

## Total cross sections for positron scattering from argon atoms at intermediate energies

S. P. Khare\*

*Centre for Interdisciplinary Studies in Chemical Physics, The University of Western Ontario,  
London, Ontario, Canada N6A 3K7*

Ashok Kumar and Kusum Lata†

*Department of Physics, Institute for Advanced Studies, Meerut University,  
Meerut 250005, Uttar Pradesh, India*

(Received 7 October 1985)

A model complex potential is employed to obtain integrated elastic cross sections, absorption cross sections, and total cross sections for positron scattering from argon atoms in 100–800 eV energy range. The total cross sections are found to be in good agreement with the experimental data for  $E \geq 300$  eV and lower than the corresponding electron cross sections over the whole energy range.

## I. INTRODUCTION

In recent years a number of theoretical investigations have been carried out for the scattering of electrons by inert gases in the intermediate energy range using the optical potential approach (see the references given by de Heer and Jansen,<sup>1</sup> de Heer, Jansen, and van der Kay,<sup>2</sup> Reitan,<sup>3</sup> and Staszewska, Schwenke, and Truhlar<sup>4</sup>). However, enough attention has not been paid to positron scattering. Only one theoretical investigation by Joachain, Vanderpoorten, Winters, and Byron<sup>5</sup> has been carried out for the positron scattering by argon atoms in the intermediate energy range. A comparison of their results for the total cross section  $Q_T$  with the experimental data<sup>6</sup> shows that the theory overestimates the cross sections over the whole energy range. Recently, Reitan<sup>3</sup> has proposed a very simple absorption potential for inert gases. He represented the complex target wave function in terms of exponential density functions fitted to the statistical Thomas-Fermi distribution. With this density function, he obtained a scattering amplitude in Glauber approximation and then used the Glauber phase shifts to generate absorption potential. For the removal of the divergence from the Glauber amplitude in the forward direction, he replaced the second-order Glauber term by the second-order Born term and then transferred the amplitude into coordinate space to obtain absorption potential. His results for electron scattering are encouraging. Hence, to examine the extent of the applicability of his absorption potential to positron scattering, we have used his expression for the absorption potential along with the expressions for the real potentials, employed by Jhanwar, Khare, and Kumar<sup>7</sup> and Khare and Kumar<sup>8</sup> for the elastic scattering of electrons by inert gases, to obtain  $Q_T$ , and also integrated elastic cross section  $Q_{el}$  and absorption cross section  $Q_{ab}$  for the positron scattering from argon atoms in the 100–800-eV energy range. We note that at present no other experimental or theoretical values exist for  $Q_{el}$  and  $Q_{ab}$ .

## II. CALCULATION, RESULTS, AND DISCUSSION

In the present investigation the optical potential  $V_{op}(r)$  is taken to be a spherically symmetric, local, energy-dependent complex potential represented by

$$V_{op}(r) = V_{00}(r) + V_{pol}(r) + iV_{ab}(r) . \quad (1)$$

As remarked above, the static potential  $V_{00}(r)$  and polarization potential  $V_{pol}(r)$  are taken to be the same as employed by Khare and Kumar<sup>8</sup> for the elastic scattering of electrons by argon atoms with appropriate sign change in the static potential. For the absorption potential, we have adopted the expression of Reitan.<sup>3</sup> However, the value of the mean excitation energy was taken to be the same as employed in the evaluation of  $V_{pol}(r)$  and was obtained with the help of the dipole sums  $L(-1)$  and  $S(-1)$  (Inokuti<sup>9</sup>). The resulting one-dimensional differential equation was solved numerically for the complex scattering matrix  $S_l$  by the Numerov method. The cross sections were then obtained with the help of the following expressions:

$$Q_{el} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |1 - S_l|^2 , \quad (2)$$

$$Q_{ab} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) (1 - |S_l|^2) , \quad (3)$$

$$Q_T = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) (1 - \text{Re} S_l) , \quad (4)$$

where  $k$  is the wave number of the incident particle. For comparison, we have also obtained  $Q_T$  for  $e^-$ -Ar scattering. For this calculation, the local exchange potential as obtained by Khare and Kumar<sup>8</sup> was also added in (1).

Figure 1 shows our present values for  $Q_T$ ,  $Q_{el}$ , and  $Q_{ab}$  as a function of positron energy. The experimental data of Kauppila *et al.*<sup>6</sup> and the theoretical values of Joachain, Vanderpoorten, Winters, and Byron<sup>5</sup> for  $Q_T$  along with  $Q_{el}$  values of Khare and Kumar,<sup>8</sup> who took  $V_{ab}(r) = 0$ , are also shown for comparison. It is evident that the present investigation overestimates  $Q_T$  at lower energies. However, for  $E \geq 300$  eV, the present values are within 10% of the experimental data. Such a behavior is not surprising, because the absorption potential of Reitan is expected to be good at higher energies. On the other hand, the values obtained by Joachain, Vanderpoorten, Winters, and Byron<sup>5</sup> are relatively better at lower energies, but their theory overestimates the cross sections, and the overestimation increases with the energy. A comparison of the present values of  $Q_{el}$  with those of Khare and Kumar shows that the effect of the absorption potential is to decrease the value of the  $Q_{el}$  over the whole energy range. This remark is found to be valid even at energies just above the threshold of the formation of the posi-

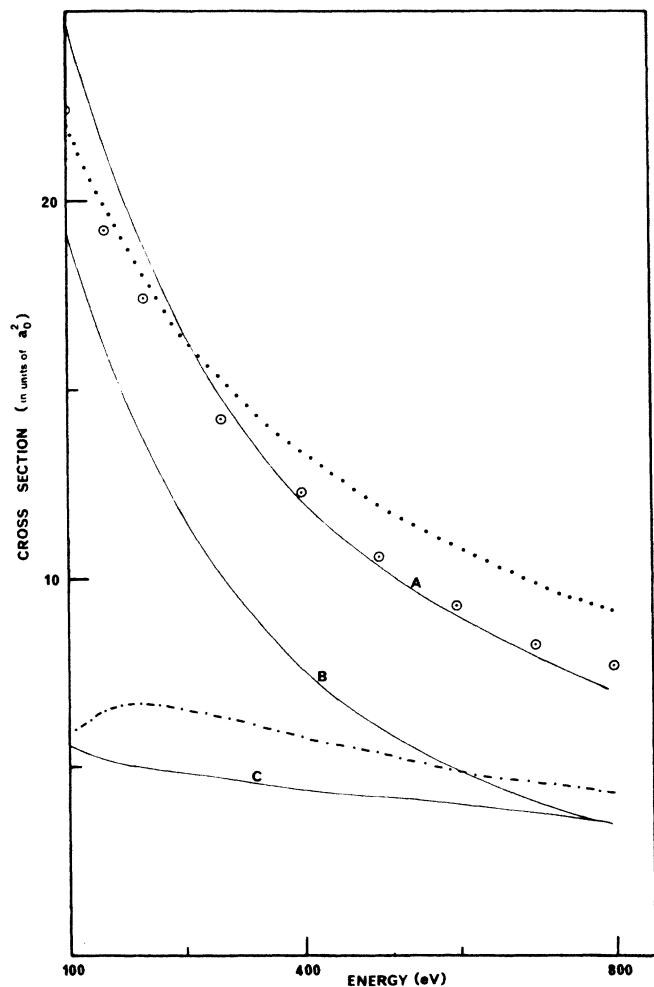


FIG. 1. Cross sections for positrons scattered by argon atoms. Solid curves *A*, *B*, and *C* denote present values of  $Q_T$ ,  $Q_{ab}$ , and  $Q_{el}$ , respectively. Dotted lines,  $Q_T$  of Joachain, Vanderpoorten, Winters, and Byron (Ref. 5); dash-dotted line,  $Q_{el}$  of Khare and Kumar (Ref. 8); dotted circles,  $Q_T$  of Kauppila *et al.* (Ref. 6).

tronium.<sup>10</sup> The recent calculation of Brown and Humberston<sup>10</sup> has shown that above the threshold of the formation of the positronium  $Q_{el}$  are less than the extrapolated values. Hence care should be observed in obtaining the cross sections for positronium formation with the help of  $Q_T$  and extrapolated values of  $Q_{el}$ . We also notice that  $Q_{ab}$  is greater than  $Q_{el}$  over the entire energy range. The difference between  $Q_{ab}$  and  $Q_{el}$  is rather large at lower energies, and it decreases rapidly with the energy. If we assume that the overestimation for  $Q_T$  at lower energies is due to a too strong absorption potential, then a milder absorption potential which will decrease the values of  $Q_T$  will also decrease the values of  $Q_{ab}$  and increase the values of  $Q_{el}$ . Thus the difference between  $Q_{ab}$  and  $Q_{el}$  will diminish.

In Fig. 2 we have shown our present values of  $Q_T$  for positron and electron scatterings by argon atoms along with the experimental data.<sup>6,11</sup> In the electron case, also, the theory overestimates the cross sections at lower energies, and the agreement between the theory and the experimental data of Kauppila *et al.*<sup>6</sup> is within 10% for  $E \geq 300$  eV. However, underestimation is noticed at higher energies. We also

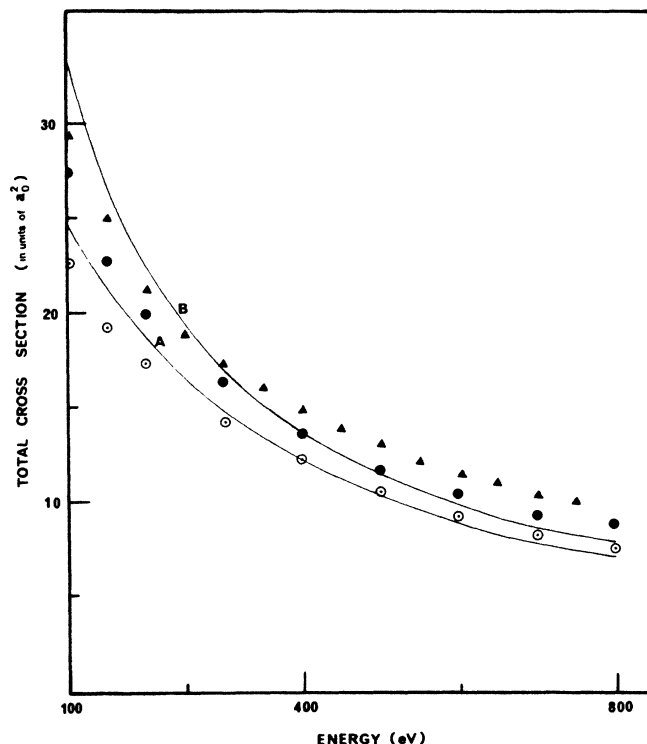


FIG. 2. Total cross sections for positrons and electrons scattered by argon atoms. Solid curves *A* and *B* denote present values for the positrons and the electrons, respectively. Dotted and solid circles, Kauppila *et al.* (Ref. 6) for the positrons and the electrons, respectively; triangles, Wagenaar and de Heer (Ref. 11) for the electrons.

notice that the values of the most recent experimental cross sections  $Q_T(e^-)$  obtained by Wagenaar and de Heer<sup>11</sup> are always higher than those of Kauppila *et al.*<sup>6</sup> Hence our theoretical values are in better agreement with this new set of experimental data at lower energies, but at higher energies the underestimation has further increased. Our theoretical values also support the experimental finding<sup>6</sup> that the curve for  $Q_T(e^-)$  does not merge with that of  $Q_T(e^+)$  even at 800 eV. Furthermore, the theoretical values of the ratio  $R = Q_T(e^-)/Q_T(e^+)$  are within 10% of the experimental values over the whole energy range. However, whereas the theoretical values of  $R$ , as expected, decrease continuously with the energy toward its asymptotic values of unity, the experimental values pass through a minimum at 400 eV. Finally, we conclude that the model potential employed in the present investigation has given satisfactory values for  $E \geq 300$  eV. Thus there is a need to refine the present model potential in such a way that better values are obtained at lower impact energies without also destroying the agreement with the experiment obtained above 300 eV.

#### ACKNOWLEDGMENTS

One of us (S.P.K.) gratefully acknowledges partial support and the hospitality extended to him by the Centre for Interdisciplinary Studies in Chemical Physics. Financial assistance from University Grants Commission (India) is also acknowledged.

\*On leave of absence from The Department of Physics, Meerut University, Meerut 250005, Uttar Pradesh, India.

†Present address: Physics Department, Birla Institute of Technology and Science, Pilani, India.

<sup>1</sup>F. J. de Heer and R. H. J. Jansen, *J. Phys. B* **10**, 3741 (1977).

<sup>2</sup>F. J. de Heer, R. H. J. Jansen, and W. van der Kay, *J. Phys. B* **12**, 979 (1979).

<sup>3</sup>A. Reitan, *Phys. Scr.* **22**, 615 (1981).

<sup>4</sup>G. Staszewska, D. W. Schwenke, and D. G. Truhlar, *Phys. Rev. A* **29**, 3078 (1984).

<sup>5</sup>C. J. Joachain, R. Vanderpoorten, K. H. Winters, and F. W. Byron, *J. Phys. B* **10**, 227 (1977).

<sup>6</sup>W. E. Kauppila, T. S. Stein, J. H. Smart, M. S. Dababneh, Y. K. Ho, J. P. Downing, and V. Pol, *Phys. Rev. A* **24**, 725 (1981).

<sup>7</sup>B. L. Jhanwar, S. P. Khare, and Ashok Kumar, *J. Phys. B* **11**, 887 (1978).

<sup>8</sup>S. P. Khare and Ashok Kumar, *Pramana* **10**, 63 (1978).

<sup>9</sup>M. Inokuti, *Rev. Mod. Phys.* **43**, 297 (1971).

<sup>10</sup>C. J. Brown and J. W. Humberston, *J. Phys. B* **18**, L401 (1985).

<sup>11</sup>R. W. Wagenaar and F. J. de Heer, *J. Phys. B* **18**, 2021 (1985).