Scattering of near-zero-energy electrons and positrons by H₂

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The parameters for S-wave elastic scattering of near-zero-energy electrons and positrons by H₂ molecules are calculated using the stabilization method with explicitly correlated Gaussians. The confined variational method is applied to optimize the Gaussians to describe the short-range interaction of incident e± with H₂ in the fixed-nuclei approximation. For e±-H₂ scattering the scattering length is substantially improved. More importantly, for e- -H₂ scattering, from first principles, the scattering length is computed as a function of the internuclear distance. In the case that the two nuclei are at the equilibrium distance the results are in a good agreement with values derived from fitting experimental total and diffusion cross sections to the modified effective range theory.

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I. INTRODUCTION

The scattering of e± from H₂ is of fundamental interest and has been the subject of intensive theoretical and experimental investigations for decades [1–23]. Due to the dual-center nature of molecular H₂, theoretical calculations for the low-energy e± scattering are much more challenging than for the scattering by He atoms. Hence there exist few well-converged first-principles calculations, even for H₂ in the fixed-nuclei approximation. In the case of low-energy scattering, the incident e± can interact with the target for a relatively long period of time before moving away. Therefore, the scattering depends significantly on the complicated correlation interaction with the target.

In this work, the low-energy e±-H₂ scattering is studied using the stabilization method [24,25] in the fixed-nuclei approximation. Explicitly correlated Gaussians (ECGs) [26–28] are chosen as basis functions, which have the advantage that the Hamiltonian matrix elements of the scattering system can be evaluated analytically. To improve the description of the complicated short-range interaction, the confined variational method is adopted to optimize the ECGs. The idea of adding a confining potential to the Hamiltonian previously has been used to study e± and positronium scattering [29–32]. For the e+ -H₂ scattering, the scattering lengths of previous ECG calculations [32] can be significantly improved by larger basis sets, by optimizing the energy of the lowest pseudostate for each confined system rather than optimizing the mean energy of the lowest two pseudostates, and by taking into account the polarization correction. For the e- -H₂ scattering, our present scattering length of 1.24a₀ is in good agreement with the values obtained by the modified effective range theory (MERT), A_{scat} = 1.27 ± 0.01a₀ [33,34], 1.29a₀ [35], and 1.30a₀ [23].

II. THEORY AND COMPUTATIONAL METHOD

Atomic units are used throughout this paper. The Hamiltonian for e±-H₂ scattering is

\[ H = -\sum_{i=1}^{3} \frac{V_i^2}{2} + \sum_{j>i=1}^{3} \frac{q_i q_j}{|\mathbf{r}_j - \mathbf{r}_i|} + \sum_{i=1}^{3} \left\{ \frac{q_i}{|\mathbf{r}_i - \mathbf{R}/2|} + \frac{q_i}{|\mathbf{r}_i + \mathbf{R}/2|} \right\} \]

where \( \mathbf{r}_i \) is the coordinate of the i-th light particle (electron or positron) relative to the midpoint of the internuclear axis, \( q_i \) is the corresponding charge, and ±\( \mathbf{R}/2 \) represents the displacement of the two protons, respectively, from the midpoint. The basis functions for the interaction region have the form

\[ \phi_k = \hat{P} \exp \left( -\frac{1}{2} \sum_{i=1}^{3} b_{k,i} |\mathbf{r}_i - \mathbf{S}_{k,i}|^2 \right) \times \exp \left( -\frac{1}{2} \sum_{i=1}^{3} \sum_{j=i+1}^{3} a_{k,ij} |\mathbf{r}_i - \mathbf{r}_j|^2 \right). \]

The vector \( \mathbf{S}_{k,i} \) displaces the center of the ECG for the i-th particle to a point on the internuclear axis, ensuring that the wave function is of \( \Sigma \) symmetry. The operator \( \hat{P} \) forces the wave function to have \( \Sigma \) symmetry. Each ECG has a total of nine parameters \( a_{k,ij}, b_{k,i}, \) and \( \mathbf{S}_{k,i} \), which are adjusted in the optimization process.

To improve the description of correlations between the incident e± and molecular electrons, a confining potential \( W_{CP}(r_i) \) for each lepton is added in the Hamiltonian, given by

\[ W_{CP}(r_i) = 0, \quad r_i < R_0, \]

\[ W_{CP}(r_i) = G(r_i - R_0)^2, \quad r_i \geq R_0, \]

where \( G \) is a small positive number, 1.55 \times 10^{-4} for e+ scattering and 6.0 \times 10^{-5} for the e- scattering. Moreover,
TABLE I. Convergence of calculations for the Σg e±H₂ system at R = 1.4a₀ with respect to the number of ECGs. Results for R = 1.45a₀, calculations by other groups, and experimental measurements are included. Energies Eₙₜₐₖ, wave numbers k, and scattering lengths Aₜₐₖ are given in atomic units.

<table>
<thead>
<tr>
<th>Nᵢₙₜₑᵢᵦ + Nₑᵡₜₑᵢᵦ</th>
<th>Eₙₜₐₖ</th>
<th>k</th>
<th>Aₜₐₖ</th>
<th>Aₜₐₖ⊥</th>
<th>Zₑᵩ</th>
<th>Zₑᵩ⊥</th>
</tr>
</thead>
<tbody>
<tr>
<td>600 + 36</td>
<td>−1.16946817</td>
<td>0.635577 × 10⁻²</td>
<td>−2.508</td>
<td>−2.763</td>
<td>14.37</td>
<td>14.59</td>
</tr>
<tr>
<td>1000 + 36</td>
<td>−1.16947050</td>
<td>0.635547 × 10⁻²</td>
<td>−2.496</td>
<td>−2.771</td>
<td>14.65</td>
<td>14.87</td>
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<tr>
<td>1400 + 36</td>
<td>−1.16947207</td>
<td>0.635530 × 10⁻²</td>
<td>−2.478</td>
<td>−2.793</td>
<td>14.62</td>
<td>14.88</td>
</tr>
<tr>
<td>2600 + 36</td>
<td>−1.16947222</td>
<td>0.635511 × 10⁻²</td>
<td>−2.450</td>
<td>−2.809</td>
<td>14.66</td>
<td>14.95</td>
</tr>
<tr>
<td>Mean value</td>
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<td>14.80</td>
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<tr>
<td>Stabilization: ECG [32]</td>
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<td>0.635551 × 10⁻²</td>
<td>−2.53</td>
<td>−2.63</td>
<td>14.74</td>
<td>14.83</td>
</tr>
<tr>
<td>Kohn: ECG [40]</td>
<td>−2.565</td>
<td>14.61</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kohn: Method of models [12,42,48]</td>
<td>−2.2</td>
<td>12.6</td>
<td></td>
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<tr>
<td>Kohn: Method of models [42]</td>
<td>0.01</td>
<td>13.5</td>
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<tr>
<td>1600 + 36</td>
<td>−1.16908917</td>
<td>0.635264 × 10⁻²</td>
<td>−2.594</td>
<td>−2.982</td>
<td>15.67</td>
<td>16.00</td>
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<tr>
<td>Mean value</td>
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<td>15.80</td>
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</tr>
<tr>
<td>Kohn: ECG [40]</td>
<td>−2.709</td>
<td>15.70</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>MERT fit [23,44]</td>
<td>−2.51</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>MERT fit [23,45]</td>
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<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>Experiment, k ≈ 0.045a₀⁻¹, R ≈ 1.448a₀ [7]</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>14.7(2)</td>
</tr>
<tr>
<td>Experiment, k ≈ 0.045a₀⁻¹, R ≈ 1.448a₀ [13]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>14.61(14)</td>
</tr>
<tr>
<td>Experiment, k ≈ 0.045a₀⁻¹, R ≈ 1.448a₀ [8]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>16.02(08)</td>
</tr>
</tbody>
</table>

R₀ must be larger than the interaction region in order to avoid disturbing the interaction between e± and target. We use R₀ = 18a₀ for all calculations presented in this article. By applying the confining potential, the continuum state problem is converted into a problem of discrete energy levels. Therefore, the basis set for the short-range interaction is optimized by minimizing the lowest energy of the confined system by the stochastic variational method [28,36,37].

To enlarge the basis, we merge several basis sets, each being well optimized for a specific interatomic distance. For e±H₂ scattering, for example, the basis sets for R = 1.4 and 1.6a₀ are merged to form the basis set of the interaction region for R = 1.4a₀. As compared to e±H₂ scattering, for e±H₂ scattering the optimization of the inner basis functions is much more time-consuming and difficult. Besides the more complicated permutation symmetry, the main reason is that the near-linear dependence frequently occurs when the size of the basis set is larger than 800. We again merge several well-optimized basis sets for different interatomic distances. For example, the basis set of the interaction region for R = 1.4a₀ is composed of the basis sets for R = 1.4, 1.6, and 1.8a₀. For some values of R the Schrödinger equation for the confined system cannot be solved with the merged basis set. However, in most cases a solution is possible when the confining potential is excluded. By adding a certain number of basis functions each time and trying to solve the Schrödinger equation without confining potential, we determine which basis functions cause the near-linear dependence. After a successful solution, we obtain the corresponding eigenenergies and eigenwave functions, which are orthonormalized to each other. The lowest eigenenergy, which is higher than the ground-state energy of fixed-nuclei H₂, becomes lower when the number of basis functions increases. Otherwise, the near-linear dependence occurs and the basis functions added in the last step must be removed. In addition, the quality of the finally selected inner basis functions is confirmed for mutual consistency by the convergence of the scattering parameters (see Tables I and II).

For scattering at very low energy, the convergence of the scattering parameters can be improved by including exterior basis sets to describe the asymptotic region, which are given by products of H₂ wave functions and Gaussians,

\[ \psi_{\text{outer}} = \psi_{\text{H}^2}(r_1, r_2) \exp \left(-\frac{1}{2} \alpha_r r_2^2 \right). \]  

(5)

The H₂ wave functions for different distances R are represented by linear combinations of 100 or 120 ECGs. For example, the calculated ground-state energy of H₂ for R = 1.40a₀ is −1.174475 54 hartree using a basis set of 120 ECGs, i.e., only 1.7 × 10⁻⁷ hartree higher than the close-to-exact value −1.174475 71 hartree [38]. The Gaussians are introduced to represent the asymptotic behavior of the incident particle. Moreover, \( \{\alpha_r\} \) is an even tempered set given by the relation \( \alpha_i = \alpha_1 / T^{i-1} \) with \( \alpha_1 = 18.59 \) and \( T = 1.435 \). A total of 36 long-range functions is added to each interaction region basis set.

The Hamiltonian matrices (excluding the confining potential) are constructed with both inner and exterior basis functions. Diagonalization leads to a set of eigenenergies and wave functions. In the stabilization method [24,25] eigenwave functions with positive energy are reasonable approximations to the exact scattering wave functions. The phase shifts are derived by a least-squares fit to the overlap of the target wave function and the wave function of the e±H₂ scattering. The overlap function

\[ C(r_3) = \int d^3 r_1 d^3 r_2 \psi_{\text{H}^2}(r_1, r_2) \psi(r_1, r_2, r_3) \]  

(6)

depends on the distance \( r_3 \) of the incident e± from the internuclear midpoint and the angle \( \theta_3 \) with respect to the internuclear axis.
TABLE II. Convergence of the calculations for the $\Sigma_g$ $e^+\cdot H_2$ system at $R = 1.4a_0$ with respect to the number of ECGs. Energies $E_{N\text{scat}}$, wave numbers $k$, and scattering lengths $A_{\text{scat}}$ are given in atomic units.

<table>
<thead>
<tr>
<th>$N_{\text{inner}} + N_{\text{outer}}$</th>
<th>$E_{N\text{scat}}$</th>
<th>$k$</th>
<th>$A_{\text{scat},\parallel}$</th>
<th>$A_{\text{scat},\perp}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000 + 36</td>
<td>$-1.16943034$</td>
<td>$0.640734 \times 10^{-2}$</td>
<td>1.161</td>
<td>1.333</td>
</tr>
<tr>
<td>1500 + 36</td>
<td>$-1.16943511$</td>
<td>$0.640723 \times 10^{-2}$</td>
<td>1.149</td>
<td>1.338</td>
</tr>
<tr>
<td>2000 + 36</td>
<td>$-1.16943541$</td>
<td>$0.640715 \times 10^{-2}$</td>
<td>1.124</td>
<td>1.353</td>
</tr>
<tr>
<td>2500 + 36</td>
<td>$-1.16943560$</td>
<td>$0.640712 \times 10^{-2}$</td>
<td>1.118</td>
<td>1.355</td>
</tr>
<tr>
<td>Mean value</td>
<td></td>
<td></td>
<td>1.24</td>
<td></td>
</tr>
<tr>
<td>MERT fit by Fedus and co-workers</td>
<td></td>
<td></td>
<td>1.30</td>
<td></td>
</tr>
<tr>
<td>MERT fit by Chang</td>
<td></td>
<td></td>
<td>1.27 ± 0.01</td>
<td></td>
</tr>
<tr>
<td>MERT fit by Fabrikant</td>
<td></td>
<td></td>
<td>1.29</td>
<td></td>
</tr>
</tbody>
</table>

During the scattering the $e^\pm$ experiences a long-range potential of which the dominating part is given by

$$V_{LR}(r_3) = -\frac{\alpha}{2r_3} - \frac{\alpha_2}{2r_3^3} P_2(\cos \theta_3) - \frac{Q}{2r_3^3} P_2(\cos \theta_3),$$

(7)

where $\alpha$ and $\alpha_2$ are the isotropic and anisotropic polarizabilities of $H_2$, respectively [34]. $P_2(\cos \theta_3)$ is a Legendre polynomial of order two and the third term represents the quadrupole potential, $Q$ being the quadrupole moment of $H_2$. For the scattering of near-zero-energy electrons on ground-state $H_2$ the $S$-wave elastic scattering dominates, while other channels as well as channel coupling effects of the orientation-dependent part of the long-range potential are negligible [39]. Thus the fixed-nuclei approximation is reasonable. The effect of isotropic potential on the phase shifts is taken into account by integrating the asymptotic form $B(\theta_3) \sin[k(r_1 + \delta_1(\theta_3))]$ of the wave functions inward to the inner boundaries of the least-squares fits, which are made over the interval $[R_1, R_2]$ at fixed values of $\theta_3$. The value of $R_1$ should be sufficiently large for the projectile and target wave functions to have minimal overlap, typically $R_1 = 15a_0$ for few-electron atomic and molecular targets. The value of $R_2$ should ensure that the probability density of the particle remains a reasonable fraction (e.g., 20%) of the peak probability density, typically $R_2 = 25$ to $30a_0$. In this work we chose $R_1 = 18a_0$ and $R_2 = 30a_0$. For the $e^+\cdot H_2$ scattering the positrons may annihilate with the electrons of $H_2$ to create photons. The annihilation parameter $Z_{\text{eff}}$, which represents the effective number of electrons available for annihilation, is determined by the normalization constant $B(\theta_3)$.

### III. RESULTS AND DISCUSSION

#### A. Near-zero-energy positron scattering from $H_2$

Table I addresses the convergence of the calculations for the $\Sigma_g$ $e^+\cdot H_2$ system at $R = 1.4a_0$ as a function of the number of ECGs, $N_{\text{inner}} + N_{\text{outer}}$, where $N_{\text{inner}}$ is the number of inner region basis functions and $N_{\text{outer}}$ is the number of outer region basis functions. The energy of the lowest state in the confining potential is given by the $E_{N\text{scat}}$ column. The wave number $k$ (in $a_0^{-1}$) refers to the lowest-energy pseudostate when the entire basis is diagonalized without confinement potential. $A_{\text{scat}}$ (in $a_0$) and $Z_{\text{eff}}$ are derived from the wave-function projections parallel ($\parallel$) and perpendicular ($\perp$) to the internuclear axis. While we optimize the basis sets for the inner region by minimizing the energy of the lowest pseudostate, in previous ECG calculations [32,40] the mean energy of the two lowest pseudostates has been minimized during the optimization. In addition, since the size of the present basis sets is larger and the polarization effect of $H_2$ is taken into account, improved results can be expected.

As the number of basis functions increases, $E_{N\text{scat}}$, $k$, $A_{\text{scat}}$, and $Z_{\text{eff}}$ change monotonically; see Table I. The inner basis set is optimized for $R = 1.4a_0$ up to a size of 1400. For calculating the scattering parameters with the stabilization method 1200 basis functions optimized for $R = 1.6a_0$ are added, which improves the results by about 0.5% to 1% though the corresponding $E_{N\text{scat}}$ is just slightly lower than for 1400 basis functions. As compared to the previous ECG calculation in Ref. [32], our $A_{\text{scat},\parallel}$ is 3% larger and our $A_{\text{scat},\perp}$ is 7% smaller. As expected, the difference between these two quantities grows when the number of basis functions increases. Armour and co-workers have obtained $A_{\text{scat}}$ and $Z_{\text{eff}}$ by the Kohn variational method [41–43]. Their phase shift for $k = 0.01a_0^{-1}$ gives a scattering length of $-2.56a_0$ [42]. Fedus and co-workers have obtained MERT scattering lengths of $-2.51a_0$ and $-3.13a_0$ [23] by fitting the experimental data of Hoffmann and co-workers [44] and Karwasz and co-workers [45], respectively. The fit values are close to the limits of our $A_{\text{scat},\parallel}$ and $A_{\text{scat},\perp}$ for $R = 1.45a_0$ (i.e., almost the equilibrium distance 1.448$a_0$). The experimental $Z_{\text{eff}} = 14.7$ [7], 16.02 [8],

![FIG. 1. (Color online) Scattering length $A_{\text{scat}}$ as a function of the angle $\theta_3$ for $e^+\cdot H_2$ scattering.](https://example.com/figure1.png)
FIG. 2. (Color online) Annihilation parameter $Z_{\text{eff}}$ as a function of the angle $\theta_3$ for $e^+\text{-H}_2$ scattering.

and 14.61 [13] are included in Table I for comparison, showing reasonable agreement with the theoretical results. As pointed out earlier [32], the variation among the experimental values is probably related to different densities of the H$_2$ gas [8].

Figures 1 and 2 present for $e^+\text{-H}_2$ scattering the scattering length $A_{\text{scat}}$ and annihilation parameter $Z_{\text{eff}}$ as a function of the angle $\theta_3$, respectively, for different values of $R$. Due to the symmetry plane passing through the center-of-mass of the molecule perpendicular to the molecular axis, the values for $\theta_3$ and $\pi - \theta_3$ are the same and we can restrict the plots to the range $0 \leq \theta_3 \leq \pi/2$. Corresponding plots of $A_{\text{scat}}$ and $Z_{\text{eff}}$ as a function of the internuclear distance $R$ are given in Figs. 3 and 4, respectively, separately for $\theta_3 = 0$ and $\theta_3 = \pi/2$. The minimum in the scattering length around $R \approx 3.4a_0$ indicates the formation of a virtual state [32,46]. The effect of the polarization on the scattering length lies within a range of 1% to 5% for $1a_0 \leq R \leq 4a_0$. For $R = 1.4a_0$, for example, it is 3.0%. Since $A_{\text{scat},||}$ and $A_{\text{scat},\perp}$ for the same $R$ deviate by not more than 13% throughout all calculations, the near-zero energy $e^+\text{-H}_2$ scattering can be approximately described by a system of spherical symmetry.

B. Near-zero-energy electron scattering from H$_2$

Table II addresses the convergence of the calculations for the $\Sigma_g^- e^-\text{-H}_2$ system for $R = 1.4a_0$ as a function of the number of ECGs. For an increasing number of short-range basis functions $A_{\text{scat},||}$ decreases while $A_{\text{scat},\perp}$ increases monotonically. For low-energy electron scattering by nonpolar molecules, the total and diffusion cross sections can be approximately expressed as a function of the wave number $k$. The fitting parameters include the scattering length $A_{\text{scat}}$, which largely depends on the short-range interaction. By fitting the experimental diffusion cross sections of Crompton and co-workers [3], Chang found $A_{\text{scat}} = 1.27 \pm 0.01a_0$ [33,34].

FIG. 3. (Color online) Scattering length $A_{\text{scat}}$ as a function of the internuclear distance $R$ for $e^+\text{-H}_2$ scattering.

FIG. 4. (Color online) Annihilation parameter $Z_{\text{eff}}$ as a function of the internuclear distance $R$ for $e^+\text{-H}_2$ scattering. The experimental values are those from Table I.

FIG. 5. (Color online) Scattering length $A_{\text{scat}}$ as a function of the angle $\theta_3$ for $e^-\text{-H}_2$ scattering.
and Fabrikant estimated $A_{\text{scat}} = 1.29 a_0$ [35]. The small difference is mainly due to the fact that Chang determined the isotropic part of the polarizability as $\alpha = 5.4 \pm 0.1 a_0^2$, whereas Fabrikant used $\alpha = 5.18 a_0^2$. Fedus and co-workers obtained $A_{\text{scat}} = 1.30 a_0$ and $\alpha = 5.314 a_0^2$ [47]. All three MERT values of $A_{\text{scat}}$ are within the range of our $A_{\text{scat}|\parallel}$ and $A_{\text{scat}|\perp}$.

Figure 5 presents for $e^{-}\text{H}_2$ scattering the scattering length $A_{\text{scat}}$ as a function of the angle $\theta$. The difference between $R = 1.4$ and $1.45 a_0$ is less than 0.5%, whereas for $e^{-}\text{H}_2$ scattering this difference is about 6.0%. According to Fig. 5, the mean scattering length is $1.24 a_0$, in agreement with the accurate MERT values within 3% to 4% [23,34,35]. Since the size of the optimized basis set for the $e^{-}\text{H}_2$ system (1400) is much larger than that for the $e^{-}\text{H}_2$ system (1000), it is likely that the accuracy of our calculations in the former case is better than 4%. This indicates that the uncertainty of the experimental scattering lengths is large. Figure 6 gives $A_{\text{scat}|\parallel}$ and $A_{\text{scat}|\perp}$ as functions of the internuclear distance $R$. As compared to the $e^{+}\text{H}_2$ scattering, the effect of polarization is much larger for the $e^{-}\text{H}_2$ scattering. The polarization correction lies within a range of 8% to 35% for $1.4 a_0 \leq R \leq 3.6 a_0$. For $R = 1.4 a_0$, for example, it is 8.5%. Since the convergence is slower for $A_{\text{scat}|\parallel}$ than for $A_{\text{scat}|\perp}$ for each $R$ when the number of basis functions increases, we expect that $A_{\text{scat}|\perp}$ is less accurate, especially for large $R$. In addition, it is less accurate for large $R$ than for small $R$. $A_{\text{scat}|\perp}$ shows a tendency to decrease when $R$ increases, reaching a minimum at $R = 3.2 a_0$. On the other hand, $A_{\text{scat}|\perp}$ increases slightly for increasing $R$, with a maximum at $R = 3.2 a_0$.

IV. CONCLUSION

To conclude, the near-zero-energy $e^{\pm}\text{H}_2$ scattering has been studied by the stabilization method with ECGs. For $e^{+}\text{H}_2$ scattering, the presented results are significantly more accurate than previous ECG calculations [32,40], as well as Kohn variational calculations [41,43]. The results of $A_{\text{scat}}$ agree with MERT values. In addition, the obtained values for $Z_{\text{eff}}$ are compatible with the experiment. In particular, the success of the $e^{+}\text{H}_2$ calculations testifies the potential of merged basis sets for different distances $R$. This strategy also turns out to be very useful for $e^{-}\text{H}_2$ scattering, as it avoids near-linear dependencies for increasing basis size. Our results represent a first principles determination of the scattering length without model potentials. The calculated mean scattering length at $R = 1.45 a_0$ shows good agreement with MERT values [23,34,35].

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