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Resonances of positronium complexes

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Resonances of electron-positron complexes are studied by the stochastic variational method combined with the complex scaling method. Several low-lying resonances in the positronium negative ion are obtained. One *P*-state and nine *S*-state resonances of the positronium molecule are predicted below the $\mathrm{Ps}(n=1)+\mathrm{Ps}(n=4)$ threshold. The structure of some of these resonances is analyzed.

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Recent developments in the use of low-energy positron beams have led to a growing interest in positronium (Ps) related investigation such as the Bose-Einstein condensation of Ps [1] and the spectroscopy of Ps complexes and positronic atoms [2]. The possibility of using Ps gas is expected to yield direct information on the Ps molecule formation.

Among electron-positron complexes [3], only the positronium negative ion, Ps^-, has been experimentally confirmed to date [4] except for the well-known Ps. Despite the theoretical conclusion that the positronium molecule Ps_2 forms a bound system (disregarding the electron-positron pair annihilation), its existence has not yet been experimentally confirmed. The ground state (g.s.) of Ps_2 has attracted continual theoretical interest, and its energy has been calculated accurately. Furthermore, it has been confirmed theoretically [5] that Ps_2 has only four bound states, three $L^\pi=0^+$ [6], and one 1^- state [7]. The latest calculation with the stochastic variational method (SVM) indicates that the binding energy of the g.s. of Ps_2 from the dissociation threshold into two Ps atoms is 0.435 eV, while the 1^- state lies at 4.506 eV above that dissociation threshold. The latter was found to be stable against the autodissociation from the symmetry consideration of the system but decays via the pair annihilation as well as the dipole transition to the g.s.

Though there exist only a few bound states in Ps^- and Ps_2, the existence of resonances may be countless. For example, in analogy to the Rydberg series [8], which are formed by the positron attaching to the H^- ion, Ps_2 may have resonances of the Ps^-+e^+ structure. Since several Ps+Ps thresholds are open below the Ps^-+e^+ threshold, it would, however, be natural to expect that resonances of the Ps-Ps type appear first at low excitation energies instead of the Ps^-+e^+ series. The study of resonances is not only important for the spectroscopy of the Ps complexes but is also interesting theoretically, especially in highly nonadiabatic systems such as Ps_2 because it is unknown beforehand which degree of freedom is responsible for the resonating motion in such systems. Calculations of the *S*-state resonance parameters of Ps^- and Ps_2 were done in Refs. [9–11] with the complex scaling method (CSM) [12]. Most calculations done so far have limitations in imposing the proper symmetries of the constituent particles and/or in considering states with nonzero angular momenta at least in Ps_2. This study shows that the SVM combined with the CSM (SVM+CSM) facilitates the calculation of the resonance parameters of more complex and general systems reliably.

The most standard approach to find a resonance is a coupled-channels method, but a generalization of bound-state solutions to resonances has always attracted much interest because of its simplicity. The real stabilization method [13] and the method of analytic continuation in the coupling constant [14] are such examples. Predicting the resonance width requires complex energy calculations at some stage. The CSM is widely used for this purpose in atomic [15,16] and nuclear physics [17]. A complex absorbing potential method [18] has recently been proposed. Its application has so far been limited to simple cases. These methods work for narrow resonances and have been mostly applied to two- and three-body systems because it is hard to obtain precise solutions even for bound-state solutions beyond the three-body system. Recently an SVM with correlated Gaussians [19] has been used successfully in the diverse problems of many-particle systems. The secret of the accuracy is the use of the correlated basis and the careful optimization of nonlinear parameters, which characterize the basis states.

In the CSM, the coordinate $\boldsymbol{r}$ is rotated as $\boldsymbol{r}\to\boldsymbol{r}e^{i\theta}$ by a transformation $U(\theta)$. The rotated resonance wave function may be expanded in terms of square-integrable basis functions just as a bound-state solution is expanded,

$$U(\theta)\Psi_R(\boldsymbol{x})=\sum_{i=1}^{\mathcal{K}} C_i(\theta)\mathcal{P}\psi_i(\boldsymbol{x})\chi, \tag{1}$$

where $\boldsymbol{x}=\{\boldsymbol{x}_1,\boldsymbol{x}_2,\cdots,\boldsymbol{x}_{N-1}\}$ is a set of the relative coordinates, $\mathcal{P}$ is a projector onto states with proper symmetry, and χ is a spin function. Linear parameters $C_i(\theta)$ are obtained as the solution of the equation

$$\sum_{j=1}^{\mathcal{K}} \langle\mathcal{P}\psi_i\chi|U(\theta)HU^{-1}(\theta)|\mathcal{P}\psi_j\chi\rangle C_j(\theta) =E^\theta\sum_{j=1}^{\mathcal{K}} \langle\mathcal{P}\psi_i\chi|\mathcal{P}\psi_j\chi\rangle C_j(\theta). \tag{2}$$

If the solution corresponds to a resonance exactly, the eigenenergy E^θ should not depend on θ but actually depends

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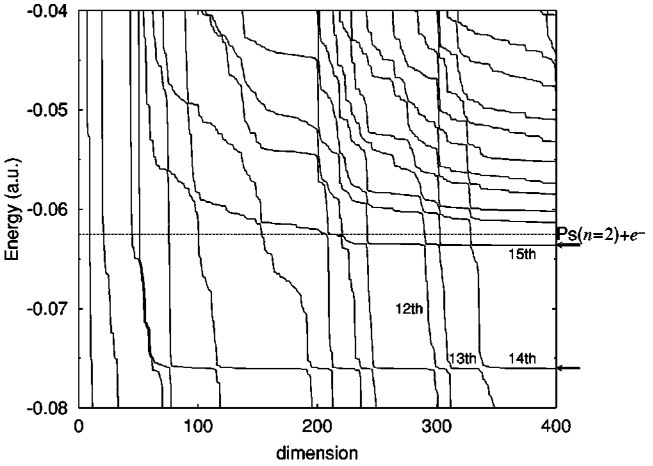

FIG. 1. Trajectories of the Ps^- states with ${}^1S^{\mathrm{e}}$ symmetry as a function of the basis dimension. Each trajectory has a plateau around the resonance energy. Some trajectories are labeled by their sequence numbers.

slightly on it as well as on what basis elements are employed. Such eigenenergy E^θ that is stationary with respect to θ has been identified as giving the resonance parameter. A similar procedure was employed in Refs. [10,11,15].

Hylleraas-type functions are frequently used as basis functions in atomic systems. Correlated Gaussians are used here because they facilitate the calculation of matrix elements for larger systems and high angular momenta, and moreover, provide solutions with high accuracy [19]. The basis function ψ_i is given as follows:

$$\psi_i(\boldsymbol{x}) = |\boldsymbol{v}_i|^L Y_{LM}(\hat{\boldsymbol{v}}_i)\exp\left\{-\frac{1}{2}\sum_{j,k=1}^{N-1} A_{i_{jk}}\boldsymbol{x}_j\cdot\boldsymbol{x}_k\right\}, \tag{3}$$

where a vector $\boldsymbol{v}_i = \Sigma_{j=1}^{N-1} u_{i_j}\boldsymbol{x}_j$ is introduced to describe a nonspherical orbital motion [20]. The elements $A_{i_{jk}}$ of an $(N-1)\times(N-1)$ symmetric matrix A_i together with the coefficients u_{i_j} are variational parameters.

The SVM+CSM procedure is exemplified in Ps^-. The projector $\mathcal{P}$ is just the antisymmetrizer for the two electrons. The relative coordinates chosen are $\boldsymbol{x}_1 = \boldsymbol{r}_{e_1^-} - \boldsymbol{r}_{e^+}$ and $\boldsymbol{x}_2 = \frac{1}{2}(\boldsymbol{r}_{e_1^-} + \boldsymbol{r}_{e^+}) - \boldsymbol{r}_{e_2^-}$. The spin function with an electron singlet state is chosen to be $\chi = |\uparrow\Uparrow\downarrow\rangle - |\downarrow\Uparrow\uparrow\rangle$, where $\uparrow$ ($\downarrow$) denotes the spin-up (spin-down) state of electrons, and $\Uparrow$ denotes the positron spin-up state. Figure 1 shows the energy ($\theta=0$) versus the basis dimension $\mathcal{K}$, which is increased one by one following the SVM procedure. ${}^1S^e$ (${}^3S^e$) denotes an S-wave ($L=0$) positive-parity state with an electron singlet (triplet) state. The energy plateaux are seen at, e.g., $E = -0.076$ and -0.064 atomic units (a.u.) below the $\mathrm{Ps}(n=2)+e^-$ threshold. This first step serves to select the basis set, which is to be used in the expansion (1). The wave function $\tilde{\Psi}_R$ and the energy corresponding to the stabilized solution with a large dimension (say, $\mathcal{K}=400$) approximate those of the resonance well (cf. Table I) if the resonance width is narrow.

TABLE I. Resonances of Ps^-. E_R and Γ denote the resonance energy and width. The first four resonances are in ${}^1S^{\mathrm{e}}$, while the last three in ${}^3S^{\mathrm{e}}$.

Present		Ref. [9]	
$-E_R$ (a.u.)	Γ (a.u.)	$-E_R$ (a.u.)	Γ (a.u.)
0.0760297	4.236×10^{-5}	0.0760305(20)	$4.275(100)\times10^{-5}$
0.063667	8.99×10^{-5}		
0.0353329	7.68×10^{-5}	0.0353425(50)	$7.25(50)\times10^{-5}$
0.029845	5.52×10^{-5}		
0.0635373564	8.1×10^{-9}		
0.062505	7.4×10^{-5}		
0.02935176	2.0×10^{-5}		

The next step is to calculate E^θ by solving Eq. (2) with the basis functions found in the first step. Figure 2 displays the trajectory of the 14th eigenstate in Fig. 1 as a function of θ (in rad) from 0 to 0.4 in steps of 0.01. The variation $d|E|/d\theta$ becomes a minimum at $E = (-0.07603, -2.1\times10^{-5})$ a.u., which gives the resonance parameter. The accuracy of the calculation has been checked by looking at the stability of the resonance parameters against the increase of the basis dimension.

Table I compares the resonance parameters calculated by the SVM+CSM with those of Ref. [9]. Two resonances below the $\mathrm{Ps}(n=2)+e^-$ threshold and two resonances below the $\mathrm{Ps}(n=3)+e^-$ threshold were obtained. Two of them are in good agreement with Ref. [9]. Two more resonances have been predicted by the present method. A calculation was extended to the electron-spin triplet state $\chi = |\uparrow\Uparrow\uparrow\rangle$ as well. Three resonances were identified as shown in Table I. To find the resonance at $E_R = -0.062\,505$ a.u., only 5×10^{-6} a.u. below the $\mathrm{Ps}(n=2)+e^-$ threshold, a careful calculation is necessary. The level structure has a close similarity to that of H^- [21]. The two electrons in the triplet state cannot get very close to each other, which makes the coupling to continuum states weak. This explains why the width of the triplet resonance is, in general, smaller than that of the singlet resonance.

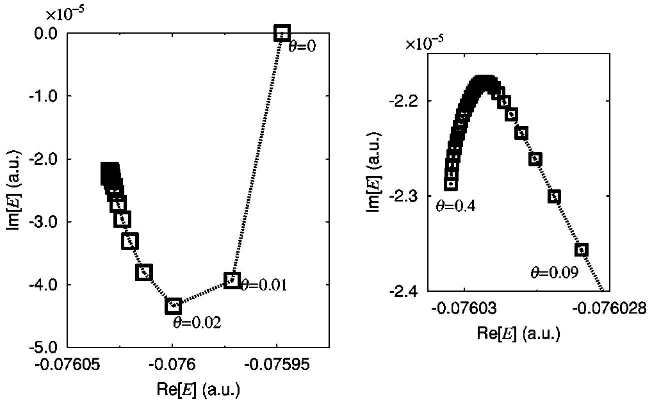

FIG. 2. Trajectories of the Ps^- resonance labeled 14th in Fig. 1 as a function of the rotation angle θ. The vicinity near the stationary point is magnified on the right.

TABLE II. Bound states and resonances of Ps_2 classified according to the D_{2d} group. E_R and Γ denote the resonance energy and the width for the autodissociation. States with unspecified Γ value correspond to a bound state.

L^π	D_{2d}	$-E_R$ (a.u.)	Γ (a.u.)
0^+	A_1	0.516003789058	
		0.3294	0.0062
		0.2924	0.0039
	B_2	0.3146733	
		0.28976	0.00014
		0.27935	0.00007
	A_2	0.27655	0.00031
	B_1	0.30814	0.00024
		0.2736	0.0017
	E	0.33027681	
		0.2939	0.0043
		0.2822	0.0017
1^-	A_1	0.287778	0.00005
	B_2	0.3344082658	

Now we look for resonances of Ps_2. The Hamiltonian for Ps_2 is invariant with respect to the interchange of the coordinates of electrons or positrons as well as the charge reversal, which provides the symmetry for the eigenstate. These eight permutations form a group isomorphic to the point group D_{2d} [6], which classifies the eigenstates according to five irreducible representations: A_1, A_2, B_1, B_2, and E. The E representation is two dimensional and gives twofold degenerate levels. The projector $\mathcal{P}$ for each irreducible representation is given as a combination of the permutations [5,6]. The spins of the electrons and the positrons compatible with the representation are determined depending on the representation. Ps_2 can form a 0^+ bound state only in A_1, B_2, and E symmetry and a 1^- bound state in B_2 symmetry.

The relative coordinates for Ps_2 are chosen as the H-type (Ps-Ps type) coordinates: $\boldsymbol{x}_1=\boldsymbol{r}_{e_1^-}-\boldsymbol{r}_{e_1^+}$, $\boldsymbol{x}_2=\boldsymbol{r}_{e_2^-}-\boldsymbol{r}_{e_2^+}$, $\boldsymbol{x}_3=\frac{1}{2}(\boldsymbol{r}_{e_1^-}+\boldsymbol{r}_{e_1^+})-\frac{1}{2}(\boldsymbol{r}_{e_2^-}+\boldsymbol{r}_{e_2^+})$. This choice does not imply, however, that Ps-Ps configurations are favored in the calculation [19]. The basis function is expressed in terms of only the relative coordinates. By subtracting the center-of-mass kinetic energy from the Hamiltonian, we can calculate the intrinsic energy of Ps_2.

Nine 0^+ resonances were confirmed as listed in Table II. Figure 3 summarizes the 0^+ spectrum of Ps_2 including the bound states. The lifetime of these resonances for the autodissociation decay is in the range of 0.004–0.4 ps, very short compared with that due to the 2γ annihilation, typically of the order of nanoseconds, which is determined by the quantity $\langle\delta(\boldsymbol{r}_{e^-}-\boldsymbol{r}_{e^+})\rangle$ [5]. The calculation of Refs. [10,11] assumed the spin-singlet state for the electrons, specified no definite spin for the positrons and imposed no symmetry between the electrons and the positrons. This means that only states with A_1, B_2, and/or E symmetry were actually considered. A state of Refs. [10,11] is, in general, a mixed state of A_1+B_2+E symmetry. The resonance with $E_R=-0.3294$ and $\Gamma=0.0056$ a.u. [11] is probably a mixed state of the two states of the present calculation, that is the A_1 resonance at $E_R=-0.3294$ a.u. and the E bound state at $E_R=-0.33027$ a.u. This conjecture is consistent with the fact that the width of Ref. [11] is 90% of that of the A_1 resonance. A state assigned as a "resonance" at $E_R=-0.313$ a.u. [11] probably corresponds to the B_2 bound state at $-0.314\,67$ a.u. The $0^+(B_2)$ state at $-0.314\,67$ a.u. and the $0^+(E)$ state at $-0.330\,27$ a.u. are both bound [5]. For example, the former state becomes bound because it cannot decay to the $Ps(1s)+Ps(1s)$ channel due to the charge parity conservation. Reference [6] also predicted the $0^+(B_2)$ and $0^+(E)$ states as metastable states at $E_R=-0.314\,468\,9$ and $-0.330\,046\,9$ a.u., respectively.

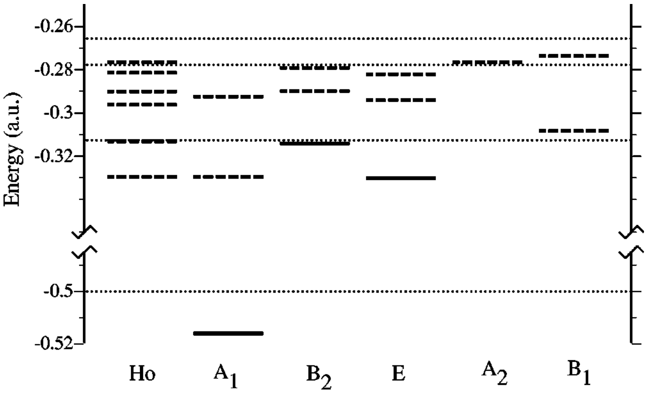

FIG. 3. 0^+ spectrum of Ps_2 classified according to the D_{2d} group. Thick solid and thick dashed lines represent bound states and resonances, respectively. Thin dashed lines represent $Ps(n=1)+Ps(n)$ thresholds. The present results are compared with those of Ref. [11] (first column), in which neither the spin of the positrons nor the charge reversal symmetry is however specified.

In order to clarify the resonance structure, we calculate the correlation function defined by $C(r)=\langle\tilde{\Psi}_R|\delta(\boldsymbol{x}_i-\boldsymbol{r})\times|\tilde{\Psi}_R\rangle$. Using $\tilde{\Psi}_R$ seems to be a good approximation for understanding the characteristic feature of the resonance. By choosing $\boldsymbol{x}_1$ and $\boldsymbol{x}_3$ for $\boldsymbol{x}_i$, the correlation function is expected to give information on what Ps states dominate and how much two Ps are separated in the resonance.

Figure 4 compares the correlation functions for the three $0^+(A_1)$ states: the g.s. (solid line), two resonances at $E_R=$

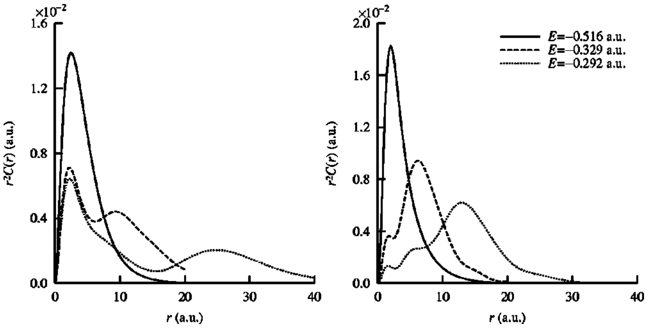

FIG. 4. Correlation functions of the three $0^+(A_1)$ states of Ps_2. Left: r corresponds to the distance between the electron and the positron. Right: r corresponds to the distance between the center of masses of the two electron-positron pairs.

TABLE III. Spectroscopic factors to dominant Ps states.

Ps_2	$-E_R$ (a.u.)	S_{1s}	S_{2s}	S_{2p}
$0^+(A_1)$	0.516	0.739	0.020	0.090
$0^+(A_1)$	0.329	0.373	0.329	0.092

-0.3294 (dashed line), and -0.2924 a.u. (dotted line). The left panel shows the function $r^2C(r)$ for $\boldsymbol{x}_1$. The g.s. has a peak at about $2a$, with a being the Bohr radius. The density, multiplied by r^2, of the Ps$(1s)$ atom has a peak at $2a$, so the g.s. of Ps_2 consists dominantly of the Ps$(1s)+$Ps$(1s)$ component. The lower resonance has two peaks at about $2.2a$ and $9.4a$, whereas the higher resonance is at about $2.2a$ and $24.8a$, respectively. The larger positions approximately correspond to the positions of the outermost peak of the $2s$ and $3s$ Ps states, $10.5a$ and $26.1a$, respectively. The main components of the resonances are thus considered Ps$(1s)$ $+$Ps$(2s)$ and Ps$(1s)+$Ps$(3s)$, respectively, but the deviation from these indicates mixtures of several components. (It should be noted that $C(r)$ does not map the e^--e^+ correlation inside one Ps pair, but has several contributions from the e^--e^+ pairs belonging to the different Ps pairs.) The right panel displays the $r^2C(r)$ for $\boldsymbol{x}_3$, which shows that the relative motion between two Ps atoms has an increasing number of peaks and an increasing spread of the distribution with increasing excitation energy.

To corroborate the above arguments, we list in Table III the examples of ''spectroscopic factors'' for a particular Ps state, defined by $S_{nl}=\Sigma_m\langle\tilde{\Psi}_R|P_{nlm}|\tilde{\Psi}_R\rangle$, where P_{nlm} $=|\psi_{\mathrm{Ps}_{nlm}}\rangle\langle\psi_{\mathrm{Ps}_{nlm}}|$. Note that $\Sigma_{nl}S_{nl}=1$. The spectroscopic factor is a measure of the strength distribution to various Ps states. A similar analysis was made for the g.s. by using the density-matrix formalism [22]. For the g.s. of Ps_2, S_{1s} is predominantly large (0.739) and other S_{nl} values are small, which is consistent with the fact that the dominant component of the g.s. is Ps$(1s)+$Ps$(1s)$. For the lowest $0^+(A_1)$ resonance, both S_{1s} and S_{2s} are by far larger than others, so this resonance is concluded to have Ps$(1s)+$Ps$(2s)$ structure.

As an example of a resonance with nonzero L value, $1^-(A_1)$ states were considered. As shown in Table II, a very narrow resonance was found lying between the Ps$(n=1)$ $+$Ps$(n=2)$ and Ps$(n=1)+$Ps$(n=3)$ thresholds.

To conclude, an SVM$+$CSM method was found to be versatile for studying resonances of e^--e^+ systems. The calculation for Ps^- confirmed the resonances were similar to H^-. Nine resonances with $L^\pi=0^+$ were identified in Ps_2. The structure of the g.s. and two resonances of A_1 symmetry were analyzed in terms of the correlation function. The method was successful in predicting the P-state resonance as well. The SVM with the correlated Gaussian basis, originally proposed for bound-state problems, works well even for selecting those basis elements that are needed to describe resonances, and by combining with some suitable methods such as the CSM it can predict resonances in complex systems with confidence.

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