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## POSITRON-ALKALI ATOM SCATTERING

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### ABSTRACT

Positron-alkali atom scattering has recently been investigated both theoretically and experimentally in the energy range from a few eV up to 100 eV. On the theoretical side calculations of the integrated elastic and excitation cross sections as well as total cross sections for Li, Na and K have been based upon either the close-coupling method or the modified Glauber approximation. These theoretical results are in good agreement with experimental measurements of the total cross section for both Na and K. Resonance structures have also been found in the  $L = 0, 1$  and  $2$  partial waves for positron scattering from the alkalis. The structure of these resonances appears to be quite complex and, as expected, they occur in conjunction with the atomic excitation thresholds. Currently both theoretical and experimental work is in progress on  $e^+$ -Rb scattering in the same energy range.

### INTRODUCTION

The study of positron-alkali scattering is of considerable interest since these atoms can be viewed as one-electron atoms with fixed cores, and hence the overall system can be considered as an effective three-body problem. The early theoretical work on  $e^+$ -alkali atom scattering was confined primarily to the simplest alkali, namely Li. Low-energy elastic scattering of positrons from Li in the energy range up to 7 eV was investigated using the polarized-orbital method by Bui and Stauffer;<sup>1</sup> they determined the elastic total and momentum transfer cross sections as well as  $Z_{\text{eff}}$ . This work was later extended to Na by Bui.<sup>2</sup>

On the other hand Sarkar *et al*<sup>3</sup> used the first Born approximation (FBA), the polarized FBA as well as the modified eikonal method to calculate the cross section for  $e^+$ -Li scattering for energies up to 500 eV. Borodonaro *et al*<sup>4</sup> and Ferrante *et al*<sup>5</sup> used the classical JWKB method to determine elastic cross sections for energies up to 7 eV for all the alkalis from Li to Cs. Except for the polarized-orbital method, all of the above methods are high-energy techniques and hence are unlikely to produce reliable results in the low-energy regime, say from 0 up to 50 eV.

In the past few years experimental measurements of the total cross section in the energy range from a few eV to nearly 100 eV have become available for  $e^+$  scattering from K,<sup>6,7</sup> Na<sup>8</sup> and Rb<sup>9</sup>. Parallel to this development there have been several elaborate close-coupling calculations of the integrated elastic and excitation cross sections for Li,<sup>10-14</sup> Na<sup>11-14</sup> and K<sup>12-15</sup> as well as more recently for Rb.<sup>16</sup> The total integrated cross section for

$e^+$  scattering from Li, Na and K has also been determined in a modified Glauber approximation<sup>17,18</sup> within the model potential approach and repeated recently for K in an improved modified Glauber approximation.<sup>19</sup> The overall agreement between theory and experiment is quite gratifying.

Resonance structures have also been found in the  $L = 0, 1$  and  $2$  partial waves in the vicinity of the atomic excitation thresholds in Li, Na and K.<sup>14,20,21</sup> The widths of these resonances are quite narrow, varying between 0.2 and 130 meV. In addition some evidence has been found for the existence of positron-alkali bound states.

Besides excitation, two more inelastic channels need to be considered, namely ionization and positronium formation. The total ionization cross section for  $e^+$ -Li scattering has been found using both the FBA as well as by distorted-wave techniques.<sup>22-23</sup>

Positron-alkali scattering is also interesting both experimentally as well as theoretically since the rearrangement channel (positronium formation) is always open. This possibility should have a pronounced influence on the elastic and various excitation cross sections at very low energy. There have been several calculations<sup>24-27</sup> of the positronium formation cross section in the alkalis based upon either the FBA or various forms of the distorted-wave approximation. However, only the two-state calculation for Li of Guha and Ghosh,<sup>28</sup> which included polarization potentials in both channels and the distorted-wave approach of Mazumdar and Ghosh,<sup>29</sup> also for Li, which determined the incident wavefunction via a polarized-orbital method are liable to prove reliable in the low-energy regime.

This review will be concerned solely with the recent theoretical treatments used to determine the integrated elastic and differential cross sections, the various excitation cross sections and the total cross section for the alkalis. A brief discussion of the resonance structures will also be presented. Whenever possible a direct comparison with experiment will be made.

### THEORY

#### The close-coupling method

The alkali atoms, to a good approximation, can be considered as one-electron systems where the valence electron moves outside a fixed or frozen core, consisting of the nucleus and the remaining electrons. Based upon this assumption the alkalis can be treated within the close-coupling framework in an analogous manner to that formulated by Percival and Seaton<sup>30</sup> for  $e^-$ -H scattering.

If the quantum numbers of the valence electron are denoted by  $n_1 l_1 m_1 m_{s_1}$  and those of the incident positron by  $kl_2 m_2 m_{s_2}$  then we can define the functions  $\Psi_\gamma$  according to

$$\Psi_\gamma(\mathbf{r}_c \sigma_c, \mathbf{r}_1 \sigma_1, \hat{\mathbf{r}}_2 \sigma_2) = \Phi(\mathbf{r}_c \sigma_c, \mathbf{r}_1 \sigma_1) Y_{l_2 m_2}(\hat{\mathbf{r}}_2) \chi_{m_{s_2}}(\sigma_2) \quad (1)$$

where  $Y_{l_2 m_2}(\hat{\mathbf{r}}_2)$  and  $\chi_{m_{s_2}}(\sigma_2)$  represent the angular momentum and spin functions of the positron and  $\mathbf{r}_c \sigma_c$  and  $\mathbf{r}_1 \sigma_1$  represent the space and spin coordinates of the core and valence electrons respectively. Here  $\gamma$  collectively represents the quantum numbers  $n_1 l_1 m_1 m_{s_1} k l_2 m_2 m_{s_2}$  and  $\Phi$  denotes the bound state wavefunction of the atom. The latter, in turn, is represented by a single Slater determinant of the individual electron orbitals.

Since spin-orbit coupling is neglected, the total orbital and spin angular momentum quantum numbers  $LSM M_S$  will be separately conserved during the collision. Consequently, calculations are simplified by using, instead of  $\gamma$ , the alternative representation  $\Gamma = n_1 k l_1 l_2 LSM M_S$ . These two representations are related by the unitary

$$\left[ \frac{d^2}{dr^2} - \frac{l_2(l_2+1)}{r^2} - 2V_c(r) + k_\nu^2 \right] F_{\nu LS}(r) = -2 \sum_{\nu'} V(\nu, \nu')_L F_{\nu' LS}(r) \quad (5)$$

where  $\nu = n_1 l_1 l_2$

$$V_c(r) = \frac{Z}{r} - \sum_{nl} 2(2l+1) y_0(nl, nl; r) \quad (6)$$

$$V(\nu, \nu')_L = \sum_{\lambda} f_{\lambda}(l_1 l_2, l'_1 l'_2; L) y_{\lambda}(n_1 l_1, n'_1 l'_1; r) \quad (7)$$

and

$$y_{\lambda}(n_1 l_1, n'_1 l'_1; r) = r^{-\lambda-1} \int_0^r P_{n_1 l_1}(x) P_{n'_1 l'_1}(x) x^{\lambda} dx + r^{\lambda} \int_r^{\infty} P_{n_1 l_1}(x) P_{n'_1 l'_1}(x) x^{-\lambda-1} dx \quad (8)$$

In the above equations the  $P$ 's are the radial atomic orbitals. The summation in equation (6) is over the core orbitals and the coefficients  $f_{\lambda}$ , given in equation (7), are defined in Percival and Seaton.<sup>30</sup>

If the  $\nu'$ th linearly independent solution for  $F_{\nu LS}(r)$  is now denoted by  $F_{\nu LS}^{\nu'}(r)$  then the appropriate scattering boundary conditions are

$$F_{\nu LS}^{\nu'}(0) = 0 \quad (9)$$

and

$$F_{\nu LS}^{\nu'}(r)_{r \rightarrow \infty} \sim \frac{1}{\sqrt{k_{\nu}}} \left[ \delta(\nu, \nu') \sin(k_{\nu} r - \frac{l\pi}{2}) + R_{\nu\nu'}^{LS} \cos(k_{\nu} r - \frac{l\pi}{2}) \right] \quad (10)$$

Here the coefficients  $R_{\nu\nu'}^{LS}$  are the corresponding elements of the reactance matrix or  $\mathbf{R}$  matrix which, in turn, is re-

transformation

$$(\gamma|\Gamma') = \delta(n_1 l_1 l_2, n'_1 l'_1 l'_2) C(l_1 l_2 L'; m'_1 m'_2 M') \times C(\frac{1}{2} \frac{1}{2} S'; m'_{s_1} m'_{s_2} M'_S) \quad (2)$$

If we now define the so-called channel functions  $\Psi_{\Gamma}$  by

$$\Psi_{\Gamma}(\mathbf{r}_c \sigma_c, \mathbf{r}_1 \sigma_1, \hat{\mathbf{r}}_2 \sigma_2) = \sum_{\gamma} (\gamma|\Gamma) \Psi_{\gamma}(\mathbf{r}_c \sigma_c, \mathbf{r}_1 \sigma_1, \hat{\mathbf{r}}_2 \sigma_2) \quad (3)$$

then the total wavefunction of the system takes the form

$$\Psi(\mathbf{r}_c \sigma_c, \mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2) = \sum_{\Gamma} \Psi_{\Gamma}(\mathbf{r}_c \sigma_c, \mathbf{r}_1 \sigma_1, \hat{\mathbf{r}}_2 \sigma_2) \frac{1}{r_2} F_{\Gamma}(r_2) \quad (4)$$

The functions  $F_{\Gamma}(r_2)$  describe the radial motion of the incident positron. The close-coupling equations are now obtained by projecting the Schrödinger equation for  $\Psi$  onto  $\Psi_{\Gamma}$ ; one thus obtains

lated to the scattering matrix  $\mathbf{S}$  and the transition matrix  $\mathbf{T}$  according to

$$\mathbf{S} = \frac{1 + i\mathbf{R}}{1 - i\mathbf{R}} \quad (11)$$

and

$$\mathbf{T} = \mathbf{S} - 1 \quad (12)$$

The total cross section for the excitation of an alkali atom from the state  $n'_1 l'_1$  to  $n_1 l_1$  is given (in units of  $\pi a_0^2$ ) by

$$\sigma(n'_1 l'_1 \rightarrow n_1 l_1) = \sum_{LS} \sum_{l_2 l'_2} \frac{(2L+1)(2S+1)}{4k_{\nu}^2 (2l'_1+1)} |T_{\nu\nu'}^{LS}|^2 \quad (13)$$

and the corresponding elastic differential cross section is given by

$$\frac{d\sigma}{d\Omega}(n_1' l_1' \rightarrow n_1 l_1) = \sum_S \frac{(2S+1)}{16k_{\nu'}^2} \left| \sum_{L_1'} (2L+1) P_L(\cos\theta) T_{\nu'\nu'}^{LS} \right|^2 \quad (14)$$

### The modified Glauber approximation

While the conventional Glauber amplitude was found to work quite well for  $e^\pm$ -atom scattering at intermediate energies<sup>31</sup> it was nonetheless shown<sup>32</sup> that it could be improved by correcting its second-order eikonal term with the counterpart of the second-Born approximation. Thus, in the so-called modified Glauber approximation, we have

$$f_{\text{MG}} = f_{\text{G}} - f_{\text{G}2} + f_{\text{B}2} \quad (15)$$

The total cross section is then obtained by means of the optical theorem,

$$\sigma = \frac{4\pi}{k_i} \Im m f(0) \quad (16)$$

where  $f(0)$  is the scattering amplitude in the forward direction without change in energy.

$$f(\theta) = -\frac{1}{2\pi} \langle \Phi_f \exp ik_f \cdot \mathbf{r}' | V_c(\mathbf{r}') | \chi_i^{(+)} \rangle - \frac{1}{2\pi} \langle \chi_f^{(-)} | V_a(\mathbf{r}, \mathbf{r}') | \Psi_i^{(+)} \rangle \quad (19)$$

Here  $\Phi_f$  is the final state atomic wavefunction and  $\Psi_i^{(+)}$  is the solution of the full Schrödinger equation of the system consisting of the incident positron plus the alkali target. The functions  $\chi_{i,f}^{(\pm)}$  are called distorted waves and, in principal, are solutions of the full Schrödinger equation with  $V(\mathbf{r}, \mathbf{r}')$  replaced by just  $V_c(\mathbf{r}')$ . The subscripts ( $i, f$ ) refer to the initial and final states of the system and the superscripts ( $\pm$ ) refer to outgoing and incoming wave boundary conditions respectively.

If the scattering amplitude is now evaluated using the Glauber technique then the first term above represents the Glauber amplitude of the core-potential scattering and the second term represents the core-corrected Glauber amplitude of the projectile scattering by the 'one-electron' atom.

## RESULTS

### Lithium

Several close-coupling calculations for the elastic cross section as well as various excitation cross sections have been performed for  $e^+$ -Li scattering by Khan *et al*<sup>10</sup> in the energy range 2–10 eV, and extended by Sarkar *et*

In the case of a larger atom (such as Na or K) one encounters serious difficulties in an eikonal-type approximation, like the modified Glauber approximation, in the evaluation of the multiple-scattering terms in the scattering amplitude. These terms arise from the scattering of the incident projectile by the core electrons of the target. In order to overcome this difficulty a model potential approach was developed by Gien<sup>33</sup> for  $e^\pm$ -alkali scattering. Here the potential which describes the scattering of the incident projectile by the alkali atom is expressed as

$$V(\mathbf{r}, \mathbf{r}') = V_a(\mathbf{r}, \mathbf{r}') + V_c(\mathbf{r}') \quad (17)$$

where, in the case of a positron

$$V_a(\mathbf{r}, \mathbf{r}') = -\left[ \frac{1}{|\mathbf{r} - \mathbf{r}'|} - \frac{1}{r'} \right] \quad (18)$$

is the scattering potential of the projectile by the 'one-electron' atom and  $V_c(\mathbf{r}')$  is the core potential of the target atom. Here  $\mathbf{r}$  and  $\mathbf{r}'$  represent the coordinates of the valence electron and the incident positron respectively.

The core potential,  $V_c$ , of the alkali<sup>+</sup> ions is also used to generate the bound-state valence orbitals of the atoms.

In terms of the two-potential formalism<sup>34</sup> the scattering amplitude can be expressed as

$a$ <sup>11</sup> to the energy range 15–100 eV. More recently Ward *et al*<sup>13</sup> have reported similar calculations in the energy range 0.5–50 eV. In each case the most elaborate calculation carried out by the above authors respectively was based upon the inclusion of the 5 atomic states (2s–2p–3s–3p–3d) in the eigenfunction expansion for the total wavefunction. In the work of Khan *et al* and Sarkar *et al* the analytic Hartree-Fock wavefunctions of Weiss<sup>35</sup> were used for the bound state orbitals whereas Ward *et al* employed both frozen-core Hartree-Fock as well as model potential wavefunctions.<sup>36</sup>

On the other hand Gien<sup>18</sup> has given results for the total cross section for  $e^+$ -Li scattering based upon the core-corrected modified Glauber approximation in the energy range from 40 to 1000 eV. So far there are no experimental measurements with which to compare.

In table 1 we present the 5-state close-coupling results referred to above for the elastic, the resonance transition and the total cross section together with the total cross section determined in the core-corrected modified Glauber approximation. These results are also shown in figure 1.

TABLE 1. Elastic, resonant excitation and total integrated cross sections ( $\pi a_0^2$ ) for  $e^+$ -Li scattering in the energy range 0.5–100 eV.

| Energy (eV) | Refs. 10, 11 |       |        | Ref. 13 |       |        | Ref. 18 |
|-------------|--------------|-------|--------|---------|-------|--------|---------|
|             | 2s-2s        | 2s-2p | Total  | 2s-2s   | 2s-2p | Total  | Total   |
| 0.5         |              |       |        | 351.95  |       | 351.95 |         |
| 1.0         |              |       |        | 212.15  |       | 212.15 |         |
| 1.5         |              |       |        | 183.58  |       | 183.58 |         |
| 2.0         |              |       |        | 169.49  | 21.24 | 190.72 |         |
| 3.0         |              |       |        | 106.87  | 72.29 | 179.16 |         |
| 4.0         | 67.79        | 78.07 | 151.10 | 71.86   | 79.09 | 160.36 |         |
| 5.0         | 48.46        | 79.10 | 135.29 | 52.11   | 81.68 | 145.11 |         |
| 7.0         | 29.14        | 73.99 | 112.80 | 31.19   | 77.61 | 121.04 |         |
| 10.0        | 17.68        | 67.33 | 94.70  | 18.13   | 68.15 | 97.27  |         |
| 15.0        | 9.93         | 56.43 | 74.89  |         |       |        |         |
| 20.0        | 7.17         | 49.53 | 63.38  | 7.51    | 47.35 | 61.00  |         |
| 30.0        | 4.97         | 38.90 | 48.16  | 5.14    | 36.54 | 45.56  |         |
| 40.0        | 4.07         | 30.14 | 37.32  | 4.08    | 29.84 | 36.68  | 35.67   |
| 50.0        | 3.37         | 24.23 | 30.00  | 3.44    | 25.21 | 30.77  | 30.82   |
| 70.0        |              |       |        |         |       |        | 24.37   |
| 80.0        | 2.37         | 14.48 | 18.25  |         |       |        |         |
| 100.0       | 1.99         | 10.63 | 13.69  |         |       |        | 18.71   |

The close-coupling results of Sarkar *et al* and Ward *et al* are in satisfactory agreement; the slight differences could be attributed to the use of different bound state wavefunctions as well as the different numerical proce-

dures used to determine the cross sections. On the other hand, the differences between the cross sections of Khan *et al* and Ward *et al* are somewhat more than what might be expected from these causes.

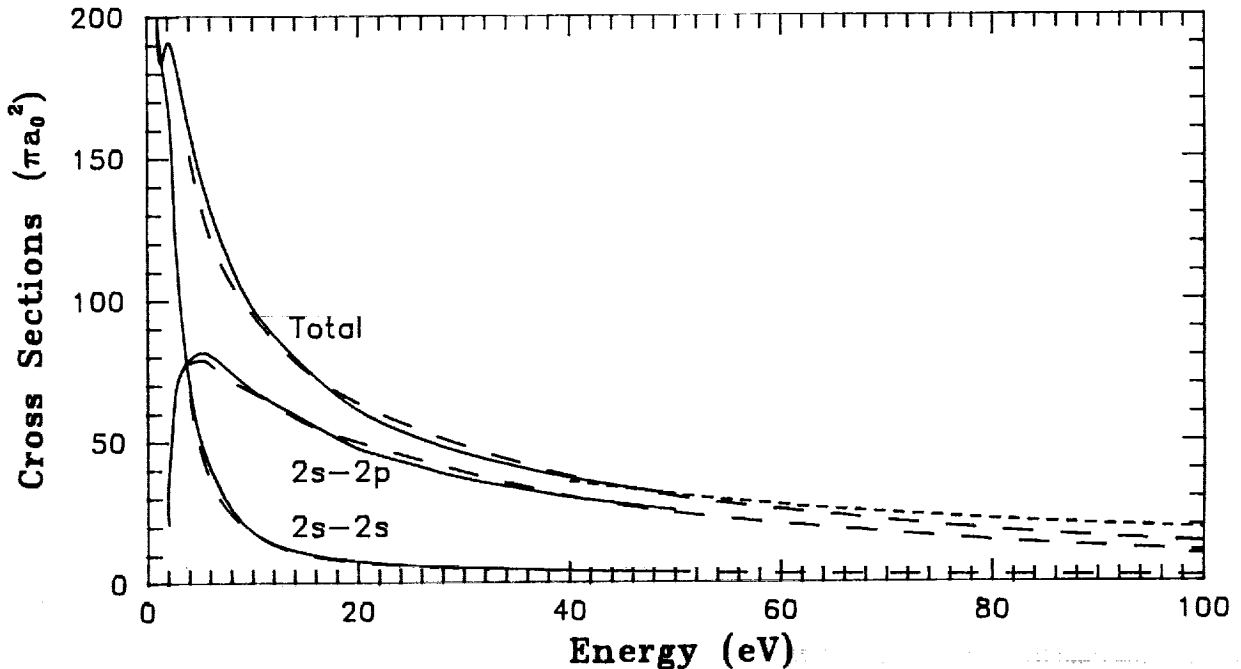


FIG. 1. The 5-state close-coupling elastic, resonance excitation and total cross section and the modified Glauber total cross section for  $e^+$ -Li scattering: (---), Khan *et al*<sup>10</sup> and Sarkar *et al*<sup>11</sup> (—), Ward *et al*<sup>13</sup> (-.-), Gien.<sup>18</sup>

The total cross sections of the core-corrected modified Glauber approximation are either comparable to or lie above the close-coupling results with the difference increasing with increasing energy. However, it should be noted that the total cross sections in the close-coupling procedure include neither excitations to bound levels with principal quantum number  $n \geq 4$  nor the ionization and positronium formation channels.

In the close-coupling calculations of positron-alkali collisions of Ward *et al*<sup>14,20</sup> and Horbatsch *et al*<sup>21</sup> a number of resonances in the  $L = 0, 1$  and  $2$  channels have been found in the vicinity of the atomic excitation thresholds. The appearance of such resonances near thresholds is well established in electron scattering from atoms and in particular from the alkalis.<sup>37,38</sup> In positron-atom scattering, resonance structures have been calculated in detail only for the  $e^+ - \text{H}$  system.<sup>39</sup> However, hydrogen is quite different from the alkalis in many ways. In particular, its energy levels are degenerate and a large contribution to its dipole polarizability can be attributed to the continuum P states. In the alkalis, whose polarizabilities are very large, over 98% of the dipole polarizability comes from just the resonant excitation transition. Also significant is the fact that in the alkalis the Ps formation channel is open at zero energy.

In the work of Ward *et al*<sup>14</sup> the  $R$  matrices obtained

from 4-state ( $2s-2p-3s-3p$ ) and 5-state close-coupling approximations were diagonalized and the eigenphase sum was computed according to

$$\sum_i \eta_{iL}(E) = \sum_i \tan^{-1}(\lambda_i) \quad (20)$$

where the  $\lambda_i$  are the eigenvalues of the respective  $R$  matrices. The resonances for which the eigenphase sum underwent a change of  $\pi$  rad were analyzed in terms of the single-resonance Breit-Wigner formula

$$\sum_i \eta_{iL}(E) = \eta_L^{(B)}(E) + \tan^{-1} \frac{\frac{1}{2}\Gamma_{BW}}{E_{BW} - E} \quad (21)$$

by means of a method described by Nesbet.<sup>37</sup> In figure 2 we show the eigenphase sum for  $L = 0$  from both 4- and 5-state close-coupling calculations based upon model potential wavefunctions. We first note that the 4-state calculation yields different results in the vicinity of the  $2p$  threshold (1.844 eV). Thus the presence of the  $3d$  orbital, as a closed channel, in the eigenfunction expansion plays a key role in developing the discontinuity present in the 4-state calculation into the usual resonance shape. Nonetheless, the eigenphase sum changes by only 2 rad at  $E_{\text{res}} = 1.86$  eV with a full width  $\Gamma = 35$  meV.

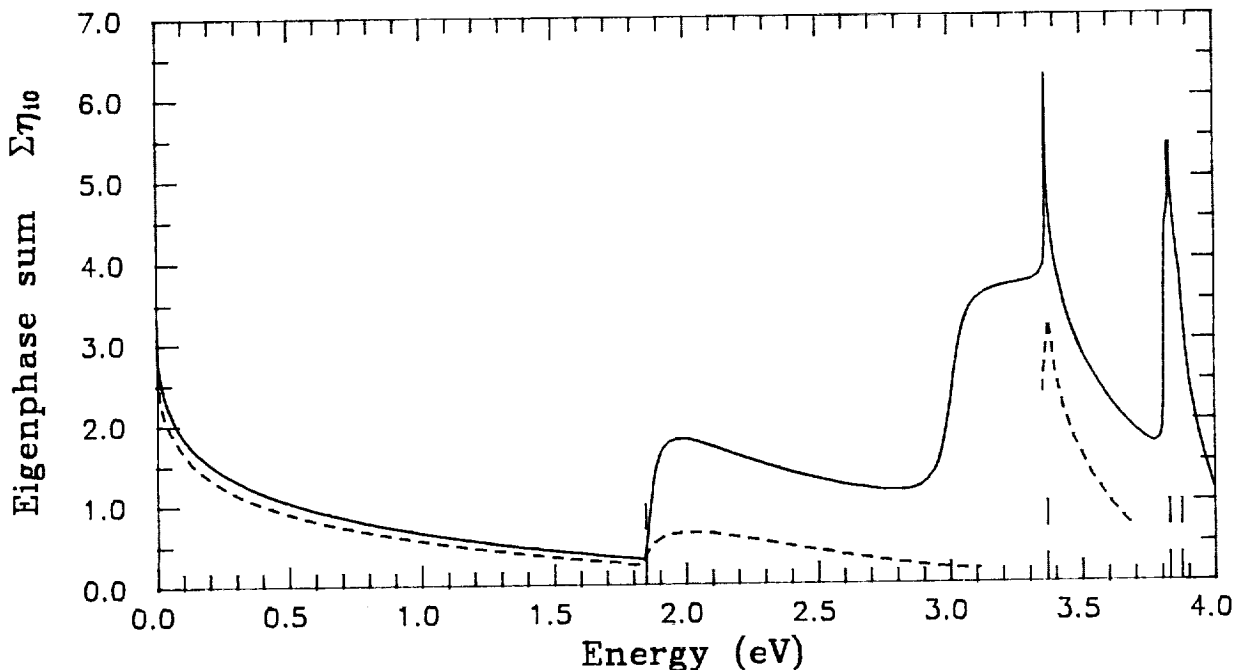


FIG. 2. The eigenphase sum for  $L = 0$ ,  $e^+ - \text{Li}$  scattering in a 5-state (—), and 4-state (---) close-coupling approximation. The dashes indicate the positions of the excitation thresholds in the model potential approximation at 1.844, 3.367, 3.829 and 3.874 eV.

As can also be seen from the figure there is a 5-state resonance below the  $3s$  excitation threshold (3.367 eV)

which is not present in the 4-state results. The resonance parameters here are  $E_{\text{res}} = 3.01$  eV and  $\Gamma = 40$  meV. A

narrow resonance,  $E_{\text{res}} = 3.365$  eV,  $\Gamma = 1$  meV occurs immediately below the 3s excitation threshold; it is present in both the 4- and 5-state eigenfunction expansions. The 5-state calculation also displays a further narrow resonance just below the 3p excitation threshold (3.829 eV) which is missing in the 4-state results. Ward *et al*<sup>14,20</sup> have shown that this general type behaviour in the  $L = 0$  channel persists in the  $L = 1$ , and 2 channels as well, not only for Li but also for Na and K.

At zero energy Ward *et al*<sup>14,20</sup> point out that the s-wave ( $L = 0$ ) phase shifts for Li, Na and K start at least at  $\pi$  rad since they begin with negative slopes (positive scattering lengths) and the polarization potential, which dominates at zero energy, is attractive. This implies the possible existence of at least one bound state in these  $e^+$ -alkali systems.

However, Ps formation is possible at zero energy and hence the shape, position and even the existence of resonances could be radically altered when this channel is properly taken into account in a calculation. The situation with respect to the existence of bound states in the  $e^+$ -alkali systems could also be altered.

#### Sodium

On the theoretical side the situation for  $e^+$ -Na scattering is somewhat the same as for lithium. Sarkar *et al*<sup>11</sup> have carried out close-coupling calculations of the elastic cross section as well as various excitation cross

sections in the energy range 4–100 eV. Similar calculations have also been reported by Ward *et al*<sup>13</sup> in the energy range 0.5–50 eV. The most elaborate calculation by Sarkar *et al* was based upon the inclusion of 4 atomic states (3s–3p–3d–4p) in the eigenfunction expansion for the total wavefunction. On the other hand, the most accurate results of Ward *et al* were based upon the 5-state expansion (3s–3p–3d–4s–4p). In the work of Sarkar *et al* the analytic Hartree-Fock wavefunction of Clementi and Roetti<sup>40</sup> was used for the ground state and the wavefunctions of Kundu *et al*<sup>41</sup> and Kundu and Mukherjee<sup>42</sup> for the excited p- and d-states respectively. The frozen-core wavefunctions of Ward *et al* were determined from the model potential of Peach.<sup>36</sup> Ward *et al* also performed a 4-state calculation but based upon the atomic states (3s–3p–3d–4s) and hence a direct comparison of their results with those of Sarkar *et al* is not possible. Nonetheless, the overall agreement between these two sets of close-coupling results is satisfactory.

Gien<sup>18</sup> has also given results for the total cross section for  $e^+$ -Na scattering based upon the core-corrected modified Glauber approximation in the energy range from 40 to 1000 eV. In table 2 we present the 4-state (Sarkar *et al*<sup>11</sup>) and 5-state (Ward *et al*<sup>13</sup>) close-coupling values for the elastic, the resonance transition and the total cross section as well as the total cross section determined by Gien<sup>18</sup> in the core-corrected Glauber approximation.

TABLE 2. Elastic, resonant excitation and total integrated cross sections ( $\pi a_0^2$ ) for  $e^+$ -Na scattering in the energy range 0.5–100 eV.

| Energy (eV) | Ref. 11 |       |        | Ref. 13 |       |        | Ref. 18 |
|-------------|---------|-------|--------|---------|-------|--------|---------|
|             | 3s–3s   | 3s–3p | Total  | 3s–3s   | 3s–3p | Total  | Total   |
| 0.5         |         |       |        | 341.24  |       | 341.24 |         |
| 1.0         |         |       |        | 205.18  |       | 205.18 |         |
| 1.5         |         |       |        | 175.53  |       | 175.53 |         |
| 2.0         |         |       |        | 189.47  |       | 189.47 |         |
| 2.5         |         |       |        | 130.92  | 48.23 | 179.15 |         |
| 3.0         |         |       |        | 110.22  | 66.11 | 176.33 |         |
| 3.5         |         |       |        | 87.52   | 67.47 | 165.75 |         |
| 4.0         | 71.48   | 66.87 | 144.19 | 73.96   | 69.25 | 159.21 |         |
| 5.0         | 54.24   | 72.37 | 137.78 | 54.13   | 69.99 | 144.71 |         |
| 7.0         |         |       |        | 33.04   | 65.91 | 121.57 |         |
| 7.5         | 30.54   | 72.80 | 120.87 |         |       |        |         |
| 10.0        | 19.78   | 65.82 | 102.54 | 19.84   | 59.21 | 98.81  |         |
| 15.0        | 11.82   | 54.56 | 74.89  |         |       |        |         |
| 20.0        | 8.84    | 46.46 | 65.04  | 8.98    | 44.61 | 63.78  |         |
| 30.0        | 6.56    | 38.67 | 51.13  | 6.49    | 35.83 | 48.50  |         |
| 40.0        | 5.41    | 33.56 | 43.04  | 5.35    | 29.93 | 39.59  | 29.62   |
| 50.0        | 4.74    | 26.52 | 34.30  | 4.67    | 25.67 | 33.61  | 26.41   |
| 70.0        |         |       |        |         |       |        | 21.68   |
| 80.0        | 3.53    | 14.25 | 19.31  |         |       |        |         |
| 100.0       | 3.04    | 11.04 | 15.30  |         |       |        | 17.18   |

However, it should be noted that, in contrast to Li, where only the elastic, and resonance transition cross sections are of significant magnitude, the other excitation cross sections in Na (i.e. 3s-3d, 3s-4s and 3s-4p) do contribute appreciably to the total cross section. When compared with the corresponding close-coupling values for the total cross section the core-corrected modified Glauber results appear to be too low at energies below 100 eV.

For Na there are the experimental data of Kwan *et al*<sup>8</sup> for the total cross section with which to compare. However, since experimentally it is not possible to discriminate against positrons scattered elastically through small angles about the forward direction, a knowledge of the elastic differential cross section enables one to estimate how much flux has been lost by means of this

effect. Thus Ward *et al*<sup>13</sup> calculated an effective elastic cross section defined as

$$\sigma_{el}^{eff} = 2\pi \int_{\theta_0}^{\pi} \sin \theta \frac{d\sigma_{el}}{d\Omega} d\theta \quad (a_0^2) \quad (22)$$

where  $\theta_0$  is the lower limit of the experimental angular discrimination. An estimate of this quantity has been made in the experimental measurements of Kwan *et al*<sup>8</sup> for several values of the energy of the incident positron. When this effective elastic cross section is added to the various excitation cross sections an effective total cross section is obtained which can, more meaningfully, be compared with the experimental data. In figure 3 we illustrate the various theoretical results referred to above for the total cross section for  $e^+$ -Na scattering together with the experimental data.

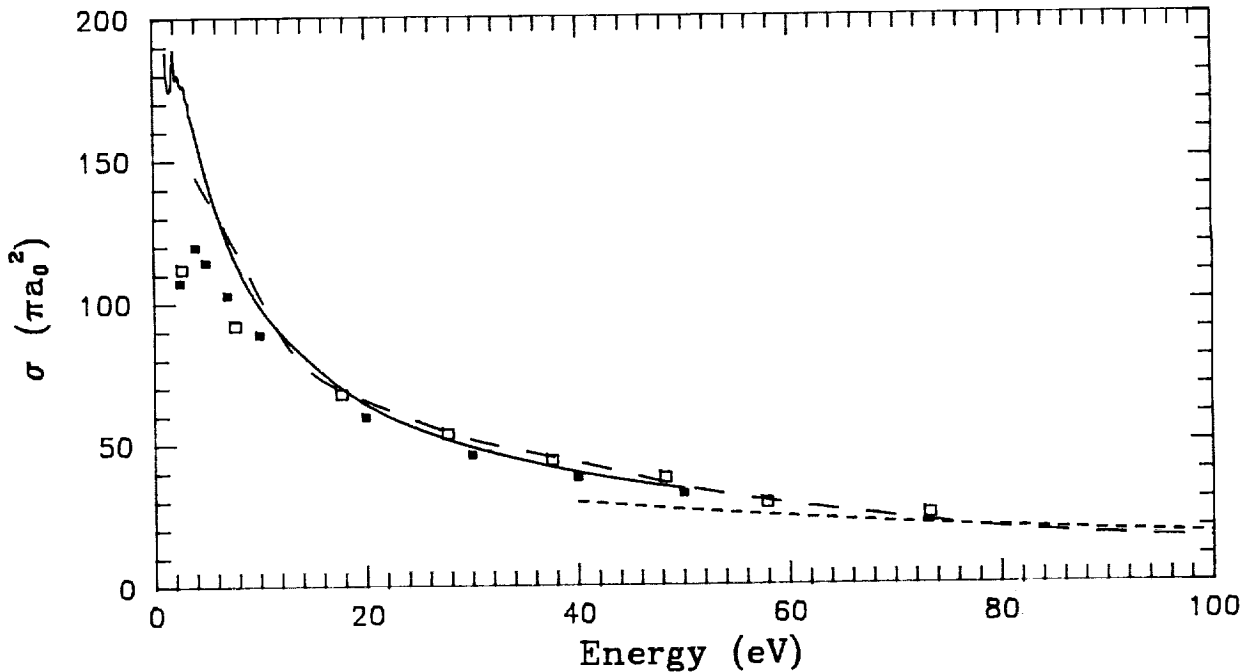


FIG. 3. The total cross section for  $e^+$ -Na scattering: (---), 4-state close-coupling approximation (CCA), Sarkar *et al*,<sup>11</sup> (—), 5-state CCA, Ward *et al*,<sup>13</sup> ■, effective 5-state CCA, Ward *et al*,<sup>13</sup> (- - -), core-corrected modified Glauber approximation, Gien,<sup>18</sup> □, experimental data, Kwan *et al*.<sup>8</sup>

The overall agreement between the *effective* total cross section of Ward *et al*<sup>13</sup> and experiment is quite satisfactory over the entire energy range below 50 eV. It should be noted that below 20 eV it becomes very important to make allowance for the fact that experimentally there is a serious loss of flux from positrons elastically scattered through small angles. However, the effective cross section is highly sensitive at low energies to the particular value used in equation (22) for the cut-off angle  $\theta_0$ . The

value of  $\theta_0$  increases rapidly as the energy decreases and hence the apparent structure in the effective cross section may be artificial.

Above 20 eV the total cross sections of Sarkar *et al*<sup>11</sup> are also in quite satisfactory agreement with experiment. On the other hand the total cross section determined in the core-corrected modified Glauber approximation by Gien<sup>18</sup> appears to be slightly too low in this energy region.

## Potassium

In the case of  $e^+$ -K scattering several close-coupling calculations of the elastic cross section as well as various excitation cross sections have been reported by Ward *et al.*<sup>12-15</sup> The most elaborate of these is a 5-state (4s-4p-5s-3d-5p) calculation, which employed model potential wavefunctions,<sup>36</sup> in the energy range 0.5 to 50 eV.

Once again Gien<sup>18</sup> has reported results for the total cross section for  $e^+$ -K scattering based upon the core-corrected modified Glauber approximation in the energy range from 40 to 1000 eV. However, more recently Gien<sup>19</sup> has repeated these calculations in an improved Glauber

approximation in the energy range from 11 to 102.5 eV. In his original work<sup>18</sup> only the contribution from the 4s intermediate state to the second Born term for one-electron atom scattering was evaluated exactly; i.e. the remaining contributions were determined via closure. In his most recent work<sup>19</sup> the contributions from the 4p and 5s as well as the 4s intermediate states have been evaluated exactly.

In table 3 we present the 5-state close-coupling values of Ward *et al.*<sup>13</sup> for the elastic, the resonance transition and the total cross section together with the total cross sections as determined by Gien<sup>18,19</sup> in the core-corrected modified Glauber approximation.

TABLE 3. Elastic, resonant excitation and total integrated cross sections ( $\pi a_0^2$ ) for  $e^+$ -K scattering in the energy range 0.5-102.5 eV.

| Energy (eV) | Ref. 13 |        |        | Refs. 18, 19 | Ref. 19 |
|-------------|---------|--------|--------|--------------|---------|
|             | 4s-4s   | 4s-4p  | Total  | Total        | Total   |
| 0.5         | 666.57  |        | 666.57 |              |         |
| 1.0         | 510.78  |        | 510.78 |              |         |
| 1.5         | 486.71  |        | 486.71 |              |         |
| 2.0         | 322.75  | 79.60  | 402.35 |              |         |
| 2.5         | 239.39  | 126.40 | 365.79 |              |         |
| 3.0         | 184.65  | 125.42 | 329.17 |              |         |
| 3.5         | 145.34  | 119.65 | 298.29 |              |         |
| 4.0         | 117.83  | 112.33 | 273.44 |              |         |
| 5.0         | 82.56   | 100.14 | 235.97 |              |         |
| 7.0         | 48.96   | 87.57  | 189.72 |              |         |
| 10.0        | 29.66   | 80.09  | 151.56 |              |         |
| 11.0        |         |        |        | 38.07        | 105.85  |
| 20.0        | 14.27   | 64.65  | 97.60  |              |         |
| 21.1        |         |        |        | 48.85        | 84.96   |
| 30.0        | 10.66   | 52.79  | 74.37  |              |         |
| 31.2        |         |        |        | 46.15        | 70.75   |
| 40.0        | 9.01    | 44.11  | 60.44  | 42.04        | 61.28   |
| 41.4        |         |        |        | 41.38        | 59.99   |
| 50.0        | 8.02    | 37.67  | 51.33  | 37.49        | 52.92   |
| 70.0        |         |        |        | 30.37        |         |
| 76.8        |         |        |        | 28.52        | 38.61   |
| 100.0       |         |        |        | 23.61        |         |
| 102.5       |         |        |        | 23.19        | 30.76   |

We first note that, similar to Na, the other excitation cross sections in K (i.e. 4s-5s, 4s-3d and 4s-5p) make an appreciable contribution to the total cross section. Secondly we see that, when the contribution to the second Born term is evaluated more precisely, the core-corrected modified Glauber approximation agrees with the close-coupling results down to 30 eV.

For K there are the experimental data of Stein *et al.*<sup>6,7</sup>

for the total cross section with which to compare. In order to obtain satisfactory agreement with experiment at low energies Ward *et al.*<sup>13</sup> again found it necessary to calculate, using equation (22), an effective elastic, and hence total cross section. In figure 4 we illustrate the above theoretical results for the total cross for  $e^+$ -K scattering together with the experimental data.



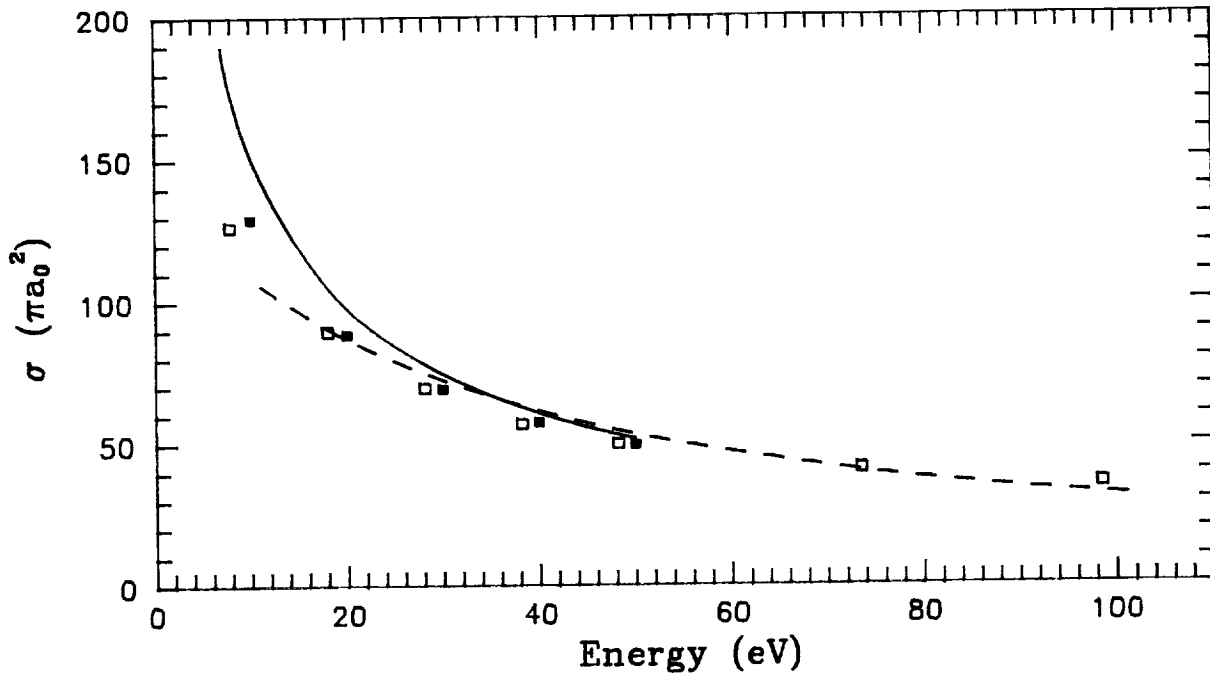


FIG. 4. The total cross section for  $e^+$ -K scattering: (—), 5-state close-coupling approximation (CCA), Ward *et al.*<sup>13</sup> ■, effective 5-state CCA, Ward *et al.*<sup>13</sup> (---), core-corrected modified Glauber approximation, Gien;<sup>19</sup> □, experimental data, Stein *et al.*<sup>6,7</sup>

Once again the overall agreement between the *effective* total cross section of Ward *et al.*<sup>13</sup> and experiment is quite satisfactory over the entire energy range below 50 eV. The improved modified Glauber approximation is similarly in quite satisfactory agreement with experiment down to about 30 eV. It is worth noting that the K cross sections are, however, much larger in magnitude than the corresponding ones for Na. This is a reflection of the larger value of the static dipole polarizability of K, namely  $293 \pm 6 a_0^3$  versus  $159 \pm 3 a_0^3$  for Na.<sup>43</sup>

#### Rubidium

Quite recently work has begun on the corresponding

5-state close-coupling calculation (5s-5p-4d-6s-6p) for  $e^+$ -Rb scattering.<sup>16</sup> In this case the bound-state wavefunctions of Rb were determined variationally by means of a polarized frozen-core Hartree-Fock technique which has previously proved to be quite successful in atomic structure calculations on Na.<sup>44,45</sup> This calculation is the only theoretical research which has been reported so far for this system.

In table 4 we present the results of this calculation for the elastic, resonance excitation and total cross section as well as the effective total cross section, as determined with the aid of equation (22), for  $e^+$ -Rb scattering.

TABLE 4. Elastic, resonant excitation and total integrated cross sections ( $\pi a_0^2$ ) for  $e^+$ -Rb scattering in the energy range 3.7-28 eV.

| Energy (eV) | Ref. 16 |       |                       |                                    |
|-------------|---------|-------|-----------------------|------------------------------------|
|             | 5s-5s   | 5s-5p | $\sigma_{\text{tot}}$ | $\sigma_{\text{tot}}^{\text{eff}}$ |
| 3.7         | 124.23  | 92.20 | 289.66                | 209.28                             |
| 5.8         | 62.76   | 76.18 | 219.07                | 170.83                             |
| 7.8         | 42.16   | 77.68 | 185.58                | 151.47                             |
| 17.8        | 17.64   | 73.12 | 114.98                | 102.69                             |
| 28.0        | 12.79   | 60.27 | 86.12                 | 80.31                              |

Once again we observe that the other excitation cross sections in Rb (i.e. 5s-4d, 5s-6s and 5s-6p) make a significant contribution to the total cross section. We also note that at 3.7 eV nearly 2/3 of the elastic scattering flux will not be detected experimentally and that this fraction increases to 4/5 at 7.8 eV. Nonetheless, the effective total cross section as predicted by this 5-state close-coupling approximation is monotonically increasing as the energy of the incident positron decreases. This be-

haviour is in contrast to the experimental data of Stein *et al*<sup>9</sup> which has a maximum in the low energy regime. In figure 5 we present the corresponding elastic differential cross section at several energies. These cross sections are, as expected, highly peaked in the forward direction and possess a minimum between 35 and 40° which is then followed by one or more secondary maxima. This overall behaviour pattern of the differential cross section is typical of all the alkalis studied so far.<sup>13,14,28,29</sup>

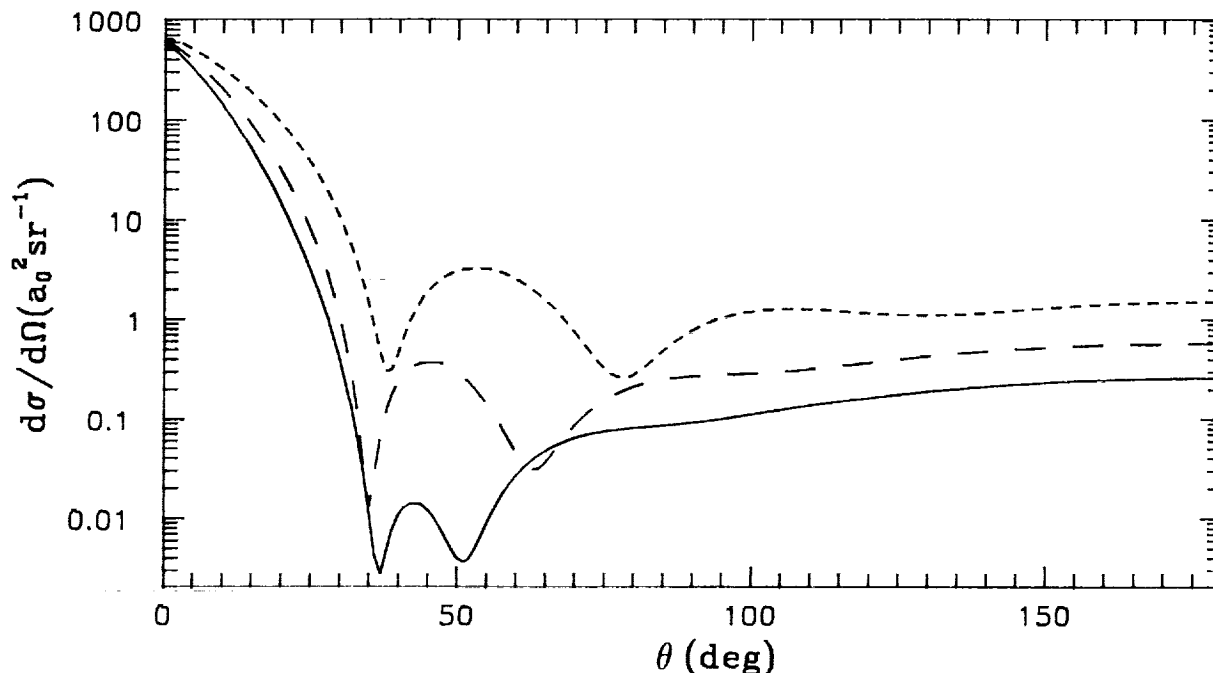


FIG. 5. The elastic differential cross section for  $e^+$ -Rb scattering in a 5-state close-coupling approximation: (---), 3.7 eV; (- - -), 5.8 eV; (—), 7.8 eV.

## CONCLUSIONS

The effective total cross sections, as determined in a 5-state close-coupling procedure, are in quite satisfactory agreement with the experimental data for Na and K; the exception to this is Rb. When the second Born term in the core-corrected modified Glauber approximation is evaluated accurately this approach will also yield total cross sections in agreement with experiment down to relatively low energies. For the alkalis, Li, Na and K, the close-coupling approximation predicts an extensive series of resonance structures associated with the atomic excitation thresholds and holds forth the possibility of true bound states in these  $e^+$ -alkali systems. The same situation will no doubt be true for the remaining alkalis.

However, the most important theoretical problem re-

maining in low-energy  $e^+$ -alkali scattering is the accurate inclusion of the positronium formation channel; ionization is, of course, also important. The incorporation of these two channels into, say, a close-coupling calculation, could have a major effect upon the resulting cross sections at lower energies and could seriously influence the various resonance structures as well as alter the situation with respect to the existence of bound states in the  $e^+$ -alkali systems

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