Zero- and negative-energy solutions of the coupled *T*-matrix equations: Application to positronium-hydrogen singlet scattering

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Analytical and numerical schemes to solve the coupled-channel *T*-matrix equations at zero and negative energies are presented and the methodology is applied to the Ps-H system. Using a recent approach of potential simulation technique inside the *T*-Matrix method, improved predictions on the scattering length ($3.89a_0$) has been made by reproducing the binding energy (1.067 eV) from direct solutions of the *T*-matrix equations at zero and negative energies, respectively.

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I. INTRODUCTION

In practice, the coupled-channel scattering *T*-matrix equations are solved at nonzero positive energies and the informations on the scattering length and any possible projectile-target bound state are made using the effective-range expansion of the positive-energy phase shifts to zero and negative energies, respectively [1]. In our previous studies [2–4], we also applied the same procedure and predicted the scattering length and binding energy for the Ps-H system. However, the binding energy of PsH is quite large (-1.066 eV) [5–9] and thus the effective-range expansion mentioned above may not be a suitable procedure and could lead to procedural error [10].

Nevertheless, it is possible to solve the *T*-matrix equations at zero and negative energies and predict the scattering length and binding energy directly from the solutions. In this work, we present the details of solving the coupled-channel *T*-matrix equations at negative and zero energies and apply the formulation to the Ps-H singlet scattering.

Ore [11] first predicted that the singlet channel of PsH can form a chemically stable bound state with a binding energy of 1.066 eV. Drachman and Houston [12,13] predicted that the system can possess an *S*-wave resonance in the singlet channel at 4.45 eV; the binding energy and the scattering length in their calculation were 0.672 eV and $5.33a_0$ (see also Ref. [10]). Using a similar basis set to that of DH but including explicit electron-electron correlation terms, Ho [14,15] found the *S*-wave resonance energy to converge to 4.01 eV and the binding energy to converge to 1.05 eV. Later on, Yan and Ho [7] improved these variational predictions further and arrived at 4.006 eV for the resonance and 1.0666 eV for the binding. Among other predictions for the binding energy, Frolov and Smith [5] obtained a value of 1.065 eV while Usukura *et al.* [6] obtained 1.0666 eV. Later, considering relativistic effect, Yan and Ho [8] found the binding energy to reduce to 1.064 eV. These calculations, particularly those of Ho [14] and Yan and Ho [7], demonstrate that if the theory is converged, PsH might give rise to a binding energy ~ 1.066 eV and *S*-wave resonance energy ~ 4.0 eV. However, these calculations do not address the scattering length (a^+). In recent variational calculations, Adhikari and Mandal [16] obtained $3.45a_0$ while Ivanov *et al.* [17,18] obtained $4.34a_0$ for a^+. Using an *R* matrix, Blackwood *et al.* [19,20] obtained a scattering length of $4.41a_0$ and found that it is accompanied by a binding energy of 0.994 eV and a resonance energy of 4.31 eV. The binding and resonance of the *R*-matrix calculation indicate that the theory is yet to be fully converged and that the scattering length of $4.3a_0$ or $4.4a_0$ could converge further.

Here, we improve upon previous works [2–4] by (1) solving the coupled *T*-matrix equations at zero and negative energies (instead of using the effective-range expansion) so that the results reveal the correct values for the model and (2) addressing the convergence pattern of the potential simulated *T*-matrix formalism (PSTMF) [21]. In PSTMF, effectively an adjustable model exchange-correlation potential is added to the input potential of the *T*-matrix equation, which is then fixed through the simulation of the solution to some precisely known physical parameter. Once the potential is optimized, other scattering parameters are calculated. Convergence of the model is tested by repeating the procedure with addition of channels. In our calculation, we find an *S*-wave resonance energy of 4.06 eV and a singlet scattering length of $3.89a_0$, when the *T*-matrix pole (corresponding to binding) is simulated in between $E=-1.066$ eV to 1.067 eV.

II. THEORY

In a coupled-channel formalism the space part of the total wave function of the Ps (χ_ν) and H (ϕ_μ) system is expanded as

$$\Psi^{\pm}(\mathbf{x},\mathbf{r}_1,\mathbf{r}_2)=\sum_{\mu}\sum_{\nu}\{F_{\mu\nu}(\mathbf{s}_1)\chi_\nu(\mathbf{t}_1)\phi_\mu(\mathbf{r}_2) \pm F_{\mu\nu}(\mathbf{s}_2)\chi_\nu(\mathbf{t}_2)\phi_\mu(\mathbf{r}_1)\}, \quad (1)$$

where $\mathbf{x}$ is the positron coordinate; $\mathbf{r}_1$, $\mathbf{r}_2$ are the electron coordinates; $\mathbf{s}_i=(\mathbf{r}_i+\mathbf{x})/2$, $\mathbf{t}_i=(\mathbf{r}_i-\mathbf{x})$; $i=1,2$. $F_{\mu\nu}$ is the motion of the moving positronium. The corresponding spin-averaged *T*-matrix equations are represented as [22–24]

$$f^{\pm}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k})=\mathcal{B}^{\pm}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k})-\frac{1}{2\pi^2}\sum_{\nu''}\sum_{\mu''}\int d\mathbf{k}'' \times\frac{\mathcal{B}^{\pm}_{\mu'\nu',\mu''\nu''}(\mathbf{k}',\mathbf{k}'')f^{\pm}_{\mu''\nu'',\mu\nu}(\mathbf{k}'',\mathbf{k})}{k^2_{\nu''\mu''}-k''^2+i0}. \quad (2)$$

Here, $k^2_{\nu''\mu''}=2m/\hbar^2\{E-\epsilon_{\nu''}-\mathcal{E}_{\mu''}\}$; $\mathbf{k}_{\nu''\mu''}$, $\mathbf{k}$, and $\mathbf{k}'$ are on-shell momenta and $\mathbf{k}''$ is off-shell momentum. m is the mass of Ps. E is the total energy of the system; $\epsilon_{\nu''}$, $\mathcal{E}_{\mu''}$, represent the binding energies of Ps and H, respectively. $\mathcal{B}^{\pm}$ are the spin-averaged input potentials to the coupled equations for the singlet $(+)$ and triplet $(-)$ channels and are given by

$$\mathcal{B}^{\pm}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k})=B^{d}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k})\pm B^{e}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k}), \quad (3)$$

B^d and B^e correspond to the Born amplitudes for the direct and exchange transitions, respectively. B^d can be recast exactly as [25,26]

$$B^{d}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k})=-\frac{4}{q^2}\int \chi_{\nu'}(\mathbf{t}_1)(e^{i\mathbf{q}\cdot\mathbf{t}_1/2}-e^{-i\mathbf{q}\cdot\mathbf{t}_1/2})\chi_{\nu}(\mathbf{t}_1) \times d\mathbf{t}_1\int \phi_{\mu'}(\mathbf{r}_2)e^{i\mathbf{q}\cdot\mathbf{r}_2}\phi_{\mu}(\mathbf{r}_2)d\mathbf{r}_2, \quad (4)$$

where $\mathbf{q}=\mathbf{k}-\mathbf{k}'$. Expression (4) is arrived at giving a transformation $\{\mathbf{x},\mathbf{r}_1\}\rightarrow\{\mathbf{s}_1,\mathbf{t}_1\}$ to the Born amplitude and integrating the resulting expression over d^3s_1. B^e, the exchange potential, has an exact form as follows:

$$B^{e}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k})=-\frac{1}{\pi}\int e^{i\mathbf{k}'\cdot\mathbf{s}_2}\chi_{\nu'}(\mathbf{t}_2)\phi_{\mu'}(\mathbf{r}_1)[H'_0-H_0 + V']e^{i\mathbf{k}\cdot\mathbf{s}_1}\chi_{\nu}(\mathbf{t}_1)\phi_{\mu}(\mathbf{r}_2)d\mathbf{x}d\mathbf{r}_1d\mathbf{r}_2, \quad (5)$$

where V' is the interaction potential between Ps and H in the primed $(\mu'\nu')$ channel; H_0 and H'_0 are the unperturbed Hamiltonians in the initial and the primed channel [27]. For simulation purposes, B^e is taken as [2–4]

$$B^{e}_{\mu'\nu',\mu\nu}(\mathbf{k}',\mathbf{k})=\frac{4}{\langle D\rangle}\int \chi_{\nu'}(\mathbf{t}_1)e^{i\mathbf{q}\cdot\mathbf{t}_1/2}\chi_{\nu}(\mathbf{t}_1)d\mathbf{t}_1 \times\int \phi_{\mu'}(\mathbf{r}_2)e^{i\mathbf{q}\cdot\mathbf{r}_2}\phi_{\mu}(\mathbf{r}_2)d\mathbf{r}_2, \quad (6)$$

where $\langle D\rangle=(k^2+k'^2)/8+C[(\alpha^2_{\mu'}+\alpha^2_{\mu})/2+(\beta^2_{\nu'}+\beta^2_{\nu})/2]$; with α^2_{μ} corresponding to the square of the momentum eigenvalue of the electron in the μth state H atom and β^2_{ν} is the same for the electron in the νth state Ps atom. C is the parameter that is varied to simulate the potential so that the T-matrix solution fits with some known physical parameter (here Ps-H binding energy).

To recast the T-matrix equations (2) into one-dimensional partial-wave form, suitable to solve numerically at zero incident energy, we take the following partial-wave expansion:

$$f^{\pm}_{n'l'm_{l'},nlm_l}(\mathbf{k}',\mathbf{k})=\sum_J\sum_M\sum_L\sum_{M_L}\sum_{L'}\sum_{M_{L'}} \times\langle L'l',M_{L'}m_{l'}|JM\rangle Y^{*}_{L'M_{L'}}(\hat{\mathbf{k}}') \times\langle Ll,M_Lm_l|JM\rangle Y_{LM_L}(\hat{\mathbf{k}}) \times\bar{f}^{\pm}_J(n'l'L'k',nlLk), \quad (7)$$

which differs from our earlier expansion [2,27] by a factor of $1/\sqrt{kk'}$, and recast Eq. (2) as

$$\bar{f}^{\pm}_J(\tau',k';\tau,k)=\bar{\mathcal{B}}^{\pm}_J(\tau',k';\tau k)-\frac{1}{2\pi^2}\sum_{\tau''}\int dk''k''^2 \times\frac{\bar{\mathcal{B}}^{\pm}_J(\tau',k';\tau'',k'')\bar{f}^{\pm}_J(\tau'',k'';\tau,k)}{k^2_{\tau''}-k''^2+i0}. \quad (8)$$

For elastic channel and zero incident energy, k''^2 cancels out in the Kernel and the equation reduces to

$$\bar{f}^{\pm}_J(\tau',k';\tau,k)=\bar{\mathcal{B}}^{\pm}_J(\tau',k';\tau k)-\frac{1}{2\pi^2}\sum_{\tau''} \times\int dk''\bar{\mathcal{B}}^{\pm}_J(\tau',k';\tau'',k'')\bar{f}^{\pm}_J(\tau'',k'';\tau,k), \quad (9)$$

where $\tau\equiv(n,l,L)$; n,l are principal and orbital quantum number for the ν-th state Ps atom (or for the μth state H atom). In Eq. (7), excitations of Ps ($\nu'\equiv nlm;\mu'\equiv 100$) or H ($\nu'\equiv 100;\mu'\equiv nlm$) were considered at a time for the coupling scheme [28]. L is the partial wave for the moving Ps. The elastic cross section (in units of πa_0^2) is given by

$$\sigma_{el}(k^2)=\sum_J\frac{2J+1}{4\pi^2}\left[\frac{1}{4}|\bar{f}^{+}_J(\tau,k;\tau,k)|^2+\frac{3}{4}|\bar{f}^{-}_J(\tau,k;\tau,k)|^2\right]; \quad (10)$$

superscripts "$\pm$" correspond to singlet $(+)$ and triplet $(-)$ channels.

For negative energies (E), momenta are complex and we need to solve the LS equation for arbitrary real but off-shell momenta. At negative energies, the Green function is nonsingular and we solve the following modified equation:

$$\bar{f}^{\pm}_J(\tau',p';\tau,p)=\bar{\mathcal{B}}^{\pm}_J(\tau',p';\tau p)+\frac{1}{2\pi^2}\sum_{\tau''}\int dk''k''^2 \times\frac{\bar{\mathcal{B}}^{\pm}_J(\tau',p';\tau'',k'')\bar{f}^{\pm}_J(\tau'',k'';\tau,p)}{k^2_{\tau''}+k''^2} \quad (11)$$

for off-shell momenta p, p'. At negative energies, the pole(s) of the T matrix, if exists, corresponds to the bound state(s).

TABLE I. Scattering length (a) in a.u. and binding energy (E_B) in eV for static-exchange (1CH), 3-Ps-state (3CH), and 5-state (5CH) models [28]: (a) results with the parameter $C=0.785$ as in Ref. [2] but using zero- and negative-energy solutions of the T matrix. (b) Previous results [2] using the effective-range expansion.

	1CH	3CH	5CH
a^+	(a) 4.044	3.843	3.662
	(b) 4.05	3.85	3.74
E_B	(a) 0.254	1.20	1.28
	(b) 0.254	0.97	1.05

III. RESULTS AND DISCUSSIONS

First we solve negative-energy and zero-energy T-matrix equations for the well-established static-exchange (SE) model of Ps-H scattering to compare the present numerical procedures vis-a-vis others. For the SE model, the zero-energy T-matrix equation (9) gives a scattering length of $7.272a_0$ compared to that of $7.275a_0$ calculated by Hara and Fraser (HF) [29,30] and $7.25a_0$ calculated by Campbell *et al.* [25]. Present result is almost in full agreement with the HF result. At negative energies, Eq. (11) provides a T-matrix pole at $E=-0.254$ eV for the SE model (thus binding energy $=0.254$ eV). HF do not calculate the binding energy and Campbell *et al.* [25] report a binding energy of 0.264 eV for the SE model. The difference is considered to be due to numerical procedures. The numerical solution scheme of the T-matrix integral equations, employed here, is unconditionally stable and does not depend on any external boundary conditions, as the latter are implicitly embedded in the equations. Also, integral equation approach is devoid of any accumulation error characteristic of a differential or integro-differential equation and thus could be preferred.

We now apply these direct-solution techniques to potential simulated T-matrix equations and recalculate the scattering length and binding energies. In Table I, we provide the present results in row (a). In row (b), we provide the old values obtained by using the effective-range expansion [2–4].

Table I shows that effective-range expansion could be a good approximation when the binding energy is small (e.g., the 1CH case). For substantially large binding energies (~ 1 eV), the percentage of error in the effective-range expansion method is quite high (about 20%) and is not suitable for PsH, as perceived.

To resolve this error with the binding energy, we now calculate the T-matrix pole position directly and predict the correct (upto third decimal place) binding energy of the model. For 1CH, when the pole is simulated within -1.066 eV to -1.067 eV (exact binding energy is believed to be 1.0666 eV [7]), the corresponding coupled T-matrix equations are solved at zero and positive energies to get the scattering length and other scattering parameters including the resonance. The procedure is repeated with addition of channels and the results are tabulated in Table II.

Results demonstrate that when the binding energy pole is simulated in between -1.066 and -1.067 eV, the singlet scattering length consistently converges to $3.887a_0$ and the resonance energy appears at 4.06 eV. The resonance energy 4.06 eV differs from the accurate prediction of 4.006 eV [7] by only 1% and is expected to be fairly converged in the model as the change from 2CH to 3CH result is $\sim 1\%$. Neither of the variational calculations, which predict the scattering length of $3.45a_0$ [16] and $4.34a_0$ [17], provide the S-wave resonance energy that could have been an indicator of the level of convergence. In a recent 14Ps14H R-matrix calculation [19] the Belfast group has found that a scattering length of $4.41a_0$ is accompanied by a binding energy of 0.994 eV and a resonance energy of 4.31 eV. The broader dynamical picture (binding, resonance, scattering length) provided by the R-matrix results, suggests that the theory, although, has made a significant advancement to the *ab initio* calculation, the result is yet to be fully converged, and that the scattering length of $4.41a_0$ has scope for further convergence. Thus the present result of $3.89a_0$ for the scattering length which is associated with a binding energy of 1.066 eV and a resonance energy of 4.06 eV could be considered as a step forward in this direction. In Table III, we quote the low-energy phase shifts for future reference and comparison.

TABLE II. Scattering lengths (a.u.) and binding energies (eV) for PsH.

	1CH	2CH	3CH	Accurate result
$T(E)$ pole at $E=$	1.066–7	1.066–7	1.066–7	1.0666 [6,7]
Fitted with $C=$	0.7732	0.7895	0.790	
a^+	3.939	3.888	3.887	3.5–4.3
E_r		4.10	4.06	4.006 [7]

Results in Table III, demonstrate the convergence pattern of the low-energy singlet phase shifts. Difference between 2CH and 3CH model results are within 0.05% and thus the 3CH phase shifts are assumed to be fairly converged in the present scheme.

In summary, we present a theoretical scheme to perform solution of coupled integral T-matrix equations at zero energy and negative energies and apply them to have direct prediction of the scattering length and binding energy for the singlet Ps-H system. We replace our previous estimates on binding energy and scattering length by precise determination of the T-matrix pole at negative energies and zero-

TABLE III. Phase shifts for Ps-H singlet scattering with incident energies ($E=6.8k^2$ eV).

k	1CH	2CH	3CH
Pole of $T(E)$ at $E=$	1.066–7	1.066–7	1.066–7
Fitted with $C=$	0.7732	0.7895	0.790
0.1	2.7536	2.7587	2.7589
0.2	2.3965	2.4071	2.4074
0.3	2.0861	2.1032	2.1036
0.4	1.8236	1.8487	1.8492
0.5	1.6031	1.6396	1.6402
0.6	1.4170	1.4742	1.4749

energy cross sections. In our model, the singlet scattering length converges to $3.89a_0$ and the *S*-wave resonance energy converges to 4.06 eV when the binding energy pole is precisely fixed within 1.066−7 eV.

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