Hyperspherical coupled-channel calculations of positronium formation in low-energy positron-helium collisions

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(Received 26 June 1995; revised manuscript received 2 August 1996)

The hyperspherical coupled-channel method is applied to the positron-helium scatterings in a low-energy region below 54.4 eV. An independent electron model is used for the helium atom under the approximation that the active electron is bound by a central model potential. All the hyperspherical adiabatic states associated with Ps(n,ℓ; n=1-4, ℓ=0-2) and He($1sn\ell$; n=1-5, ℓ=0-3) in the separated-atom limit are coupled for the expansion of the scattering equation, which is solved by means of a hybrid procedure of the diabatic-by-sector and the conventional adiabatic-basis-expansion methods. Excellent agreement is obtained with experiment for the positronium formation. [S1050-2947(96)06612-7]

PACS number(s): 34.70.+e, 36.10.Dr

I. INTRODUCTION

Scattering problems of few-body systems interacting through Coulomb potentials have been a long-standing subject of atomic physics in both theoretical and experimental research. Positronium formation is one of the most attractive processes among them, since exotic-particle scattering shows properties absent in ordinary particle scattering. The rapid progress of positron sources in the last decade has made the experimental study more and more feasible, and cooperative development of theoretical study is urgently desired.

Recently Igarashi and Toshima [1] have demonstrated that the hyperspherical coupled-channel method is a powerful theoretical approach to the study of positronium formation in positron-hydrogen collisions. Later the method was successfully extended to the process of antihydrogen formation [2] and to muon transfer between hydrogen isotopes [3]. Zhou and Lin [4] also studied positron-hydrogen scattering using the hyperspherical approach in a different representation of the adiabatic states. One of the merits of the hyperspherical coordinate method is that the Jacobi coordinate systems in the entrance and the rearranged channels can be unified into a common six-dimensional coordinate space and consequently the coupled scattering equations do not possess a nonlocal potential, which appears in the ordinary coupled-channel or close-coupling (CC) treatment of two-center rearrangement collisions and makes it very difficult to solve the multichannel coupled-equations accurately.

The application of the hyperspherical coordinate approach to scattering problems has been confined within three-body systems so far. The next desirable extension of the method is to the study of a two-electron atom target such as a helium atom, for which we have to deal with four bodies at least. Unfortunately solving the hyperspherical equations directly for four-body systems is not easy for scattering problems at present even if we use fast modern vector processors. An independent-electron approximation has often been used successfully for collision problems of two-electron systems. Even for ion-atom collisions, for which the treatment can be simplified by adoption of the impact-parameter method, the implementation of direct two-electron code encounters some difficulties [5].

In this study we use a model potential representation for the study of positronium formation from a helium atom. Hewitt, Noble, and Bransden [6] recently studied the same process using a model potential representation in the framework of the conventional close-coupling approximation. Although satisfactory agreement was obtained with measured values for some of the processes, the basis set they used for the expansion was not large enough to ensure that the expansion was well converged. In the previous studies [1–3] we showed that the hyperspherical coupled-channel method achieves much better convergence for rearrangement collisions than the conventional close-coupling method based on the atomic-orbital expansion. It is interesting to see how well the method can be extended to two-electron systems within an independent-electron approximation. Atomic units are used unless otherwise stated explicitly.

II. THEORY AND CALCULATIONS

We apply the hyperspherical coupled-channel method to positron-helium scattering in a collision energy range below 54.4 eV. The helium atom is treated as a single-electron atom in which the electron is moving under the influence of

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TABLE I. Eigenenergies of the bound states obtained by the model potential (1).

n	ℓ	Energy (a.u.)
1	0	-0.9047
2	0	-0.1574
2	1	-0.1277
3	0	-0.0644
3	1	-0.0564
3	2	-0.0555

a central potential from the He^+ core [7].

$$V_e(r) = -\frac{1}{r} - \frac{a+br}{r}\exp(-\beta r), \tag{1}$$

where $a=1.0$, $b=0.4143$, and $\beta=2.499$ [7]. This potential gives satisfactorily accurate energies of the ground state and singly excited states as shown in Table I. The accuracy of the eigenenergies of bound states is a very important factor in the calculation of collision processes, and the model potential method often gives better cross sections than the representation by the Hartree-Fock wave functions, which always give much worse eigenvalues. The interaction between the positron and the He^+ core is approximated by a static potential that is an average of the sum of the Coulomb potentials from the passive electron and from the helium nucleus over a simple hydrogenic distribution of an effective charge $Z_{eff}=27/16$ [6]. In this quasi-three-particle system, the Jacobi coordinates of the initial channel $(\mathbf{R}_T,\mathbf{r}_T)$ and of the final channel $(\mathbf{R}_P,\mathbf{r}_P)$ can be defined similarly to those for positron-hydrogen collisions [1]. The hyperradius ρ is related to the Jacobi coordinates as follows:

$$\mu\rho^2 = \mu_T R_T^2 + m_T r_T^2 = \mu_P R_P^2 + m_P r_P^2, \tag{2}$$

where m_T and m_P are the reduced masses of the helium atom and the positronium, and μ_T and μ_P the reduced masses for the relative motion in the entrance and the positronium formation channels, respectively. μ is an arbitrary parameter that has a dimension of mass and we set $\mu=1$ hereafter for simplicity. After separation of the center-of-mass motion of the total system, the kinetic-energy operator of the quasi-three particles is given by

$$T = -\frac{1}{2}\left(\frac{d^2}{d\rho^2} + \frac{5}{\rho}\frac{d}{d\rho} - \frac{\mathbf{\Lambda}^2}{\rho^2}\right). \tag{3}$$

Here the five-dimensional grand-angular-momentum operator Λ is given explicitly by

$$\mathbf{\Lambda}^2(\Omega) = -\frac{1}{\sin^2\phi_c\cos^2\phi_c}\left(\frac{d}{d\phi_c}\sin^2\phi_c\cos^2\phi_c\frac{d}{d\phi_c}\right) + \frac{\ell_{R_c}^2}{\cos^2\phi_c} + \frac{\ell_{r_c}^2}{\sin^2\phi_c}, \tag{4}$$

where the hyperangle ϕ_c is defined by

$$\tan\phi_c = \sqrt{m_c}r_c/\sqrt{\mu_c}R_c \tag{5}$$

and c denotes either T or P. The variable Ω represents the set of five angular-variables, ϕ_c, $\hat{r}_c$, and $\hat{R}_c$, and ℓ_{R_c} and ℓ_{r_c} are the angular-momentum operators in the ordinary three-dimensional space for the coordinates R_c and r_c, respectively.

The following procedure is analogous to the treatments used for the positron-hydrogen collisions [1] and for the muon transfer [3]. We solve the scattering equation

$$\left[-\frac{1}{2}\left(\frac{d^2}{d\rho^2} + \frac{5}{\rho}\frac{d}{d\rho}\right) + h_{ad}(\rho,\Omega) - E\right]\Psi(\rho,\Omega) = 0, \tag{6}$$

where

$$h_{ad} = \frac{\mathbf{\Lambda}^2}{2\rho^2} + V(\rho,\Omega), \tag{7}$$

and $V(\rho,\Omega)$ is the sum of the interaction potentials. The adiabatic basis functions are constructed by diagonalizing h_{ad} variationally in terms of Slater-type orbitals. $16s$, $11p$, $9d$, and $8f$ Slater orbitals are used on the helium side and $16s$, $11p$, and $9d$ Slater orbitals on the positronium side. The energy eigenvalues of the adiabatic potentials show good convergence for these Slater orbitals. The top three digits of the eigenvalue of the highest level used for the expansion mentioned below do not change for adding another five Slater orbitals to each angular momentum and better convergence is obtained for the lower levels.

The entire region of ρ is divided into a large number of small sectors, and the scattering wave function is expanded as a linear combination of basis functions that are adiabatic or diabatic locally in each sector. Namely, we have chosen a series of points of ρ in the range $0<\rho<\rho_{end}$, where ρ_{end} is the end point of integration. Then the boundaries of each sector are fixed to be the midpoints of these points. An adiabatic basis function at a point, ρ_k for instance, is used as a diabatic basis function throughout the sector if the corresponding state has an avoided crossing with another potential curve while the ordinary adiabatic representation is used if the state has no avoided crossing in the sector.

$$\phi_i^k(\rho,\Omega) = \begin{cases} \varphi_i(\rho,\Omega) & \text{if } \varphi_i \text{ has no avoided crossing,} \\ \varphi_i(\rho_k,\Omega) & \text{otherwise.} \end{cases} \tag{8}$$

The representation of each state is chosen independently in each sector; adiabatic representation is used in some sectors and diabatic representation is used in the other sectors for the same level. Substitution of the expansion

$$\Psi^k = \sum_i \frac{F_i^k(\rho)}{\rho^{5/2}}\phi_i^k(\rho,\Omega) \tag{9}$$

into the scattering equation (12) gives a set of coupled equations in a matrix representation for each sector;

$$\left(-\frac{1}{2}\frac{d^2}{d\rho^2} - E\right)\mathbf{F}^k = (S^k)^{-1}\left(-U^k + P^k\frac{d}{d\rho} + \frac{1}{2}Q^k\right)\mathbf{F}^k, \tag{10}$$

with

$$S_{ij}^k = \langle \phi_i^k | \phi_j^k \rangle, \tag{11}$$

$$P_{ij}^k = \left\langle \phi_i^k \left| \frac{d}{d\rho} \phi_j^k \right. \right\rangle, \tag{12}$$

$$Q_{ij}^k = \left\langle \phi_i^k \left| \frac{d^2}{d\rho^2} \phi_j^k \right. \right\rangle, \tag{13}$$

$$U_{ij}^k = \left\langle \phi_i^k \left| h_{ad} + \frac{15}{8\rho^2} \right| \phi_j^k \right\rangle. \tag{14}$$

Here $\mathbf{F}^k$ is a column vector whose ith component is the function $F_i^k(\rho)$. The overlap matrix S is diagonal in the subspace of the adiabatic states $\varphi_i(\rho;\Omega)$ and in that of the diabatic states $\varphi_i(\rho_k;\Omega)$. Note that the coupled equations (10) are exact except that the expansion of the wave function equation (9) is truncated up to a finite number. The matrix elements (12) and (13) are zero when the ket state ϕ_j^k is diabatic and the matrix (14) is diagonal when both the bra and ket states are adiabatic. The solution in the interval around ρ_k is matched to the solution in the adjacent sector around the next point ρ_{k+1} at the boundary $\rho_m = (\rho_k + \rho_{k+1})/2$ by requiring that the wave functions and their derivatives are smoothly connected. It is evident that the transformation matrix for the matching is diagonal among the components of the adiabatic basis functions. The solution in each sector is propagated to the next sector successively up to the outermost boundary $\rho = \rho_{end}$. The hyperspherical representation is projected onto the Jacobi representation in the last sector before the reactance matrix K is extracted from the asymptotic form of the scattering wave function [1].

III. RESULTS AND DISCUSSION

We set $\rho_{end} = 420$ and divided the interval $[0,\rho_{end}]$ into 1300 sectors, the widths of which were increased smoothly from the smallest value 0.002 near the origin for going to outer sectors. The ρ_{end} value was large enough to get reliable cross sections. Tentatively we enlarged ρ_{end} to 470 and confirmed that most of the cross sections change less than 1%. Only some small components corresponding to excitation to highly excited states changed by 2–3%. To see the convergence of the cross section for the number of the adiabatic basis functions, we employed two types of basis function set for comparison. The set A includes all the adiabatic states associated with Ps(n=1-3) and He($1sn\ell$; n=1-4) in the separated-atom limit. In the other set B the states associated with Ps($4s$,$4p$,$4d$) and He($5s$,$5p$,$5d$,$5f$) are added to the basis of the set A. For either set the same number of basis functions are used for the expansion in all the sectors to make the loss of the flux small even when high-lying states become closed at large ρ. The partial-wave expansion of the scattering wave is carried out up to the total angular momentum $J=7$. The maximum value $J=7$ is large enough to get converged cross sections in the energy range $E \leqslant 54.4$ eV. The unitarity of the S matrix is checked at each energy and the inaccuracy is kept less than 0.1% at the highest collision energy. The unitarity is maintained better as the collision energy decreases. The formation and excitation cross sections are multiplied by a factor of 2 for the account of the two electrons of the helium atom. Since the spin interaction is not taken into account explicitly in this study, all the electronic states belong to the singlet state throughout the collision.

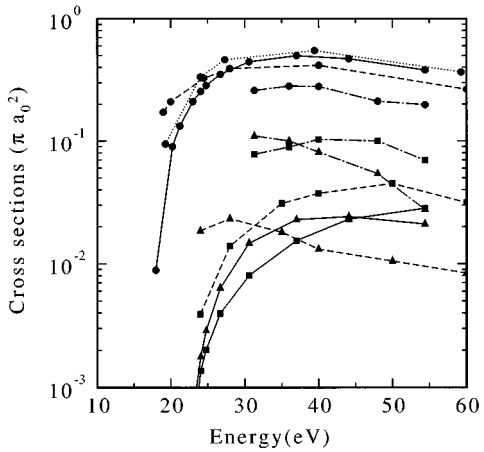

FIG. 1. Positronium formation cross sections in πa_0^2. Solid lines, the present hyperspherical coupled-channel method; dotted-dashed lines, the close-coupling calculations of Hewitt, Noble, and Bransden [6]; dashed lines, the distorted-wave calculations of Khan and co-workers [8]; dotted line, the distorted-wave calculations of Mandal, Guha, and Sil [9]. Curves connecting circles, squares, and triangles are for the formation of the ground state, the $2s$ state, and the $2p$ state, respectively.

Figure 1 shows cross sections for positronium formation into $1s$, $2s$, and $2p$ individual states. The basis set B is used for the calculations in this figure. The present cross sections for formation to the ground state are close to those of Khan, Ghosh, and Mazumdar [8] and Mandal, Guha, and Sil [9], who both used the distorted-wave approximation. Since the distorted-wave formalism is based on the perturbation theory that is essentially a high-energy approximation, the agreement between the two theoretical cross sections seems to be fortuitous. In fact, the close-coupling calculations of Hewitt, Noble, and Bransden, which can be regarded as more reliable than the perturbative treatment in this low-energy region, show poorer agreement with the present results, though the relative energy dependences of the three cross section curves are very similar. On the other hand, the cross sections for formation of the $n=2$ excited states show rather large disagreement with one another for both the energy dependence and the absolute values. At the energy of 30 eV, the cross sections of Hewitt, Noble, and Bransden are larger than ours by one order of magnitude.

The dependence of the formation cross sections on the basis functions is shown in Fig. 2. The formation cross sections for the ground state are almost identical for the two choices of the sets A and B and we can conclude that the values are well converged. On the other hand, the cross sections for the excited states are reduced considerably for going from set A to set B at high energies. It is not physically sound that the cross sections for $n=3$ are larger than those for $n=2$. Recently Errea *et al.* [11] reported similar behavior of the cross sections for the calculations of the electron capture in $He^{2+}+H$ collisions. According to their interpretation, ionization flux, which becomes larger than the electron-

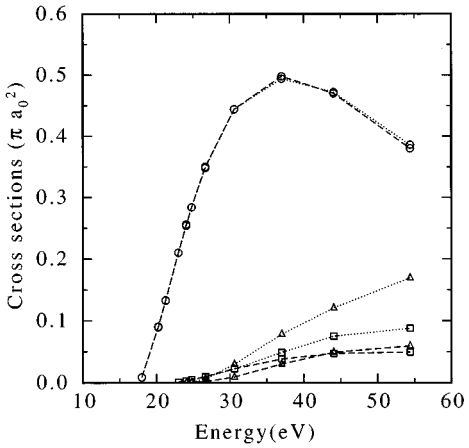

FIG. 2. The dependence of the formation cross sections on the size of the basis functions. The dotted lines are for the basis A and the dashed lines are for the basis B. Curves connecting circles, squares, and triangles are for the formation of the ground state, the $n=2$ state, and the $n=3$ state, respectively.

capture flux at high energies, is accumulated into the highest bound states if nonadiabatic couplings with continuum states are not properly taken into account, and, consequently, the capture cross sections in high-lying bound states are overestimated. Since all the adiabatic states in our calculations are connected with bound states of the positronium or the helium atom in the separated-atom limit, we conceive that the same enhancement of the population of the excited states has occurred in the present calculations.

In Fig. 3 we present the total formation cross sections of the two CC calculations and compare them with the measurements of Fromme *et al.* [10]. The present total cross sections are summed over all the positronium bound states included in the basis set B. The cross sections of Hewitt, Noble, and Bransden are extrapolated from their sum over $1s$, $2s$, and $2p$ states assuming the n^{-3} distribution law. The agreement of the present cross sections with the measurements is satisfactory, while the cross sections of Hewitt, Noble, and Bransden fail to reproduce them above 40 eV. The unsatisfactory energy dependence of their cross sections in this energy region is due to the large contribution of their $2s$ and $2p$ cross sections, which show a different energy dependence from other theoretical curves. Since the present cross sections for the formation of the $n=4$ excited states may be overestimated as stated in the preceding paragraph, we also present formation cross sections summed over $n=1$-3 states only. The agreement with the measured values has become even better.

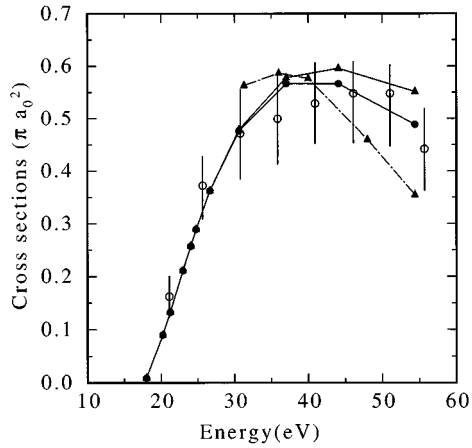

FIG. 3. The total formation cross sections in πa_0^2. Solid lines, present hyperspherical coupled-channel calculations; dotted-dashed line, close-coupling calculations by Hewitt, Noble, and Bransden. The solid line connecting solid circles gives cross sections summed over all the positronium bound states in the basis set B and the solid line connecting triangles gives cross sections summed over $n=1$–3 states only. The dotted-dashed line connecting solid triangles shows extrapolated cross sections of Hewitt, Noble, and Bransden assuming the n^{-3} law for the estimate of contribution of excited states with $n \geqslant 3$.

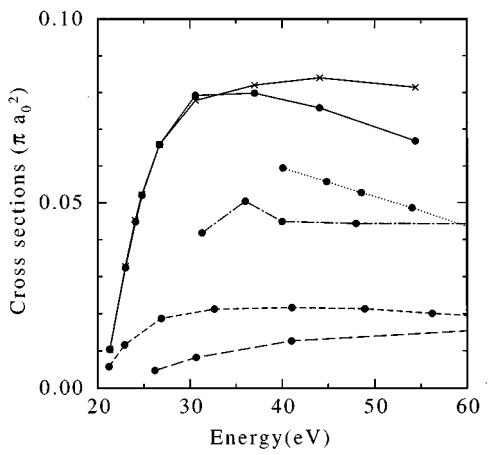

FIG. 4. Cross sections for excitation of He($2\ ^1S$) in πa_0^2. Solid line, present hyperspherical coupled-channel calculations (base B); dotted-dashed line, close-coupling calculations of Hewitt, Noble, and Bransden [6]; dotted line, close-coupling calculations of Willis and McDowell [14]; dashed line, the random-phase approximation of Varracchio [12]; long-dashed line, the distorted-wave approximation of Parcell, McEachran, and Stauffer [13]. The solid line connecting crosses is the present calculation for the base A.

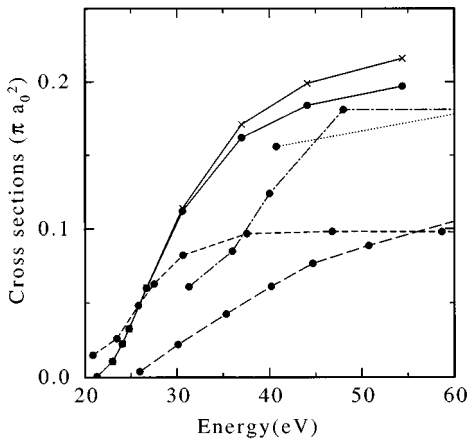

FIG. 5. The same as Fig. 4 but for the excitation of He($2\ ^1P$).

TABLE II. Positronium formation cross sections (πa_0^2) for $e^+ + He(1\,^1S)$ collisions. *A* and *B* denote the basis sets for the coupled equations (see the text) and the numbers in square brackets give the powers of 10 to be multiplied.

Energy (eV)	1*s*		2*s*		2*p*	
	A	*B*	*A*	*B*	*A*	*B*
18.0	8.94[-3]	8.86[-3]				
20.3	9.04[-2]	8.98[-2]				
21.3	1.33[-1]	1.32[-1]				
23.0	2.10[-1]	2.10[-1]	4.30[-4]	4.30[-4]	6.24[-4]	6.28[-4]
24.1	2.56[-1]	2.54[-1]	1.35[-3]	1.36[-3]	1.76[-3]	1.77[-3]
24.8	2.84[-1]	2.84[-1]	2.20[-3]	2.02[-3]	2.88[-3]	2.88[-3]
26.7	3.48[-1]	3.50[-1]	3.78[-3]	3.96[-3]	5.64[-3]	6.34[-3]
30.6	4.44[-1]	4.44[-1]	6.84[-3]	8.04[-3]	1.56[-2]	1.47[-2]
37.0	4.94[-1]	4.98[-1]	1.23[-2]	1.54[-2]	3.66[-2]	2.28[-2]
44.1	4.72[-1]	4.70[-1]	2.30[-2]	2.30[-2]	5.20[-2]	2.42[-2]
54.4	3.86[-1]	3.80[-1]	3.34[-2]	2.84[-2]	5.44[-2]	2.10[-2]

TABLE III. Excitation cross sections (πa_0^2) for $e^+ + He(1\,^1S)$ collisions. *A* and *B* denote the basis sets for the coupled equations (see the text) and the numbers in square brackets give the powers of 10 to be multiplied.

Energy (eV)	2*s*		2*p*	
	A	*B*	*A*	*B*
21.3	1.04[-2]	1.04[-2]	4.44[-3]	4.26[-3]
23.0	3.28[-2]	3.24[-2]	1.07[-2]	1.07[-2]
24.1	4.52[-2]	4.48[-2]	2.26[-2]	2.26[-2]
24.8	5.22[-2]	5.20[-2]	3.26[-2]	3.26[-2]
26.7	6.58[-2]	6.58[-2]	6.02[-2]	6.00[-2]
30.6	7.78[-2]	7.92[-2]	1.14[-1]	1.11[-1]
37.0	8.20[-2]	7.98[-2]	1.71[-1]	1.62[-1]
44.1	8.40[-2]	7.58[-2]	1.99[-1]	1.84[-1]
54.4	8.14[-2]	6.68[-2]	2.16[-1]	1.97[-1]

The $2\,^1S(1s2s)$ and $2\,^1P(1s2p)$ excitation cross sections are shown in Figs. 4 and 5. We see that larger discrepancy exists for the $2\,^1S$ excitation cross sections. Varracchio [12] used the random-phase approximation in the framework of the many-body perturbation theory. Parcell, McEachran, and Stauffer [13] calculated the cross sections by a distorted-wave approximation. Both theories are high-energy approximations and the reliability of these methods is not high in this low-energy region. Willis and McDowell [14] employed a single-center close-coupling method including pseudostates for the account of the polarization effect of the target helium atom. In the present calculations the polarizations of the target atom and the rearranged positronium are taken into account automatically by the adoption of the adiabatic basis functions in the hyperspherical representation. Hewitt, Noble, and Bransden [6] used a similar model potential to ours, and thus the disagreement of the two calculations arises from the difference of the theoretical description of the scattering problem and of the employed basis functions. We have used larger number of basis function for the expansion. Although the two close-coupling calculations of Hewitt, Noble, and Bransden and Willis and McDowell show mutual agreement; this does not mean that their calculations have achieved good convergence since both the methods are based on a similar formalism in terms of the unperturbed-atomic-orbital expansion. The polarization of the target helium atom is only partly taken into consideration by inclusion of a few pseudostates. The disagreement of the $2\,^1P$ excitation cross sections in Fig. 5 is smaller but the differences are not small enough to regard all the calculations as consistent. The $2\,^1S$ state is strongly coupled with the $2\,^1P$ state which has larger excitation cross sections. The polarization effect mixes these states easily and makes the $2\,^1S$ excitation cross sections more sensitive to the accuracy of employed approximations than the $2\,^1P$ excitation cross sections. Tables II and III summarize the present formation and excitation cross sections.

The convergence for the size of the coupled equations becomes worse for both the formation and the excitation as the collision energy increases. The present description of the scattering wave function is essentially based on the expansion in terms of adiabatic channel functions regardless of whether we use locally diabatic or adiabatic basis functions in each sector. When the incident velocity of the projectile is much larger than the average velocity of the target electron, the distortion of the internal electronic state is generally small and the representation by the atomic orbital is acceptable. If we use the adiabatically distorted-wave functions at such high energies, we need more basis functions to achieve convergence than in using unperturbed atomic orbitals. The interpretation of Errea *et al.* [11] for the overpopulation of high-lying states is another aspect of the same characteristics of the adiabatic-base expansion in a high-energy region. From these considerations we do not proceed to apply the present hyperspherical CC method to high energies above 54.4 eV.

In Fig. 6 we present the summed $2\,^1S$ and $2\,^1P$ excitation cross sections together with the measured values of Mori and

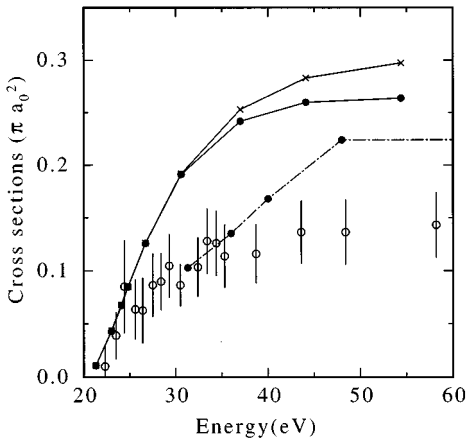

FIG. 6. The sum of $2\,^1S$ and $2\,^1P$ excitation cross sections. The notations of the theoretical curves are the same as in Figs. 4 and 5. Open circles are the measured values of Mori and Sueoka [15].

Sueoka [15]. All of the theoretical cross sections are larger than the experimental data. In the framework of the independent electron model, little account is taken of the *dynamical* correlation effect between the active and passive electrons, which can not be discriminated distinctly from the static correlation effect. The disagreement between the present results and the measured values is partly due to the defect of the independent-electron approximation. In the case of the formation, the dynamical correlation can be considered to be less important since it becomes small after the electron has been captured by the positron.

IV. SUMMARY

We have applied the hyperspherical coupled-channel method to two-electron systems within an independent-electron approximation. The helium atom is approximated as a quasi-one-electron atom with a central model potential. Good agreement is obtained with the experiment for the positronium formation cross sections but the present excitation cross sections to $2\,^1S$ and $2\,^1P$ states are larger than the measurements by a factor of 2. A better treatment for the two-electron atom is required to clarify the cause of the discrepancy with the measurement.

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