathbf{J} \times \mathbf{B}_{\text{ext}}) + \mathbf{J} \times (\mathbf{r}' \times \mathbf{B}_{\text{ext}}) \right] dV' \\
+ \frac{1}{2} \iiint_{\Omega} \left[ \mathbf{r}' \times (\mathbf{J} \times \mathbf{B}_{\text{ext}}) - \mathbf{J} \times (\mathbf{r}' \times \mathbf{B}_{\text{ext}}) \right] dV' \tag{B.14}
\]

Then by using the vector cyclic identity (A.147) and the anti-commutativity of cross product, we finally obtain

\[
\mathbf{\tau}_m = \frac{1}{2} \iiint_{\Omega} \left[ (\mathbf{r}' \times \mathbf{J}) \times \mathbf{B}_{\text{ext}} \right] dV' = \frac{1}{2} \iiint_{\Omega} \left[ \mathbf{J} \times (\mathbf{r}' \times \mathbf{J}) \right] \times \mathbf{B}_{\text{ext}} \equiv \mathbf{m} \times \mathbf{B}_{\text{ext}} \tag{B.15}
\]

which is conceptually equivalent to the result obtained in electrostatics.

Using the general result (B.13) we will deduce the dipole for planar loops, (2.81). Consider Fig. B.2, which shows a planar loop (taken to be circular here). Using (2.58) in (B.13), we can write

\[
\mathbf{m} = \frac{1}{2} \int_L \mathbf{r}' \times I d\ell \tag{B.16}
\]

From vector analysis, we know that the area of the triangle made by vectors \(\mathbf{A}\) and \(\mathbf{B}\) is given by

\[
|S| = \frac{1}{2} |\mathbf{A} \times \mathbf{B}| \tag{B.17}
\]
Letting $A = r' = r''$ and $B = d\ell$, we obtain the differential area $d\ell$ as $|dS| = \frac{1}{2} |r' \times d\ell|$. Hence we can write (B.16) as a surface integral

$$|m| = I \left| \oint_{\Sigma} dS \right|$$

where we have taken $I$ outside the integral since it is uniform. Since the loop is planar, the dipole moment is perpendicular to the plane of the loop and thus we can write the last integral as

$$m = I \oint_{\Sigma} dS = IS \quad \text{(B.18)}$$

which is the desired result.

![Figure B.2: Current-carrying loop representation of a magnetic dipole.](image)

To find the field produced by the source in the dipolar approximation, we start by taking the curl of (B.12)

$$\mathbf{B}(r) \equiv \nabla \times \mathbf{A}(r) = \frac{\mu_0}{4\pi} \nabla \times \left( m \times \frac{r}{r^3} \right) \quad \text{(B.19)}$$

To that end, we invoke the vector identity (A.160) to obtain

$$\nabla \times \left( m \times \frac{r}{r^3} \right) = m \left( \nabla \cdot \frac{r}{r^3} \right) - \frac{r}{r^3} (\nabla \cdot m) \hat{r} + \left( \frac{r}{r^3} \cdot \nabla \right) m \hat{r} - (m \cdot \nabla) \frac{r}{r^3} = m \left( \nabla \cdot \frac{r}{r^3} \right) - (m \cdot \nabla) \frac{r}{r^3}$$

where we used the fact that $m$ is constant for a give current configuration. Moreover, since $r = \sqrt{x^2 + y^2 + z^2} \neq 0$, we can write

$$\nabla \cdot \left( \frac{r}{r^3} \right) = \frac{\partial}{\partial x} \left( \frac{x}{r^3} \right) + \frac{\partial}{\partial y} \left( \frac{y}{r^3} \right) + \frac{\partial}{\partial z} \left( \frac{z}{r^3} \right) = \left( -\frac{3}{2} \frac{x^2}{r^5} + \frac{1}{r^3} \right) + \left( -\frac{3}{2} \frac{y^2}{r^5} + \frac{1}{r^3} \right) + \left( -\frac{3}{2} \frac{z^2}{r^5} + \frac{1}{r^3} \right) = 0 \quad \text{(B.20)}$$
Also
\[
(m \cdot \nabla) \frac{r}{r^3} = m_x \left[ \frac{\partial}{\partial x} \frac{r}{r^3} \right] + m_y \left[ \frac{\partial}{\partial y} \frac{r}{r^3} \right] + m_z \left[ \frac{\partial}{\partial z} \frac{r}{r^3} \right]
\]
\[
= m_x \left[ \left( \frac{-3}{r^5} + \frac{1}{r^3} \right) a_x - \frac{3}{2} \frac{x^2}{r^5} a_y - \frac{3}{2} \frac{2x y}{r^5} a_z \right] + m_y \left[ \cdots \right] + m_z \left[ \cdots \right]
\]
\[
= -3 \frac{2m_x}{r^3} \mathbf{r} + \frac{m_x}{r^3} a_x - \frac{3m_y}{r^3} \mathbf{r} + \frac{m_y}{r^3} a_y - \frac{3m_z}{r^3} \mathbf{r} + \frac{m_z}{r^3} a_z
\]
\[
= \frac{1}{r^3} [-3 (m \cdot \hat{r}) \hat{r} + \mathbf{m}]
\] (B.21)

Using the last three results in (B.19) yields the important expression of the dipolar field outside the current distribution
\[
\mathbf{B} = \frac{\mu_0}{4\pi} \left[ \frac{3 (\hat{r} \cdot \mathbf{m}) \hat{r} - \mathbf{m}}{r^3} \right]
\] (B.22)

**Magnetic Poles Model**

To derive the dipolar field expression, consider Fig. B.3, which shows two oppositely charged monopoles of magnitude \(Q_m\) centered around the origin with a separation vector \(\ell\).

![Figure B.3: Magnetic poles representation of a magnetic dipole.](image)

Outside the dipole, there are no free currents and thus \(\mathbf{H}\) is irrotational and we can use the results in 2.2.2.4. In particular
\[
\mathbf{H} = -\nabla V_m
\] (B.23)
\[
\nabla^2 V_m = 0
\] (B.24)
We may then define the magnetic scalar potential in the same way as in electrostatics

\[ V_m(r) = C \frac{Q_m}{r} \quad (B.25) \]

where \( C \) is a constant to be determined. From the principle of superposition, the potential at point \( P \) is the sum of both potentials

\[ V_m(r) = CQ_m \left[ \frac{1}{r_1} - \frac{1}{r_2} \right] \quad (B.26) \]

where \( r_1 \) and \( r_2 \) are the distances between \( P \) and \(+Q_m\) and \(-Q_m\), respectively. Now, we try to find expressions in terms of \( \ell \) and the angle \( \theta \). The law of cosines (Fig. B.4) allows us to write

\[
\begin{align*}
r_1 &= \sqrt{r^2 + \left( \frac{\ell}{2} \right)^2 - 2r \left( \frac{\ell}{2} \right) \cos \theta} = r \sqrt{1 + \frac{\ell^2}{4r^2} - \frac{\ell}{r} \cos \theta} = r \sqrt{1 + x_1} \quad (B.27) \\
r_2 &= \sqrt{r^2 + \left( \frac{\ell}{2} \right)^2 - 2r \left( \frac{\ell}{2} \right) \cos (\pi - \theta)} = r \sqrt{1 + \frac{\ell^2}{4r^2} + \frac{\ell}{r} \cos \theta} = r \sqrt{1 + x_2} \quad (B.28)
\end{align*}
\]

where \( x_1 = \frac{\ell^2}{4r^2} - \frac{\ell}{r} \cos \theta \) and \( x_2 = \frac{\ell^2}{4r^2} + \frac{\ell}{r} \cos \theta \). Then (B.26) becomes

\[ V_m(r) = C \frac{Q_m}{r} \left[ \frac{1}{\sqrt{1 + x_1}} - \frac{1}{\sqrt{1 + x_2}} \right] \quad (B.29) \]

**Figure B.4:** The law of cosines for calculating one side of a triangle when the opposite angle and the other two sides are known.

Since we are mostly interested in far field behavior, we will try to approximate the results and arrive at a simpler expression. One way is to use the Binomial expansion

\[ (1 + x)^n = 1 + nx + \frac{n(n - 1)}{2} x^2 + \frac{n(n - 1)(n - 2)}{6} x^3 + \cdots \quad (B.30) \]

which converges for \( n < 0 \) if \( |x| < 1 \). The series can then be truncated for very small value of \( x \) to obtain

\[ (1 + x)^n \approx 1 + nx \quad (B.31) \]
Using the last relation in (B.29) with \( n = -1/2 \)

\[
V_m(r) = C \frac{Q_m}{r} \left[ \left( 1 - \frac{1}{2} x_1 \right) - \left( 1 - \frac{1}{2} x_2 \right) \right]
\]

\[
= C \frac{Q_m}{r} \left[ \frac{1}{2} (x_2 - x_1) \right]
\]

\[
= C \frac{Q_m}{r} \left[ \frac{1}{2} \left( \frac{\ell^2}{Ar^2} + \frac{\ell}{r} \cos \theta - \frac{\ell^2}{Ar^2} + \frac{\ell}{r} \cos \theta \right) \right]
\]

\[
= C \frac{Q_m}{r} \left[ \frac{\ell}{r} \cos \theta \right]
\]

\[
= C \frac{Q_m \ell \cos \theta}{r^2}
\]

(B.32)

Since \( \ell \cos \theta = \ell \cdot a_r = \ell \cdot (r/r) \), we can rewrite the last result as

\[
V_m(r) = C \frac{Q_m \ell \cdot r}{r^3} = C \frac{m \cdot r}{r^3}
\]

(B.33)

where

\[
m = Q_m \ell
\]

is defined as the magnetic dipole. Using the scalar potential expression (B.33) along with (B.23) and (2.60), we can show that

\[
\mathbf{B} = -\mu_0 \nabla \left( C \frac{m \cdot r}{r^3} \right) = -\mu_0 C \frac{3 (\hat{r} \cdot m) \hat{r} - m}{r^3}
\]

(B.35)

which is consistent with (B.22) if and only if \( C = \frac{1}{4\pi} \). Under this choice we obtain the scalar potential\(^4\)

\[
V_m(r) = \frac{m \cdot r}{4\pi r^3}
\]

(B.36)

which we can use along with both (B.23) and (2.60) to find the dipolar field

\[
\mathbf{B} = \frac{\mu_0}{4\pi} \left[ \frac{3 (\hat{r} \cdot m) \hat{r} - m}{r^3} \right]
\]

(B.37)

Before concluding this appendix, we point a subtle issue concerning the interior fields. By looking at the expression of the dipolar fields (B.22) and (B.37), one might conclude that both models are identical. However, one should not jump to such conclusions so fast as the expressions give the dipolar fields outside the dipoles, and not everywhere. Looking at the current loop model (Fig. 2.15a), the field lines internal to the dipole point in the same direction as those external to it. However, for the magnetic poles (Fig. 2.15b), the field lines between the magnetic poles point in the opposite direction as those outside. Apparently there is a discrepancy, and in contrast to the expression of the external fields,

\(^4\)It can be easily shown that it indeed satisfies Laplace’s equation (2.64).
those for the internal region has to be different. In fact, in both expressions, $r = 0$ is a
singularity of the field, and there will be an ambiguity in interpreting the result at that
point. It can be shown (see [166, 169]) that for the current loop model, the true dipolar
field is given by

$$B = \frac{\mu_0}{4\pi} \left[ \frac{3 (\mathbf{\hat{r}} \cdot \mathbf{m}) \mathbf{\hat{r}} - \mathbf{m}}{r^3} + \frac{8\pi}{3} \mathbf{m} \delta (r) \right]$$

(B.38)

whereas for the magnetic poles model

$$B = \frac{\mu_0}{4\pi} \left[ \frac{3 (\mathbf{\hat{r}} \cdot \mathbf{m}) \mathbf{\hat{r}} - \mathbf{m}}{r^3} - \frac{4\pi}{3} \mathbf{m} \delta (r) \right]$$

(B.39)
Appendix C

Box-Muller Transform

Computer generated random numbers are crucial elements in computer simulations and they occur in many applications including stochastic physical processes, protecting private messages (cryptography), finance, or even video games. Almost all random number generation on computers is done using algorithms to produce a stream of numbers from $\mathcal{U}(0, 1)$, i.e. from a uniform distribution on the interval $(0, 1)$. However, in many physical processes, one might need to generate random numbers with Gaussian (normal) distribution. Although one could use some approximate methods based on the Central Limit Theorem (CLT) [216] to approximate the normal distribution $\mathcal{N}(0, 1)$, it is better to resort for more accurate and computationally-efficient methods. Box-Muller transform [273] provides an efficient algorithm to generate Gaussian pseudo-random numbers\(^1\) given a source of uniform pseudo-random numbers. It is a brilliant method to overcome the difficulty that arises when using the inverse transform sampling, i.e. when trying to invert the distribution function to obtain a normal distribution from a standard uniform

$$F(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-x'^2/2} \, dx'$$

(C.1)

which has no closed form. Box-Muller transform solves this by producing a two-dimensional bivariate normal distribution from a two-dimensional uniform distribution. It is based on the premise that, given a distribution function, one can use the fundamental transformation law of probabilities [274] to obtain a transformation function for the distributions, i.e. a transformation that maps the random numbers from distribution to the other (Fig. C.1).

\(^1\)In reality, most random numbers used in computer programs are pseudo-random, which means they are generated in a predictable fashion using a mathematical formula.
Let $X$ be a random variable with a random deviate $x \in \mathbb{R}$ whose probability density is $p_X(x)$, and let $f : X \to Y$ by a map such that another random variable $Y$ is given by

$$Y = f(X) \quad \text{(C.2)}$$

The fundamental transformation law of probabilities yields

$$|p_Y(y) dy| = |p_X(x) dx| \quad \text{(C.3)}$$

or

$$p_Y(y) = p_X(x) \left| \frac{dx}{dy} \right| \quad \text{(C.4)}$$

which is the desired probability density of $y$.

The idea above can be generalized to more than one dimension. In particular, in two dimensions, one has the two-dimensional random variable $X = (X_1, X_2)$, having the random deviates $x = (x_1, x_2) \in \mathbb{R}^2$, whose probability density is given by $p_X(x)$. If another random variable is given by the transformation $f : X \to Y$, viz.

$$Y_1 = f_1(X_1, X_2) \quad \text{(C.5)}$$

$$Y_2 = f_2(X_1, X_2) \quad \text{(C.6)}$$
obeying
\[ \begin{align*}
    dy_1 &= df_1(x_1, x_2) = \frac{\partial f_1}{\partial x_1} dx_1 + \frac{\partial f_1}{\partial x_2} dx_2 \\
    dy_2 &= df_2(x_1, x_2) = \frac{\partial f_2}{\partial x_1} dx_1 + \frac{\partial f_2}{\partial x_2} dx_2
\end{align*} \] (C.7)

then fundamental transformation law of probabilities yields
\[ \begin{align*}
    |p_X(y_1, y_2) dy_1 dy_2| &= |p_X(x_1, x_2) dx_1 dx_2| \\
    p_Y(y_1, y_2) &= p_X(x_1, x_2) dx_1 dx_2 \frac{dy_1 dy_2}{dy_1 dy_2}
\end{align*} \] (C.9)

or
\[ \begin{align*}
    p_Y(y_1, y_2) &= p_X(x_1, x_2) \\
 \end{align*} \] (C.10)

which is the desired joint probability density of \( y \). The volume elements in the two-dimensional space given above are related by
\[ dy_1 dy_2 = \det (J_f) dx_1 dx_2, \]
where \( J_f \) is the Jacobi of the map \( f : \mathbf{X} \rightarrow \mathbf{Y} \) given by
\[ J_f = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} \] (C.11)

Now, consider the two uniform deviates \( x_1, x_2 \in \mathcal{U}(0,1) \) and the transformations
\[ \begin{align*}
    y_1 &= \sqrt{-2 \ln x_1} \cos (2\pi x_2) \\
    y_2 &= \sqrt{-2 \ln x_1} \sin (2\pi x_2)
\end{align*} \] (C.12, C.13)

To find the Jacobian, we start by calculating the partial derivatives
\[ \begin{align*}
    \frac{\partial f_1}{\partial x_1} &= \frac{-1}{x_1 \sqrt{-2 \ln x_1}} \cos (2\pi x_2), \quad \frac{\partial f_1}{\partial x_2} = -2\pi \sqrt{-2 \ln x_1} \sin (2\pi x_2) \\
    \frac{\partial f_2}{\partial x_1} &= \frac{-1}{x_1 \sqrt{-2 \ln x_1}} \sin (2\pi x_2), \quad \frac{\partial f_2}{\partial x_2} = -2\pi \sqrt{-2 \ln x_1} \cos (2\pi x_2)
\end{align*} \] (C.14, C.15)

which yields the Jacobian
\[ \det (J_f) = \det \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = 2\pi e^{-\frac{y_1^2+y_2^2}{2}} \] (C.16)

Now, on the basis of the fundamental transformation law of probabilities, one has to consider the inverse of the Jacobian, viz.
\[ \frac{1}{\det (J_f)} = \frac{1}{2\pi e^{-\frac{y_1^2+y_2^2}{2}}} = \frac{1}{2\pi} e^{-\frac{(y_1^2+y_2^2)}{2}} = \frac{1}{\sqrt{2\pi}} e^{-\frac{y_1^2}{2}} \frac{1}{\sqrt{2\pi}} e^{-\frac{y_2^2}{2}} \] (C.17)
which clearly shows (in one-dimension) that $y_1$ and $y_2$ are \textit{independently} distributed according to the normal distribution.
LIST OF SUBMITTED PUBLICATIONS


[277] Andrew D. Kent. Spins dynamics in nanomagnets.


