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We studied e^+-Li and e^+-Na scattering using the close coupling approximation in the static and coupled static expansion schemes. The effect of the positronium formation on the elastic channel is found to be strong in both cases. In the case of the lithium atom the effect is dramatic; the inclusion of the positronium formation channel transforms the purely repulsive effective e^+-Li S wave (static) potential to a predominantly attractive (coupled static) potential. In this case, in the static model $\delta(0) - \delta(\infty) = 0$, whereas in the coupled static model $\delta(0) - \delta(\infty) = \pi$. According to Levinson's theorem this suggests the presence of a S wave bound or continuum bound state in the e^+-Li system.

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The close-coupling approximation scheme (CCA) provides a practical framework for dealing with electron-atom and positron-atom scattering. Unlike the variational calculations, CCA deals with rearrangement and elastic channels in an unified way and provides results for ionization and positronium formation. The main framework for positron-atom scattering has been the CCA scheme. This approach has been frequently used in e^+-H and e^+-He scattering[1–10].

Recently, there has been experimental[11,12] and theoretical activities in positron-alkali-metal-atom scattering[13–20]. The CCA scheme has been employed in the theoretical studies. However, due to technical difficulties it is not easy to include the rearrangement positronium (Ps) formation channels in the case of these large atoms. Hence most of the CCA calculations have neglected these channels. There has been some calculations including the positronium formation channel employing simple atomic wave functions[20]. Even in these calculations a systematic study of the effect of the positronium formation channel in positron-alkali-metal-atom scattering has not been made. In the present letter we make such a study of the positronium formation channel in the CCA treatment of positron-lithium and positron-sodium scattering employing realistic atomic wave functions. It should be noted that any meaningful CCA calculation of positron-alkali-metal-atom scattering should include the positronium formation channel, as this channel is already open at the elastic scattering threshold.

We studied e^+-Li and e^+-Na scattering using the CCA approach in the static and coupled static expansion schemes. The effect of the positronium formation on the elastic channel is found to be strong in both cases. In the case of the lithium atom the effect is dramatic; the inclusion of the positronium formation channel transforms the purely repulsive efective e^+-Li S wave (static) potential to a predominantly attractive (coupled static) potential. In this case, in actual calculation we find that in the static model $\delta(0) - \delta(\infty) = 0$, whereas in the coupled static model $\delta(0) - \delta(\infty) = \pi$. In both cases $\delta(E)$ is the S wave phase shift at energy E. In any positron-atom scattering this finding is completely new and for S wave elastic scattering one always had $\delta(0) - \delta(\infty) = 0$. Levinson has shown that for a short range local potential[21]

$$\delta(0) - \delta(\infty) = N\pi, \tag{1}$$

where N is the number of bound, continuum bound, or the (Pauli) forbidden states of the system. Larger the N the stronger is the attraction in the system. This means that the inclusion of the positronium formation channel in the CCA approach to the elastic e^+-Li scattering will result in strong attraction.

In the following we give the details of the e^+-Li equations we use. In the case of e^+-Na scattering the equations can be similarly written down. In the CCA approach the total wave function for the positron-lithium-atom system is written as[13]

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{x}) = \sum_i \Phi_i(\vec{r}_1,\vec{r}_2,\vec{r}_3)F_i(\vec{x}) + \sum_\nu \Phi^+_{1s}(\vec{r}_1,\vec{r}_2)\eta_\nu(\rho)G_\nu(\vec{R}), \tag{2}$$

with

$$\rho = |\vec{x} - \vec{r}_3|, \qquad R = |\vec{r}_3 + \vec{x}|/2, \tag{3}$$

where $\vec{r}_i (i = 1,2,3)$ are the coordinates of the atomic electrons and $\vec{x}$ is the positron coordinate. Here $\Phi_i(\vec{r}_1,\vec{r}_2,\vec{r}_3)$ and $\eta_\nu(\vec{\rho})$ are the ith and νth eigenstates of the lithium and the positronium atom systems, respectively. The ground state wave function of the lithium ion is described by $\Phi^+_{1s}(\vec{r}_1,\vec{r}_2)$, $F_i(\vec{x})$ describes the motion of the incident positron and $G_\nu(\vec{R})$ describes the relative motion between the positronium and the lithium ion. In our treatment we plan to include only one term in each sum of Eq. (2), e.g., the ground states of both lithium and positronium atoms.

We shall be working with the usual coupled scattering integral Lippmann-Schwinger type equations of the CCA approach which are written in the following form:[1-10]

$$f_{\beta\alpha}(\vec{k}',\vec{k}) = f^B_{\beta\alpha}(\vec{k}',\vec{k}) - \frac{1}{4\pi^2\mu_\nu}\sum_\nu \int d\vec{k}'' \frac{f^B_{\beta\nu}(\vec{k}',\vec{k}'')f_{\nu\alpha}(\vec{k}'',\vec{k})}{E + i0 - E_n}. \tag{4}$$

Here $f_{\beta\alpha}(\vec{k}',\vec{k})$ is the scattering amplitude for transition from channel α to channel β, $\vec{k}$ and $\vec{k}'$ are the relevant relative momenta in these channels, μ_ν is the reduced mass in channel ν, $f^B_{\beta\alpha}(\vec{k}',\vec{k})$ is the corresponding Born amplitude. The partial wave expansion of $f_{\beta\alpha}(\vec{k}',\vec{k})$ from the initial state $|lm>$ to the final state $<l'm'|$ is given by

$$f_{\beta\alpha}(\vec{k}',\vec{k}) = \frac{1}{(kk')^{1/2}}\sum_{JM}\sum_{L,M_L}\sum_{L',M_{L'}} < L'l'M_{L'}m'|JM >< LlM_Lm|JM > \times T^J_{\beta\alpha}(\tau'k',\tau k)Y^*_{L'M_{L'}}(\hat{k}')Y_{LM_L}(\hat{k}), \tag{5}$$

where L and M_L are orbital angular momentum and projection of the incident state, and J and M are the total angular momentum and projection, $< LlM_Lm|JM >$ is the usual Clebsch-Gordan coefficient. A similar partial wave expansion holds for the Born term. Also, τ stands for the collective quantum numbers (n,l,m), n being the principal quantum number.

After partial wave analysis the coupled integral equations become

$$T^J_{\beta\alpha}(\tau'k',\tau k) = B^J_{\beta\alpha}(\tau'k',\tau k) + \frac{1}{2\pi^2}\sum_\nu \int k''^2 dk'' \frac{B^J_{\beta\nu}(\tau'k',\tau''k'')T^J_{\nu\alpha}(\tau''k'',\tau k)}{k''^2 - k^2_\alpha - i0}. \tag{6}$$

The partial wave projection for the Born term in this equation is given by

$$B^J_{\beta\alpha}(\tau'k',\tau k) = \frac{(kk')^{1/2}}{2J+1}\sum_{MM_LM_{L'}}\sum_{mm'} < L'l'M_{L'}m'|JM >< LlM_Lm|JM > \times \int d\vec{k}d\vec{k}'Y^*_{L'M_{L'}}(\hat{k}')Y_{LM_L}(\hat{k})f^B_{\beta\alpha}(\vec{k}',\vec{k}). \tag{7}$$

The elastic scattering phase shift for the elastic channel denoted by suffix 1 is defined by

$$\delta_J = \frac{1}{2}\arctan\left[\frac{Re(T^J_{11})}{2\pi - Im(T^J_{11})}\right], \tag{8}$$

where T^J_{11} is the on-shell elastic t matrix element.

The positronium formation cross section is given by

$$\sigma_{12} = \frac{1}{k^2}\sum_J \frac{2j+1}{4\pi}|T^J_{12}|^2 \tag{9}$$

where the suffix 2 denotes the rearrangement channel for positronium formation.

The Born martix element for the elastic channel is given by

$$f^B_{11}(\vec{k}_f,\vec{k}_i) = -\frac{1}{2\pi}\int e^{i\vec{k}_i\cdot\vec{x}}\Phi^*_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3)\left[\frac{Z}{x} - \frac{1}{|\vec{x}-\vec{r}_1|} - \frac{1}{|\vec{x}-\vec{r}_2|} - \frac{1}{|\vec{x}-\vec{r}_3|}\right] \times \Phi_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3)d\vec{r}_1d\vec{r}_2d\vec{r}_3d\vec{x}. \tag{10}$$

In this equation Z is the number of atomic electrons and $\vec{k} = \vec{k}_i - \vec{k}_f$. The lithium wave function is given by

$$\Phi_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = u_{1s}(\vec{r}_1)u_{1s}(\vec{r}_2)u_{2s}(\vec{r}_3) \tag{11}$$

where the atomic orbitals for the 1s and the 2s electrons are given by

$$u_{ns}(\vec{r}) = \sum_{i=1}^{6} a_i(ns)r^{(m_i-1)}e^{-\lambda_i r}Y_{00}(\hat{r}). \tag{12}$$

The Born matrix element for the positronium formation channel is given by

$$f^B_{21}(\vec{k}_f,\vec{k}_i) = -\frac{1}{\pi}\int e^{i\vec{\rho}\cdot\vec{x}}e^{-i\vec{k}_f\cdot\vec{r}_3/2}\eta^*_{1s}(|\vec{x}-\vec{r}_3|)\Phi^*_{Li^+}(\vec{r}_1,\vec{r}_2)\left[\left(\frac{Z}{x} - \frac{Z}{r_3}\right) - \left(\frac{1}{|\vec{x}-\vec{r}_1|} - \frac{1}{|\vec{r}_3-\vec{r}_1|}\right) - \left(\frac{1}{|\vec{x}-\vec{r}_2|} - \frac{1}{|\vec{r}_3-\vec{r}_2|}\right)\right]\Phi_{2s}(\vec{r}_1,\vec{r}_2,\vec{r}_3)d\vec{r}_1d\vec{r}_2d\vec{r}_3d\vec{x}. \tag{13}$$

In this equation $\vec{\rho} = \vec{k}_i - \vec{k}_f/2$. The lithium ion wave function is taken to be given by

$$\Phi_{Li^+}(\vec{r}_1,\vec{r}_2) = u^+_{1s}(\vec{r}_1)u^+_{1s}(\vec{r}_2) \tag{14}$$

where the atomic orbitals are given by

$$u^+_{1s}(\vec{r}) = \sum_{i=1}^{4} a_i^+(1s)e^{-\lambda_i r}Y_{00}(\hat{r}). \quad (15)$$

The constants for this wave function are taken from Ref.[22]. In the calculation it is assumed that only the $2s$ electron participates in the positronium formation.

The resulting partial wave scattering integral equation for the t matrix is solved by the standard matrix inversion technique[1–8, 23]. It was also solved by a subtraction technique[24, 25] and both methods yielded identical results. The subtraction technique uses the solution of an auxiliary real Γ matrix equation and troubles with the principal value integral and inversion of a large complex matrix is largely avoided in this approach. As the subtraction tecchnique uses a real integral equation in place of the usual complex Lippmann-Schwinger equation for the t matrix, it yields numerically stable results with fewer integration mesh points. Finally, in the subtraction technique the complex on-shell t matrix is constructed algebraically using a complex integral over the real on-shell Γ matrix. This is the first application of the subtraction technique in atomic scattering. A detailed description of this application will be published elsewhere.

Similar Born terms appear in the case of the sodium atom. However, in this case the atomic wave function is taken to be that of a hydrogen-like atom with only one electron in the $3S$ state given by

$$\phi_{3s}(r) = \frac{1}{\sqrt{(4\pi)}} \sum_{i=1}^{8} c_i(3s)r^{(m_i-1)}e^{-\lambda_i r} \quad (16)$$

The constants of the wave functions are taken from Clementi and Roetti[22]. We do not explicitly show the equations for the Born term in the case of the sodium atom. However, it is interesting to point out that in the calculation of the Na($3s$)-Na($3s$) Born amplitude all the 11 electrons have been taken into account.

First, we exhibit results of e^+-Li scattering. In Figs. 1 and 2 we exhibit the results of elastic scattering phase shifts in S and P waves for static and coupled static calculations. In both cases the energy dependence of the static phase shift is weak in nature, but the coupled-static phase shift varies rapidly with energy. In the S wave case there is a jump of π in the coupled-static phase shift as energy varies from 0 to ∞. There is no such jump in the static S wave phase shift. This finding is not only new, but is also unexpected in view of available results in positron-atom scattering in the case of other atoms.

In the case of e^+-Li scattering the coupled-static phase shift is positive upto an incident positron energy of 5 eV indicating the presence of overall attraction at low energies in the elastic channel. However, at higher energies the phase shift is negative reflecting a repulsive

effective potential. In the configuration space this means that the S wave effective positron-lithium potential is attractive at large distances and possesses a repulsive core at small distances. This jump of π in the coupled-static phase shift has interesting consequence on the Levinson's theorem (1): the number N of bound, or continuum-bound, or forbidden states in this case is one[21]. It is not clear whether one has a real bound state in the e^+-Li system. Whether it is a real bound state or not $N = 1$ in Eq. (1) will mean much more attraction in the elastic channel[21]. Hence the effect of the positronium formation channel on the elastic process is dramatic as we shall see in the consideration for the cross section in the following.

In Fig. 3 (a) we plot the S (static and coupled static) and P (coupled static) wave elastic cross sections for e^+-Li scattering. At low energies the S wave coupled-static cross section is much (about ten times) larger than the static cross section reflecting the strong effect of the positronium formation channel. This was already implicit in Table I of Basu and Ghosh[13]. There it has been found that the inclusion of the Ps(1s) channel has dramatic effect on the elastic channel; whereas the $2p$ channel only has small contribution once the Ps(1s) channel is included. At about 5 eV the S wave coupled static cross section is zero. This is a consequence of having zero elastic scattering phase shift at this energy. The dramatic enhancement of the elastic S wave cross section with the inclusion of the positronium formation channel at low incident energies reflects the fact that the lithium atom is a highly polarizable target. The P wave coupled-static cross section is very small compared to S wave cross sections at low energies due to the centrifugal barrier in this case but at moderate energies it could be higher as we see in Fig. 3 (a).

In Fig. 3 (b) we exhibit the coupled-static positronium formation cross section in S and P waves. Both exhibit broad resonance-like behavior in the energy range 20–50 eV. The appearance of resonance in the positronium formation is, however, not new. Resonances have been reported in positronium formation in positron-hydrogen scattering[26]. Qualitatively, in e^+-Li scattering the S and P wave cross sections for positronium formation are similar.

Next we present results for e^+-Na scattering. In Fig. 4 the S wave static and coupled static elastic scattering phase shifts are plotted. In this case there is strong effect of positronium formation at low (¡ 50 eV) energies. However, the effect is much less pronounced than in the case of positron-lithium scattering.

In Fig. 5 (a) we plot the S (static and coupled static) and P (coupled static) wave elastic cross sections for e^+-Na scattering. Compared to e^+-Li scattering, at low energies, the effect of the positronium formation channel is less pronounced. At low energies, the S

wave coupled-static cross section is (about six times) larger than the static cross section in this case. However, apart from this quantitative difference, Fig. 5 (a) is quite similar to Fig. 3 (a) where the same results are plotted in the case of e^+-Li scattering. Again the P wave coupled-static cross section is very small compared to S wave cross sections at low energies due to the centrifugal barrier in this case but at moderate energies it could be larger.

In Fig. 5 (b) we exhibit the coupled-static positronium formation cross section in S and P waves. Both exhibit broad resonance-like behavior in the energy range 20–150 eV. Qualitatively, the S and P wave cross sections for positronium formation are similar.

The present results are in fair agreement with previous calculations. However, in previous calculations phase shifts were not plotted. Also, a quantitative comparison of results of various calculations is not to the point, because different approximations were employed in various calculations. For example, the atomic wave functions used by Basu and Ghose[13, 20] are different from those employed in the present calculation. However, the qualitative features of these two calculations are similar whenever results are available. The calculation of Ghosh et al.[14, 15] and Ward et al.[18] did not include the positronium formation channel. As we are studying the importance of the positronium formation channel, it is not fair to compare these two calculations.

In conclusion, we have exhibited the strong effect of the positronium formation channel in positron-lithium and positron-sodium scattering. In the case of positron-lithium scattering the effect of the positronium formation channel is dramatic on S wave elastic scattering. Inclusion of this channel changes the Levinson's theorem for this process. The parameter N denoting the number of bound, continuum-bound, or forbidden states changes from 0 to 1 as the positronium formation channel is included. To the best of our knowledge in all positron-atom calculations reported so far one has $\delta(0) - \delta(\infty) = 0$, and not π as in the present study of e^+-Li scattering. This implies very strong attraction and a dramatic change of the S wave elastic e^+-Li scattering cross section. Previous calculations on this system have observed this large effect on the phase shift[13]. We present results of S and P wave phase shifts, elastic and rearrangement cross sections for both positron-lithium and positron-sodium scattering.

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Figure Caption

1. S wave static (full line) and coupled static (dashed line) elastic scattering phase shifts at various energies for positron-lithium scattering.

2. P wave static (full line) and coupled static (dashed line) elastic scattering phase shifts at various energies for positron-lithium scattering.

3. S wave static (full line), coupled static (long dashed line), and P wave coupled static (short dashed line) (a) elastic and (b) positronium formation cross sections at various energies for positron-lithium scattering. Note that there is no positronium formation in the static model.

4. S wave static (full line) and coupled static (dashed line) elastic scattering phase shifts at various energies for positron-sodium scattering.

5. S wave static (full line), coupled static (long dashed line), and P wave coupled static (short dashed line) (a) elastic and (b) positronium formation cross sections at various energies for positron-sodium scattering. Note that there is no positronium formation in the static model.

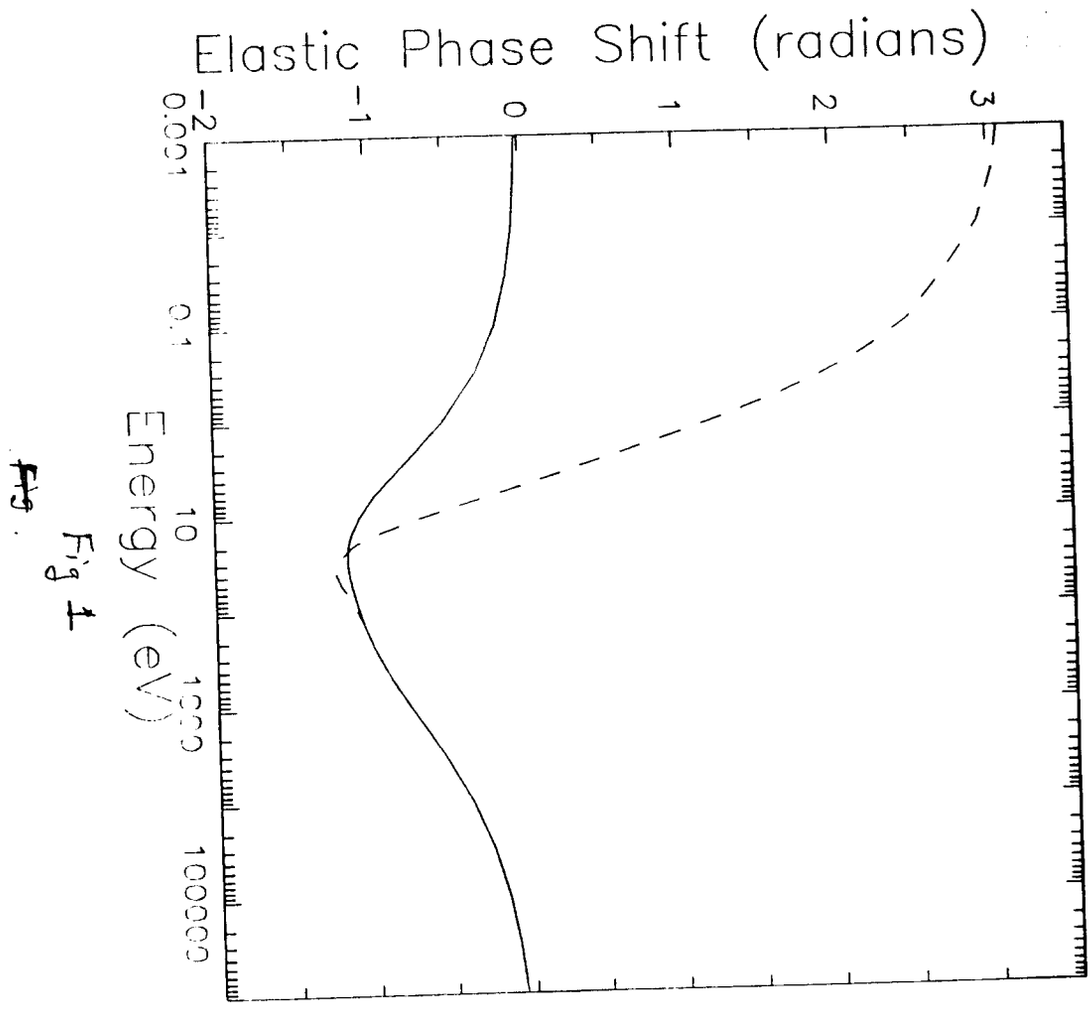

Fig 1

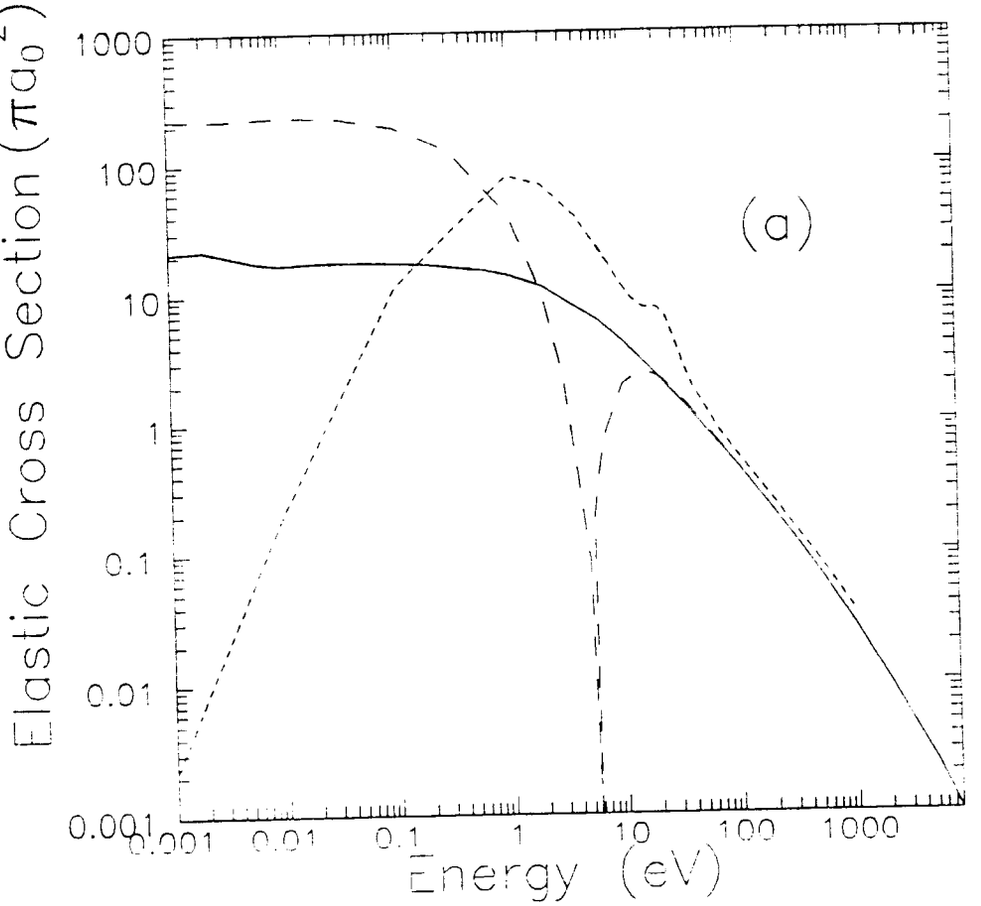
Elastic Cross Section (πa_0^2)
1000
100
10
1
0.1
0.01
0.001
(a)
0.001
0.01
0.1
1
10
100
1000
Energy (eV)

Fig 3a

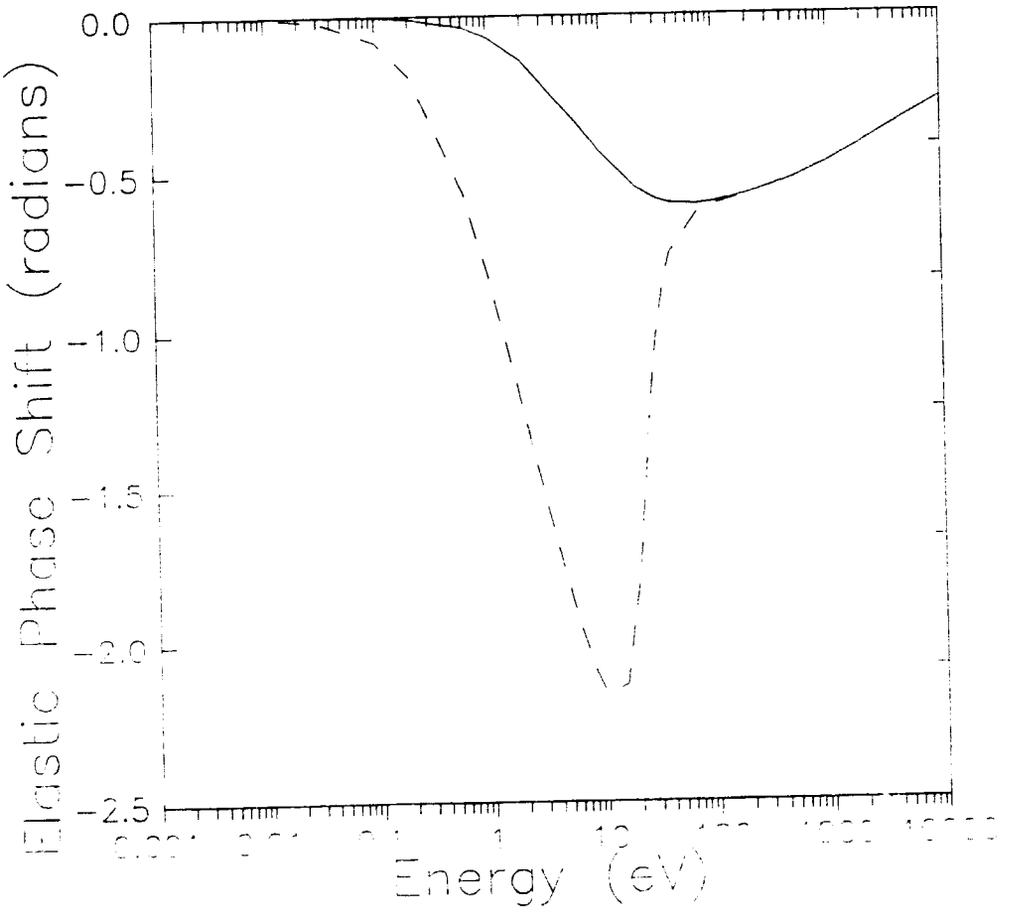
Elastic Phase Shift (radians)
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
Energy (eV)

Fig 2

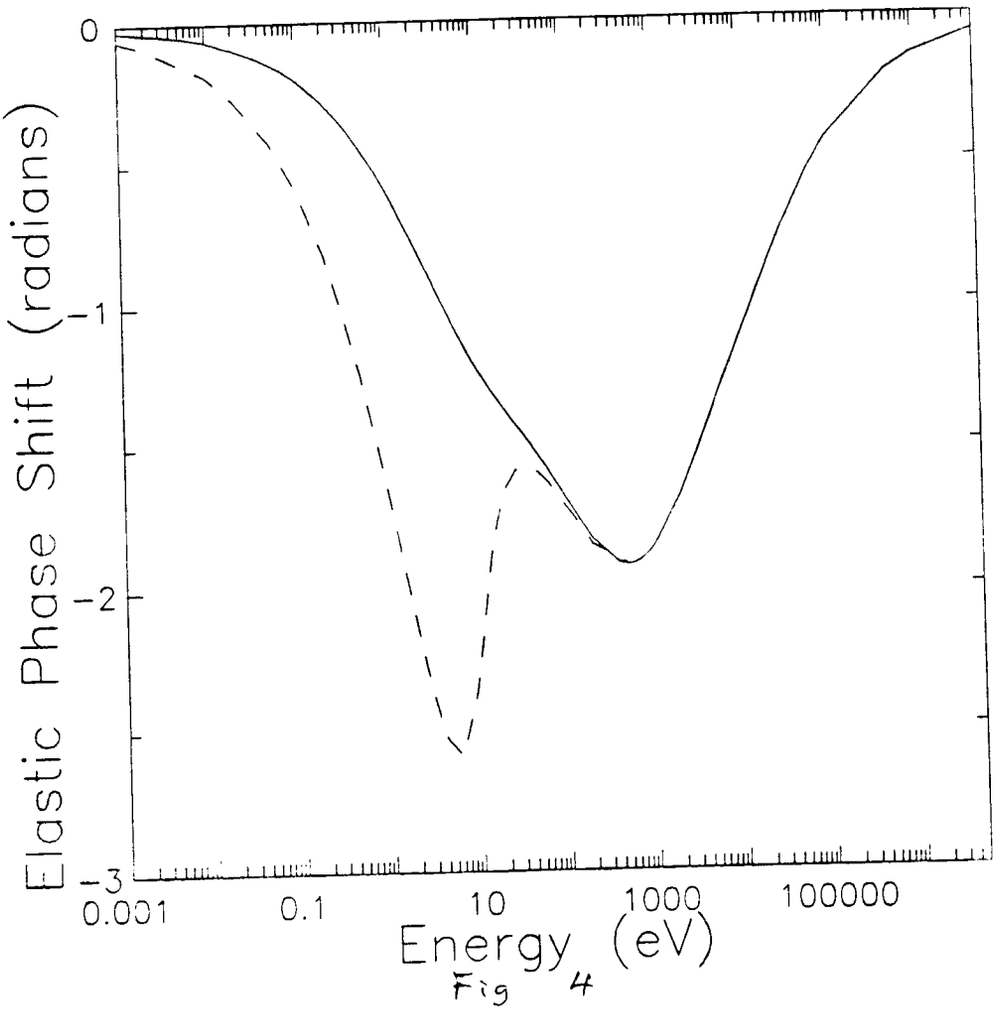
Elastic Phase Shift (radians)
0
-1
-2
-3
0.001
0.1
10
1000
100000
Energy (eV)

Fig 4

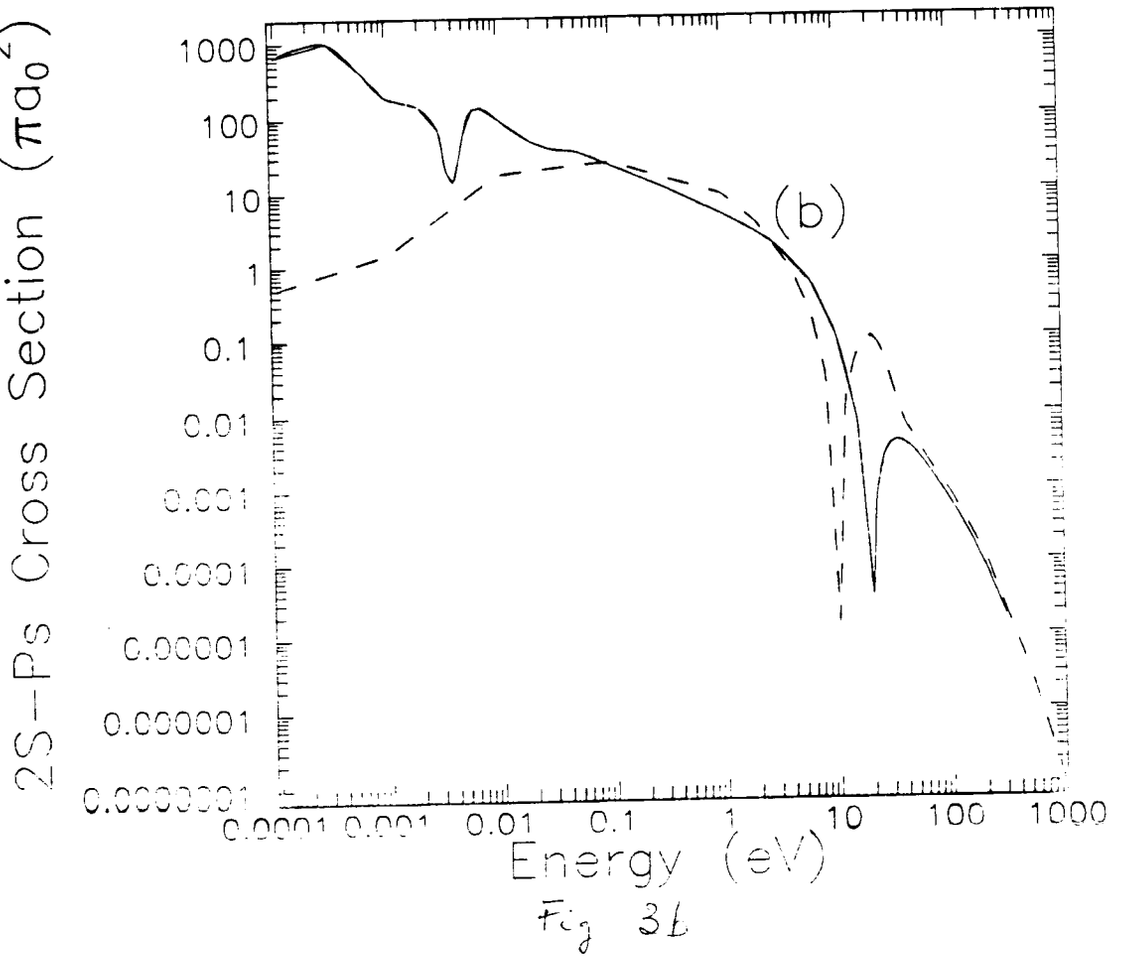
2S-Ps Cross Section (πa_0^2)
1000
100
10
1
0.1
0.01
0.001
0.0001
0.00001
0.000001
0.0000001
0.0001
0.001
0.01
0.1
1
10
100
1000
(b)
Energy (eV)

Fig 3b

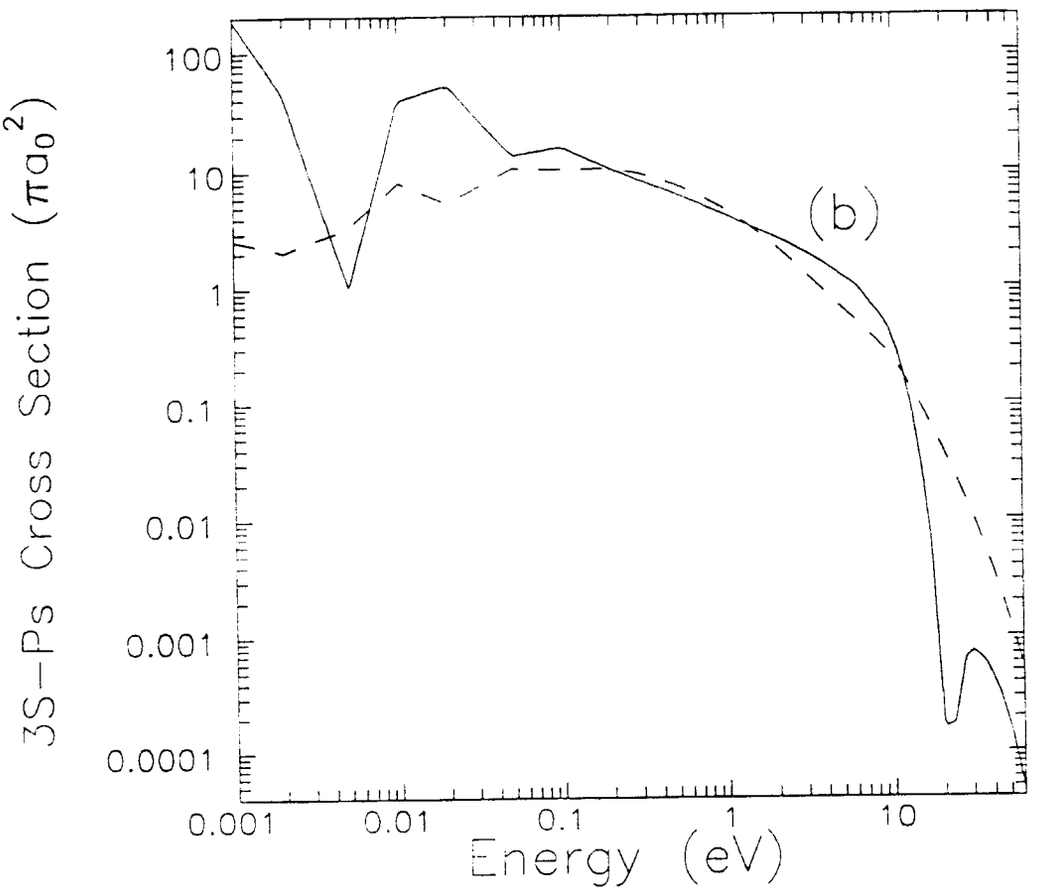
3S–Ps Cross Section (πa_0^2)
100
10
1
0.1
0.01
0.001
0.0001
0.001
0.01
0.1
1
10
Energy (eV)
(b)

Fig 5b

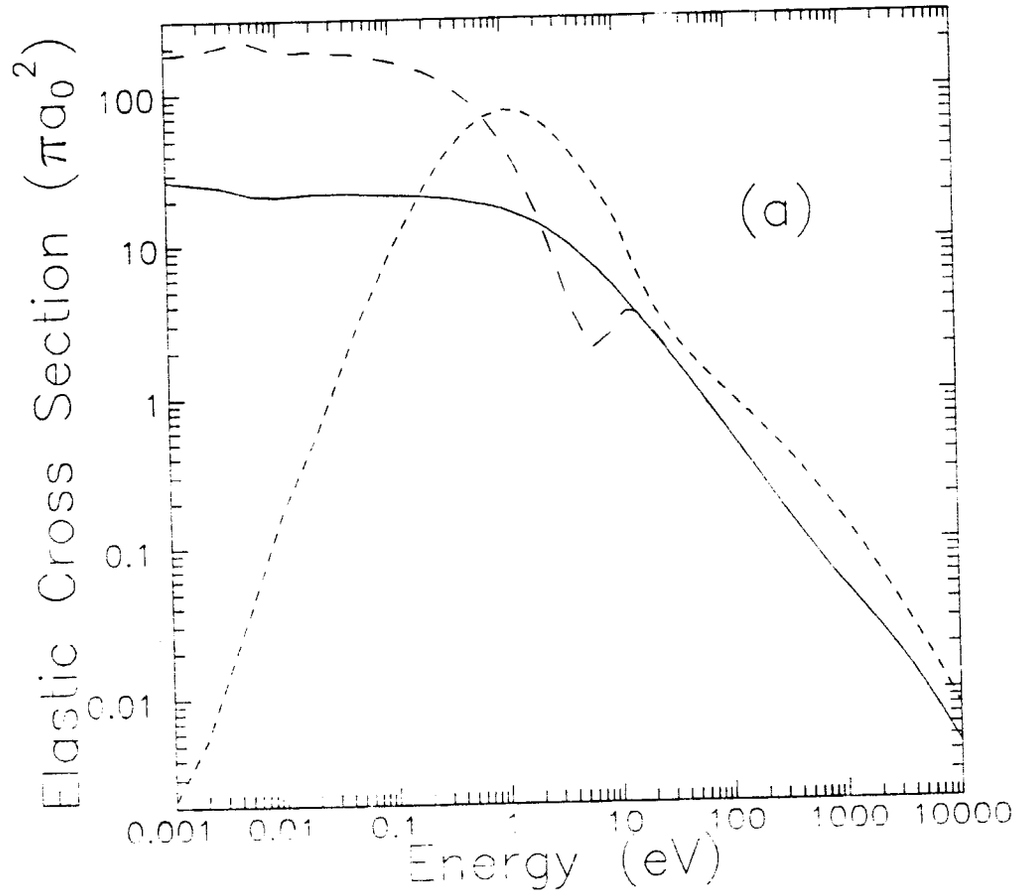
Elastic Cross Section (πa_0^2)
100
10
1
0.1
0.01
0.001
0.01
0.1
1
10
100
1000
10000
Energy (eV)
(a)

Fig 5a