# Lowest open channels, bound states, and narrow resonances of dipositronium

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The constraints imposed by symmetry on the open channels of dipositronium has been studied, and the symmetry-adapted lowest open channel of each quantum state has been identified. Based on this study, the existence of two more $0^+$ bound states has been theoretically confirmed, and a $0^+$ narrow resonance has been predicted. A variational calculation has been performed to evaluate the critical strength of the repulsive interaction. Two $0^-$ states are found to have their critical strengths very close to 1, they are considered as candidates of new narrow resonances or loosely bound states.

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## I. INTRODUCTION

Since positrons can be easily created in the processes of high-energy collisions, the molecules formed by electrons and positrons are believed to exist in nature. Half a century ago the existence of the positronium molecule, namely, the dipositronium $Ps_2$ has already been predicted [1] and has been first calculated via a variational procedure [2]. Since the lifetime of the ground state of $Ps_2$ is very short (it is only 0.906 ns[3]) due to the $e^-$-$e^+$ annihilation, it has not yet been observed experimentally. In recent years, this problem has attracted increasing attention following the ability to create cold positron beams tunable over a wide energy range [4], and the increasing ability to carry out accurate theoretical calculations [3,5–10]. In addition to the ground state, an angular momentum $L=1$ and parity $\Pi=-1$ bound excited state has also been predicted [10]. The other excited states are believed to be resonances.

Of course any resonance would collapse via at least one open channel. However, whether a state is allowed to enter into an open channel is not only determined by energy but also by symmetry. In fact, as we shall see, the states with a specific set of quantum numbers are allowed by symmetry to get access to only a few specific open channels. Thus, for a given state, it is important to make sure which open channel is the lowest one allowed by symmetry, that is called a symmetry-adapted lowest open channel (SLOC). If a state has its energy lower than the SLOC, it would be definitely bound, because it has no channel to collapse. If a state has its energy a little higher than the SLOC and if there is a barrier to hinder the wave function from leaking into the channel, it would appear as a narrow resonance. The barrier may have different origin, what is concerned here is the centrifugal barrier as discussed later. If the barrier does not exist or if the energy is much higher than the SLOC, the state would be a broad resonance. When a resonance has a very broad width, it is very difficult to be detected, and thus the existence of this resonance is meaningless. In other words, only the resonances with narrower widths are interesting.

The main aim of this paper is the identification of the SLOC, this is the base for the further study of the dipositronium. Additionally, based on the SLOC and on other existing data, the existence of a few more bound states and resonances has been confirmed. Furthermore, a few candidates of bound states or resonances has been suggested based on an evaluation. The emphasis is placed on the qualitative aspect.

## II. SYMMETRY-ADAPTED LOWEST OPEN CHANNELS

Let the particles 1 and 2 be electrons and 3 and 4 be positrons, let $\mathbf{r}_a=\mathbf{r}_2-\mathbf{r}_1$, $\mathbf{r}_b=\mathbf{r}_4-\mathbf{r}_3$, $\mathbf{r}_c=1/2(\mathbf{r}_4+\mathbf{r}_3-\mathbf{r}_2-\mathbf{r}_1)$, and $r_{ji}=|\mathbf{r}_j-\mathbf{r}_i|$. The internal Hamiltonian of the dipositronium is (in a.u.)

$$H=-\left(\nabla_a^2+\nabla_b^2+\frac{1}{2}\nabla_c^2\right)+\left(\frac{1}{r_{12}}+\frac{1}{r_{34}}-\frac{1}{r_{13}}-\frac{1}{r_{14}}-\frac{1}{r_{23}}-\frac{1}{r_{24}}\right), \tag{1}$$

which is invariant with respect to the $O_3$ group and to the point group $D_{2d}$ [3]. The latter is a subgroup of $S_4$ containing eight elements, namely, 1, $p_{12}$, $p_{34}$, $p_{12}p_{34}$, $p_{13}p_{24}$, $p_{14}p_{23}$, $p_c(1324)$, and $p_c(1423)$ (where $p_{ij}$ denotes an interchange and $p_c(ijkl)$ denotes a cyclic permutation). Hence the eigenstates can be classified according to the irreducible representations of the $O_3$ and $D_{2d}$, and thereby can be denoted as $L^{\Pi}(\mu)$, where $\mu$ denotes a representation of the $D_{2d}$ group, $\mu=A_1$, $A_2$, $B_1$, $B_2$ or $E$. Let the wave function of a $L^{\Pi}(\mu)$ state be denoted as $\Psi_{L\Pi\mu}$. From the knowledge of the $D_{2d}$ group, we have [3]

$$p_{12}p_{34}\Psi_{L\Pi\mu}=\Psi_{L\Pi\mu} \quad (\text{if } \mu\neq E), \text{ or } =-\Psi_{L\Pi\mu} \quad (\text{if } \mu=E) \tag{2}$$

and

$$p_{13}p_{24}\Psi_{L\Pi\mu}=\Psi_{L\Pi\mu} \quad (\text{if } \mu=A_1 \text{ or } B_1), \text{ or } =-\Psi_{L\Pi\mu} \quad (\text{if } \mu=A_2 \text{ or } B_2). \tag{3}$$

Let the spins of the two electrons 1 and 2 be coupled to $S_1$, those of 3 and 4 be coupled to $S_2$. Obviously, Eq. (2) implies that the states with $\mu\neq E$ have $S_1=S_2$.

On the other hand, let $\Phi_{nl}$ denote an eigenstate of the positronium Ps [the ground state has $(nl)=(10)$]. For the

 

TABLE I. The SLOC and the corresponding threshold energies (in a.u.) of the $L^{\Pi}(\mu)$ states ($L \leqslant 2$) together with the eigenenergies from theoretical calculations. The partial wave given in the third column is the lowest wave.

| $L^{\Pi}$ | $\mu$ | SLOC | Threshold energy | Eigenenergy |
|---|---|---|---|---|
| $0^+$ | $A_1$ | $(10)^s(10)$ | $-0.500\,00$ | $-0.516\,003\,778$,[a] $-0.509$[b] |
| $0^+$ | $B_1$ | $(10)^s(10)$ | $-0.500\,00$ | $-0.499\,442\,8$,[c] $-0.485$[b] |
| $0^+$ | $A_2$ | $(10)^p(21)$ | $-0.312\,50$ | $-0.312\,080\,5$,[c] $-0.301$[b] |
| $0^+$ | $B_2$ | $(10)^p(21)$ | $-0.312\,50$ | $-0.314\,468\,9$,[c] $-0.307$[b] |
| $0^+$ | $E$ | $(10)^s(20)$, $(10)^p(21)$ | $-0.312\,50$ | $-0.330\,046\,9$,[c] $-0.322$[b] |
| $1^-$ | $B_2$ | $(10)^s(21)$ | $-0.312\,50$ | $-0.334\,408$,[a] $-0.326$[b] |

[a]From Ref. [10].
[b]From our evaluation.
[c]From Ref. [3].

$Ps_2 \rightarrow Ps + Ps$ dissociation channel (where the Ps may be excited), the channel wave function $\Psi_{ch}$ can be written as

$$\Psi_{ch} = [1+(-1)^{S_1}p_{12}][1+(-1)^{S_2}p_{34}] \times \{[\Phi_{nl}(\mathbf{r}_{13})\Phi_{n'l'}(\mathbf{r}_{24})]_{l_o} f_{l_R}(\mathbf{r}_{13,24})\}_L, \quad (4)$$

where $f_{l_R}$ is the wave function of relative motion and $l_R$ is the relative angular momentum. $l$ and $l'$ are coupled to $l_o$, together with $l_R$ they are coupled to $L$. From Eq. (4) we have

$$p_{13}p_{24}\Psi_{ch} = (-1)^{l+l'}[1+(-1)^{S_2}p_{12}][1+(-1)^{S_1}p_{34}] \times \{[\Phi_{nl}(\mathbf{r}_{13})\Phi_{n'l'}(\mathbf{r}_{24})]_{l_o} f_{l_R}(\mathbf{r}_{13,24})\}_L. \quad (5)$$

Furthermore, in the special case of $(nl)=(n'l')$, Eq. (4) can be rewritten as

$$\Psi_{ch} = [1+(-1)^{S_1+S_2+l_o+l_R}] \times (\{[\Phi_{nl}(\mathbf{r}_{13})\Phi_{nl}(\mathbf{r}_{24})]_{l_o} f_{l_R}(\mathbf{r}_{13,24})\}_L + (-1)^{S_1}\{[\Phi_{nl}(\mathbf{r}_{23})\Phi_{nl}(\mathbf{r}_{14})]_{l_o} f_{l_R}(\mathbf{r}_{23,14})\}_L). \quad (6)$$

Evidently, if a $L^{\Pi}(\mu)$ state is allowed to enter into a specific Ps+Ps channel, the associated $\Psi_{ch}$ must have the same $(L, \Pi, \mu)$ symmetry.

As examples, let us first study the $0^-(A_1)$ and $0^-(B_1)$ states. From Eq. (3) we have

$$p_{13}p_{24}\Psi_{ch} = \Psi_{ch}. \quad (7.a)$$

Since the $\mu = A_1$ or $B_1$ states have $S_1 = S_2$, Eq. (5) can be rewritten as

$$p_{13}p_{24}\Psi_{ch} = (-1)^{l+l'}\Psi_{ch}. \quad (7.b)$$

Comparing Eq. (7.a) with Eq. (7.b), we have

$$(-1)^{l+l'} = 1. \quad (8.a)$$

Furthermore, since we have meanwhile $S_1 = S_2$, the factor $[1+(-1)^{S_1+S_2+l_o+l_R}]$ in Eq. (6) is nonzero only if $l_R + l_o$ is even. Thus, we have

$$(-1)^{l_o+l_R} = 1, \text{ if } (nl) = (n'l'). \quad (8.b)$$

Besides, it can be proved that none of the partial waves of a $0^-$ state can be zero. The proof is as follows. Let the angular momenta corresponding to the three Jacobian vectors $\mathbf{r}_a$, $\mathbf{r}_b$, and $\mathbf{r}_c$ be denoted as $l_1$, $l_2$, and $l_3$. For $0^-$ states, any relative partial wave, say $l_1$, cannot be zero. If $l_1$ were zero, $l_2$ must be equal to $l_3$ to assure $L=0$. However, if $l_2 = l_3$, the parity must be even. Therefore, $l_1$ (or any relative angular momentum) is not allowed to be zero in $0^-$ states. Evidently, the proof is valid for any set of Jacobian coordinates. Thus we have

$$l \neq 0, \; l' \neq 0, \text{ and } l_R \neq 0. \quad (8.c)$$

Definitely, a Ps+Ps channel is accessible to the $0^-(A_1)$ or $0^-(B_1)$ states only if Eqs. (8.a)–(8.c) are satisfied. Due to these constraints, the lowest Ps+Ps channel is that having $(nl)=(n'l')=(21)$ and $l_R=1$. This channel is labeled as $(21)^p(21)$, where $p$ denotes the relative $p$ wave of the two excited positroniums, the associated threshold energy is $-0.1250$ (a.u. are used in this paper).

For the $0^-(A_2)$ and $0^-(B_2)$ states, the constraint, Eq. (8.a), should be changed to $(-1)^{l+l'} = -1$ (thus $l_R$ is even), while constraints (8.b) and (8.c) remain unchanged. Accordingly, the lowest Ps+Ps channel is the $(21)^d(32)$ channel at $-0.090\,278$. From a similar deduction, we know that the lowest Ps+Ps channels for the $0^-(E)$ states are the $(21)^d(32)$ channel and the $(21)^p(31)$ channel both at $-0.090\,278$.

Let us inspect another two-body channel, the $Ps^- + e^+$ (or $Ps^+ + e^-$) channel. It is recalled that the $Ps^-$ has only one bound state with zero angular momentum. Thus, if a $0^-(\mu)$ state entered into this channel, $l_R$ must be zero to assure $L=0$. However, $l_R=0$ is prohibited due to Eq. (8.c). Therefore, the $Ps^- + e^+$ channel is not accessible to the $0^-(\mu)$ states.

Let us inspect the $Ps + e^+ + e^-$ three-body channel. Let $l$ be the angular momentum of the Ps. Since $l=0$ is not allowed due to Eq. (8.c), the positronium in the three-body

TABLE II. The SLOC, the threshold energies, and the critical strength $\lambda_o$. The $\lambda_o$ that smaller than 0.9 is not listed.

| $L^{\Pi}$ | $\mu$ | SLOC | Threshold energy | $\lambda_o$ |
|---|---|---|---|---|
| $0^-$ | $A_1$ | $(21)^p(21)$ | −0.125 00 | 0.93 |
| $0^-$ | $B_1$ | $(21)^p(21)$ | −0.125 00 | 0.98 |
| $0^-$ | $A_2$ | $(21)^d(32)$ | −0.090 278 | 0.94 |
| $0^-$ | $B_2$ | $(21)^d(32)$ | −0.090 278 | |
| $0^-$ | $E$ | $(21)^p(31)$, $(21)^d(32)$ | −0.090 278 | 0.99 |
| $L^{\Pi}$ | $\mu$ | SLOC | Threshold energy | $\lambda_o$ |
| $1^+$ | $A_1$ | $(10)^d(32)$ | −0.277 78 | |
| $1^+$ | $B_1$ | $(10)^d(32)$ | −0.277 78 | |
| $1^+$ | $A_2$ | $(10)^p(21)$ | −0.312 50 | |
| $1^+$ | $B_2$ | $(10)^p(21)$ | −0.312 50 | |
| $1^+$ | $E$ | $(10)^p(21)$ | −0.312 50 | |
| $1^-$ | $A_1$ | $(10)^p(20)$ | −0.312 50 | 0.93 |
| $1^-$ | $B_1$ | $(10)^p(20)$ | −0.312 50 | |
| $1^-$ | $A_2$ | $(10)^s(21)$ | −0.312 50 | |
| $1^-$ | $E$ | $(10)^p(10)$ | −0.500 00 | 0.90 |
| $L^{\Pi}$ | $\mu$ | SLOC | Threshold energy | $\lambda_o$ |
| $2^+$ | $A_1$ | $(10)^d(10)$ | −0.500 00 | |
| $2^+$ | $B_1$ | $(10)^d(10)$ | −0.500 00 | |
| $2^+$ | $A_2$ | $(10)^p(21)$ | −0.312 50 | |
| $2^+$ | $B_2$ | $(10)^p(21)$ | −0.312 50 | 0.94 |
| $2^+$ | $E$ | $(10)^d(20)$, $(10)^p(21)$ | −0.312 50 | 0.93 |
| $2^-$ | $A_1$ | $(10)^p(32)$ | −0.277 78 | |
| $2^-$ | $B_1$ | $(10)^p(32)$ | −0.277 78 | |
| $2^-$ | $A_2$ | $(10)^d(21)$ | −0.312 50 | |
| $2^-$ | $B_2$ | $(10)^d(21)$ | −0.312 50 | |
| $2^-$ | $E$ | $(10)^d(21)$ | −0.312 50 | |

channel of $0^-$ states must be excited, therefore the lowest $\mathrm{Ps}+e^++e^-$ three-body channel is at $-0.0625$ [in which the Ps has $(nl)=(21)$].

The above analysis is straightforward to be generalized and thereby all the SLOC can be identified as listed in Table I (the states having sufficient data from existing theoretical calculations are listed in this table) and Table II (otherwise).

## III. DISCUSSION OF THE SPECTRUM

### A. Confirmation of new bound states and resonance

Among the states of Table I, the $0^+(A_1)$ and $1^-(B_2)$ have already been pointed out that they are bound [3,10]. For the $0^+(B_2)$ and $0^+(E)$ states, they are tentatively classified as resonant singlet and triplet spin states in the first paper of Ref. [7], and are believed to be metastable or resonance states in Ref. [3]. Now, it is clear that these two states have their energies lower than their thresholds, thus they are definitely bound.

For the $0^+(A_2)$ state, its energy is only a little higher than the threshold. Furthermore, the lowest partial wave for the relative motion of the two dissociating positroniums is $p$ wave as shown in Table I. Thus a centrifugal barrier exists to hinder the wave function from leaking out. It is recalled that the height of the centrifugal barrier of the Ps+Ps channel is $l_R(l_R+1)/(2r_{ch}^2)$, where $r_{ch}$ is roughly the sum of the radii of the two projectiles (a positronium in the ground state and the other one in the (21) excited state), and therefore would be in the order of 10. Accordingly, the height of the barrier would be in the order of 0.01 for $p$ wave. On the other hand, the energy of the $0^+(A_2)$ is only higher than the threshold by 0.0004 [3]. Thus the barrier is sufficiently high to hinder the wave function, and therefore we believe that the width of the $0^+(A_2)$ resonance is very narrow. For the $0^+(B_1)$ state, its energy is also only a little higher than the threshold. However, the lowest partial wave for the dissociation is $s$ wave, thus centrifugal barrier does not exist, and therefore the $0^+(B_1)$ is a broad resonance which is difficult to detect.

### B. Candidates of new bound states and resonances

In order to evaluate the eigenenergies of the states in Table II, a set of basis functions is introduced for the diagonalization of the Hamiltonian. It is well known that the harmonic oscillator (h.o.) states are, in general, not appropriate for the Coulomb systems, the main shortcoming is their inappropriate asymptotic behavior. However, if several set of h.o. states with different widths are used together, this shortcoming can be remarkably cured [11]. For example, let $\varphi_{nl}^{\omega_K}$ be the eigenstate of a single-particle pure harmonic oscillation with the width $\omega_K$, eigenenergy $(2n+l+3/2)\hbar\omega_K$, and with angular momentum $l\hbar$. When five sets of $\varphi_{nl}^{\omega_K}$ are used together (i.e., $\omega_K$ has five choices), and $n\leqslant 3$ is assumed for diagonalizing the Hamiltonian of a hydrogen atom, the resultant lowest energies for $l=0$, 1, and 2 states are $-0.499\,987$, $-0.124\,998$, and $-0.055\,554$, respectively, to be compared with the exact values $-0.5$, $-0.125$, and $-0.055\,556$. Therefore, we believed that, if only bound states are taken into account, and if only the qualitative aspect is concerned, several sets of h.o. states together can be used for our limited purpose.

Below, the following seven sets of basis functions:

$$\Phi_K^{\omega_K}=[\varphi_{n_1l_1}^{\omega_K}(\mathbf{r}_a)[\varphi_{n_2l_2}^{\omega_K}(\mathbf{r}_b)\varphi_{n_3l_3}^{\omega_K}(\mathbf{r}_c)]_{l_o}]L \tag{9}$$

are used together, where $\omega_K=\omega_1$ to $\omega_7$, $\omega_i/\omega_{i-1}=2.5$, and $(-1)^{l_1+l_2+l_3}=\Pi$. Based on $\Phi_K^{\omega_K}$, the basis functions of a specific representation $\mu$ can be induced by the following idempotents of the $D_{2d}$ group [3]:

$$e^{A_1}=\frac{1}{8}(1+p_{13}p_{24})(1+p_{12})(1+p_{34}), \tag{10.a}$$

$$e^{A_2}=\frac{1}{8}(1-p_{13}p_{24})(1-p_{12})(1-p_{34}), \tag{10.b}$$

$$e^{B_1}=\frac{1}{8}(1+p_{13}p_{24})(1-p_{12})(1-p_{34}), \tag{10.c}$$

$$e^{B_2}=\frac{1}{8}(1-p_{13}p_{24})(1+p_{12})(1+p_{34}), \tag{10.d}$$

TABLE III. The calculated energies $E(\lambda)$ (in a.u.) of the lowest $0^-(A_1)$ state with $\lambda=1$ and the lowest $0^-(B_1)$ state with $\lambda=0.95$ when $N_{\max}$ is given.

| $N_{\max}$ | 15 | 17 | 19 | 21 | 23 |
|---|---|---|---|---|---|
| $0^-(A_1)$ | −0.1088 | −0.1110 | −0.1128 | −0.1142 | −0.1153 |
| $0^-(B_1)$ | −0.1258 | −0.1267 | −0.1274 | −0.1279 | −0.1283 |

$$e^{E_{11}}=\frac{1}{4}(1-p_{12}p_{34}+p_{13}p_{24}-p_{14}p_{23}), \qquad (10.e)$$

$$e^{E_{22}}=\frac{1}{4}(1-p_{12}p_{34}-p_{13}p_{24}+p_{14}p_{23}). \qquad (10.f)$$

Besides, a subsidiary procedure is needed to extract a new set $\{\Psi_i\}$ from the old sets, so that the $\Psi_i$ are orthonormalized. The total number of $\Psi_i$ used for the diagonalization is determined by $N_{\max}$ which is the maximum of the sum $2(n_1+n_2+n_3)+l_1+l_2+l_3$. As examples, when $N_{\max}=23$, the number of $\Psi_i$ for the $0^-(A_1)$ and $0^-(B_1)$ states are 6655 and 7824, respectively.

Evidently, the above basis functions are designed for bound states but not for resonances. However, most states in Table II are resonances (as we shall see). In order to avoid such an awkward situation, we introduce an adjustable parameter $\lambda$ in the repulsive interactions as $\lambda(1/r_{12}+1/r_{34})$, while the attractive interactions remain unchanged. Such an adjustment does not change the threshold energies of the Ps + Ps channels. It is emphasized that the introduction of $\lambda$ does not at all alter the symmetry of the Hamiltonian, it remains to be invariant with respect to $O_3$ and $D_{2d}$. Therefore, the nature of the problem is not altered. Of course, what we really concern is the case with $\lambda$ close to 1.

Let the lowest eigenenergy of a given $(L\Pi\mu)$ symmetry be denoted as $E(\lambda)$. Then, our procedure is first to choose a $\lambda$ smaller than one so that $E(\lambda)$ is lower than the threshold of the SLOC. For example, for the $0^-(B_1)$ state, when $\lambda=0.95$, we have $E(\lambda)=-0.1282$ which is lower than the SLOC at $-0.1250$. Second, $\lambda$ is increased step by step (in each step $\lambda$ is increased by 0.01). When $\lambda$ is equal to a value $\lambda_o$ so that $E(\lambda_o)$ is lower than the threshold while $E(\lambda_o+0.01)$ is higher than the threshold, then the procedure stops and $\lambda_o$ is called as critical strength. In this way mainly bound states are concerned in the calculation. Evidently, if a state has a $\lambda_o$ much larger than one, it is deeply bound. If $\lambda_o$ is a little larger than one, it is just bound and a little lower than the dissociation threshold. If $\lambda_o$ is a little smaller than one, it is a resonance a little higher than the threshold. If $\lambda_o$ is remarkably smaller than one, the state is a high-lying resonance with a broad width, and we will neglect it.

To show the convergency of our calculation, the eigenenergies of selected states are listed at the last column of Table I (with $\lambda=1$). Besides, two series of eigenenergies are given in Table III in accord with $N_{\max}$. Owing to the difficulty in calculation, the basis functions with $N_{\max}>23$ are not adopted. The above results exhibit that the speed of convergency is not good, thus the calculated energies would not be useful if we want to know the exact locations of the levels (this is an effort beyond the aim and scope of this paper). However, if we just want to know which levels are relatively closer to their SLOC, then our results are useful.

TABLE IV. Bound states $b$ and narrow resonances $r$ of dipositronium together with their energies (in a.u.). The state lying upper is higher in energy. $\Delta$ is a small quantity (positive or negative) in the order of 0.001. The values of the energies of the $0^+$ and $1^-$ states come from the literature cited in Table I.

| $L^{\Pi}(\mu)$ | Energy | |
|---|---|---|
| $0^-(E)$ | $-0{,}090\,278+\Delta$ | $r$ or $b$ |
| $0^-(B_1)$ | $-0.1250+\Delta$ | $r$ or $b$ |
| $0^+(A_2)$ | −0.312 080 5 | $r$ |
| $0^+(B_2)$ | −0.314 468 9 | $b$ |
| $0^+(E)$ | −0.330 046 9 | $b$ |
| $1^-(B_2)$ | −0.334 408 | $b$ |
| $0^+(A_1)$ | −0.516 003 778 | $b$ |

The numerical results of $\lambda_o$ are summarized in Table II. In this table most $\lambda_o$ are remarkably smaller than one, the associated states are broad resonances and will not be further discussed. However, there are two and only two states, namely, the $0^-(E)$ and $0^-(B_1)$, have their $\lambda_o$ very close to one. They are distinguished from the others. Since, as mentioned before, all the calculated energies are a little higher than the actual values, the actual critical strength $\lambda_{\text{actual}}$ will be a little larger than the $\lambda_o$ listed in the table. Thus, the $\lambda_{\text{actual}}$ of the $0^-(E)$ and $0^-(B_1)$ will be in fact very close to one or even larger. Furthermore, the open channels of these two states have $l_R$ to be $p$ wave or higher, thus a centrifugal barrier exists. Therefore, among all the other states, these two states are candidates, they are either narrow resonances or bound states. If they are resonances, the $0^-(E)$ would emerge when two excited positroniums collide with each other [via the $(21)^p(31)$ or $(21)^d(32)$ channel]. Similarly, the $0^-(B_1)$ would emerge in the collision via the $(21)^p(21)$ channel. Once they are created, they are free from direct annihilation [12]. They would collapse either via their channel of formation, or would be transformed to a lower broad resonance via an $E1$ transition [the $0^-(E)$ would then become a $1^+(E)$, and the $0^-(B_1)$ become a $1^+(A_2)$], and then collapse via the $(10)^p(21)$ channel. Anyway, during the decay of these resonances, low-energy photons (from the above $E1$ transition and from the transition of an excited positronium to its ground state) can be detected. These low-energy photons would help the identification of these states.

## IV. FINAL REMARKS

In conclusion, the main outcome of this paper is the identification of the SLOC of dipositronium. The identification is proved to be very useful to the analysis of the existing data. Specifically, in addition to the two bound states that have been found previously, two more $0^+$ bound states have been identified, and a $0^+$ narrow resonances has been predicted. Furthermore, two $0^-$ states are found to have their energies very close to their SLOC (while the others are remarkably

higher). Besides, their SLOC contain centrifugal barrier. Thus they are either narrow resonances or loosely bound states. Since our calculation is not accurate enough, what they really are remained to be identified. Undoubtedly, the final identification of these two states is an attractive theoretical topic. In the experimental aspect, the search of the $0^+(A_2)$ resonance via the collision taking place in the $(10)^p(21)$ channel is first recommended, because its width is very narrow.

As a summary, a primary spectrum of dipositronium is proposed as shown in Table IV, where at least four bound states have been identified.

The above procedure is mainly based on symmetry consideration, the way of analysis can be generalized to study other molecules with symmetries other than $O_3$ and $D_{2d}$. In particular, the identification of the SLOC is important to the study of resonances of various molecules.

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[1] A. Wheeler, Ann. N.Y. Acad. Sci. **48**, 219 (1946).
[2] E. A. Hylleraas and A. Ore, Phys. Rev. **71**, 493 (1947).
[3] D. B. Kinghorn and R. D. Poshusta, Phys. Rev. A **47**, 3671 (1993).
[4] S. J. Gilbert, C. Kurz, R. G. Greves, and C. M. Surko, Appl. Phys. Lett. **70**, 1944 (1997).
[5] P. M. Kozlowski and L. Adamowicz, Phys. Rev. A **48**, 1903 (1993).
[6] A. M. Frolov, S. I. Kryuchkov, and V. H. Smith, Jr., Phys. Rev. A **51**, 4514 (1995).
[7] Y. K. Ho, Phys. Rev. A **39**, 2709 (1989); **48**, 4780 (1993).
[8] J.-M. Richard, Phys. Rev. A **49**, 3573 (1994).
[9] D. Bressanini, M. Mella, and G. Morosi, Phys. Rev. A **55**, 200 (1997).
[10] K. Varga, J. Usukura, and Y. Suzuki, Phys. Rev. Lett. **80**, 1876 (1998).
[11] M. Kamimura and H. Kameyama, Nucl. Phys. A **508**, 17c (1990).
[12] When only the two-photon process is assumed, the probability of annihilation is proportional to the probability of overlap of an electron with a positron $\langle \delta(\mathbf{r}_{e^+} - \mathbf{r}_{e^-}) \rangle$. If this quantity is zero, the associated state is free from direct annihilation. On the other hand, it has been stated in the text that *s*-partial wave is not allowed in $0^-$ states. However, wave function of any partial wave must be zero at $r=0$, except the *s* wave. Thus, the prohibition of the *s*-partial wave leads to $\langle \delta(\mathbf{r}_{e^+} - \mathbf{r}_{e^-}) \rangle = 0$, and therefore the $0^-$ states are free from direct annihilation.