Positronium formation in e^+-Li scattering

P. S. Mazumdar
Department of Physics, Manipur University, Canchipur, Imphal 795 003, West Bengal, India

A. S. Ghosh
Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700 032, West Bengal, India

(Received 13 March 1986)

Positronium- (Ps) formation cross sections in positron-lithium scattering have been calculated by using the distorted-wave model of Khan and Ghosh. The results for the total and differential cross section are reported. The present Ps-formation cross section decreases with the increase of the incident positron energies. At about 100 eV, Ps formation is found to be negligible.

I. INTRODUCTION

We are studying positronium (Ps) formation in positron—alkali-atom scattering. For our first attempt we choose a lithium atom as our target. Ps formation in e^+—alkali-atom scattering is exothermic and a Ps atom can be formed even at zero incident positron energy. Moreover, the recent measurement of Stein *et al.*[1] on positron-alkali scattering has renewed theoretical interest in these processes.

Guha and Ghosh[2] have investigated the e^+-Li scattering using the adiabatic couple-static approximation. They have also reported results using polarization potentials in both channels. It has been noticed by them that Ps-formation cross sections are very sensitive to the method employed (Tables II and III of Ref. 2). Moreover, the polarization potential as used by them is not accurate and the effect of long-range forces is found to be appreciable even at an incident energy of 10.0 eV, the highest energy considered by them. It may be mentioned that the coupled-static Ps formation results for e^+-H (Basu *et al.*[3]) and e^+-He (Mandal *et al.*[4]) are not in good agreement with more elaborate theoretical predictions and the available measured values (see Ghosh *et al.*[5]). Guha and Saha[6] have applied the first Born approximation (FBA) to calculate the Ps-formation cross section in e^+-Li scattering in excited *ns* states. Guha and Mandal[7] have reported FBA and distorted-wave results for Ps formation in alkali atoms excluding Li. Mandal and Guha[8] have also carried out calculations for the excited *ns* states for the above system using the FBA. In all their calculations they have used a pseudopotential (a local Hellman type) to consider the effect of the core potential. The validity of and justification for this potential are not beyond question. Moreover, it is well known that the first Born approximation may not be suitable for rearrangement processes.

The distorted-wave method is an intermediate stage between the first-order approximation and more elaborate calculations. Moreover, the Ps-formation cross sections of Khan and Ghosh,[9,10] who have applied a distorted-wave polarized-orbital method to study e^+-H and e^+-He scattering, are found to be in good agreement with the available measured values and more elaborate theoretical predictions at intermediate energies. On considering these facts we have extended the method of Khan and Ghosh to study this rearrangement process. The incident-channel wave function is obtained by employing a polarized-orbital method (POM). The alkali atom is a highly polarizable target. The simple application of the polarized-orbital method may lead to erroneous predictions. Therefore we have applied the polarized-orbital equations of Bhatia *et al.*,[11] for the good representation of our incident-channel wave function. In the calculation of the scattering amplitude, we have omitted the polarized orbital ($\Phi_{\rm pol}$) for simplicity.

II. THEORY

Let $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$, and $\mathbf{x}$ be the position vectors of the target electrons and incident positron. The wave functions of the Li atom, the Li^+ ion, and the Ps atom are denoted by $\Phi_{\rm Li}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$, $\Phi^+_{\rm Li}(\mathbf{r}_1,\mathbf{r}_2)$, and $\eta(|\mathbf{r}_1-\mathbf{r}_2|)$, respectively. The ground-state Ps-formation scattering amplitude in e^+-Li scattering may be written as (in atomic units)

$$f^{(1)}_{\rm Ps}(\theta)=-\frac{\mu_f}{2\pi}\int \Psi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{x})V(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{x}) \times\Phi_{\rm Li}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)F(\mathbf{x})d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{x}\ , \quad (1)$$

where

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{x})=e^{i\mathbf{k}_f\cdot(\mathbf{r}_3+\mathbf{x})/2}\eta(|\mathbf{r}_3-\mathbf{x}|)\Phi_{\rm Li^+}+(\mathbf{r}_1,\mathbf{r}_2)\ . \quad (2)$$

$V(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{x})$ is the interaction potential and μ_f is the reduced mass in the final channel. The calculations have been performed by assuming the overlap integrals of the $1s$ orbitals of $\Phi_{\rm Li^+}$ and $\Phi_{\rm Li}$ to be unity.

To reduce the computational labor, we have also calcu-

lated the scattering amplitude given by the relation

$$f_{\rm Ps}^{(2)}(\theta)=-\frac{\mu_f}{2\pi}\int e^{-i\mathbf{k}_f\cdot(\mathbf{r}+\mathbf{x})/2}\eta^*(|\mathbf{r}-\mathbf{x}|)V(r,x)\times\Phi_{\rm Li}(2s,\mathbf{r})F(\mathbf{x})d\mathbf{r}\,d\mathbf{x}\ , \tag{3}$$

where

$$V(r,x)=\frac{1}{x}-\frac{1}{r}+V_c(x)\ . \tag{4}$$

Here $V_c(x)$ is the core potential calculated by using the wave function of the lithium ion (Clementi and Roetti[12]). The $2s$ wave function of the valence electron is denoted by $\Phi_{\rm Li}(2s,\mathbf{r})$. The incident-channel wave function of the positron has been calculated following the method of Bhatia *et al.*[11] The scattered orbitals $u_l(x)$ [i.e., the radial part of $F(\mathbf{x})$] of e^+-Li scattering is expressed as

$$\left[\frac{d^2}{dx^2}-\frac{l(l+1)}{x^2}+k_i^2\right]u_l(x)=[V(x)+V_{\rm pol}(x)]u_l(x)\ , \tag{5}$$

where $V(x)$ and $V_{\rm pol}(x)$ are the static and polarization potentials. The static potential is obtained from the relation

$$V(x)=4\Gamma_0(1s,1s;x)+2\Gamma_0(2s,2s,x)-\frac{2z}{x}\ ,$$

with

$$\Gamma_0(nl,n'l';x)=\frac{1}{x}\int_0^\infty P_{nl}(r)P_{n'l'}(r)dr+\int_x^\infty P_{nl}(r)\frac{1}{r}P_{n'l'}(r)dr\ . \tag{6}$$

The wave functions of the Li atom and ion are taken from Clementi and Roetti.[12] The notation used here is defined by Bhatia *et al.*[11] The values of the polarization potential $V_{\rm pol}(x)$ are taken from the curve labeled "polarized orbital" (modified method) of Bhatia *et al.*[11]

It may be mentioned that the corresponding first Born amplitude may be obtained by replacing $F(\mathbf{x})$ with $e^{i\mathbf{k}_i\cdot\mathbf{x}}$, $\mathbf{k}_i$ and $\mathbf{k}_f$ being the momenta in the initial and final channels.

III. RESULTS AND DISCUSSIONS

The Ps-formation cross sections have been calculated using the two expressions [$f_{\rm Ps}^{(1)}(\theta)$ and $f_{\rm Ps}^{(2)}(\theta)$] for the scattering amplitude. It has been found that the two results differ by less than 1% from each other. The scattered orbitals $u_l(x)$ are numerically integrated using the Numerov method up to a radial distance of 40.0 a.u. The $u_l(x)$ for $x>40.0$ a.u. is calculated by replacing it with its asymptotic form. The FBA amplitudes are calculated with and without partial-wave analysis and the two results are found to be identical to three significant digits. In obtaining our results, we have replaced higher-order partial-wave contributions by those of the FBA. The distorted-wave total cross sections are obtained by the relations

$$\sigma_{\rm Ps}^{\rm DW}=\sum_{l=0}^{L}\sigma_{\rm Ps}^{\rm DW}(l)-\sum_{l=0}^{L}\sigma_{\rm Ps}^{B}(l)+\sigma_{\rm Ps}^{B}\ .$$

The differential cross section has also been obtained by replacing the higher partial waves with the corresponding FBA amplitude. However, care has been taken to ensure the following:

$$\sigma_{\rm Ps}^{\rm DW}(L-1)\simeq\sigma_{\rm Ps}^{B}(L-1)$$

and

$$f^{\rm DW}(L-1)\simeq f^{B}(L-1)\ .$$

It has been found (Khan and Ghosh[9,10]) that the present distorted-wave model is not suitable near the threshold energy. For this reason we have not calculated the cross section below an incident energy of 2.0 eV. Figure 1 depicts the present Ps-formation cross sections in the energy region 2.0–20.0 eV. The same figure also contains the predictions of the FBA and of Guha and Ghosh. The numerical values of the total Ps-formation cross sections are tabulated in Table I up to an incident energy of 100.0 eV. Figure 1 shows that the present results lie always below the FBA predictions. Above this energy, the difference

TABLE I. Positronium-formation cross section (in units of πa_0^2) in e^+-Li scattering.

Energy (eV)	FBA	Present work
2.0	115.39	104.28
3.4	68.00	56.53
5.0	40.17	32.94
7.5	19.83	16.55
10.0	10.74	9.20
13.6	4.84	4.37
20.0	1.48	1.38
30.0	0.30	0.30
50.0	0.21–1	0.29–1
100.0	0.16–2	0.43–2

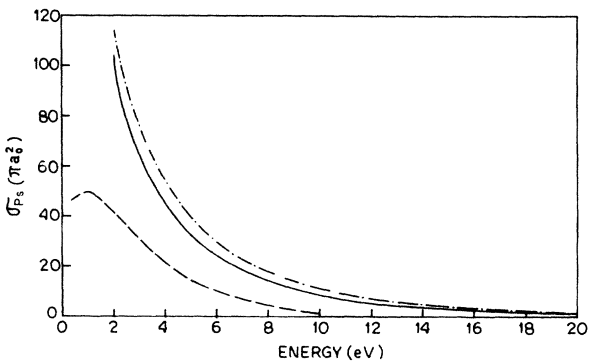

FIG. 1. Ps formation cross section (in untis of πa_0^2): ——, present results; — — —, FBA; and —·—·—·, Guha and Ghosh.

between the present and the FBA results is marginal. This feature has also been noticed by Khan and Ghosh[9,10] for the case of hydrogen and helium. The adiabatic coupled-static results of Guha and Ghosh[2] differ appreciably from the present results, the present results being always higher. The Ps-formation cross section is not appreciable at an incident energy of 100.0 eV in e^+-Li scattering. There is no reason to calculate Ps formation above this incident energy.

Three differential cross sections at 2.0, 10.0, and 20.0 eV are plotted in Fig. 2. The difference between the present and the FBA results is greatest at 2.0 eV as expected. The minimum in the differential cross section at 2.0 eV is obtained at about 50°, whereas the FBA predicts a zero in the cross section at about 44°. With increasing energy, the positions of the minimum of the present result and the zero of the FBA results are shifted towards the forward angle. Moreover, the difference between the positions of the minimum and the zero decreases with increasing energy. This conforms with the fact that the difference between the present and the FBA results decreases with increasing energy.

The accuracy of the present results cannot be ascertained with the present state of the art. It has also been pointed out that coupled-static results may not be fully reliable near the threshold energy.

The present distorted-wave results above 10 eV are in satisfactory agreement with those of Guha and Ghosh who have performed a coupled-static calculation. It has been found by Khan and Ghosh that the distorted-wave approximation is reliable in predicting the Ps formation cross section at the energy double that of the ionization threshold. The agreement between the present results with those of the coupled-static results above an incident energy of 10 eV shows the validity of the present method. Considering these facts, we conclude that the present results may be meaningful above 10 eV.

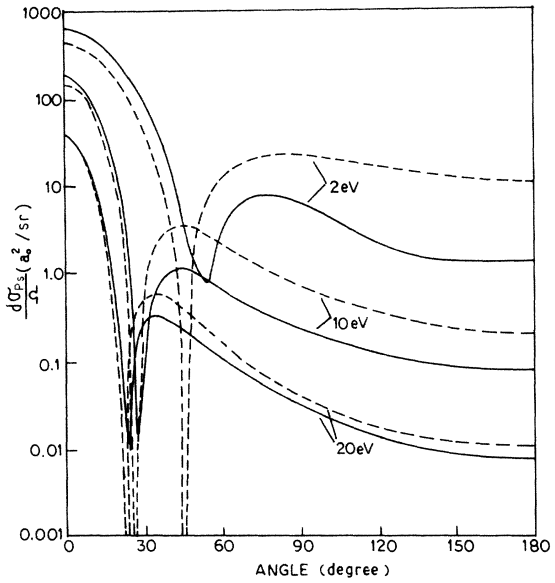

FIG. 2. Differential cross section in e^+-Li scattering at the incident energy 2.0, 10.0, and 20 eV: ——, present result and — — —, FBA.

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