Positron-impact ionization of helium in the distorted-wave polarized-orbital method

K. K. Mukherjee
Manipur Public School, Koirengei, Imphal 795 002, India

P. S. Mazumdar and S. Brajamani
Department of Physics, Manipur University, Canchipur, Imphal 795 003, India
(Received 25 January 1988; revised manuscript received 26 September 1988)

The total cross sections for positron-impact ionization of helium are evaluated by using the distorted-wave polarized-orbital method taking into account the effects of screening and final-channel distortion. The present results are in fair agreement with other elaborate theoretical calculations and experimental results.

I. INTRODUCTION

The total cross section (TCS) for the positron-impact ionization of helium was measured by Suekoa,[1] Diana *et al.*,[2] and Fromme *et al.*[3] Apart from the semiempirical estimates of the TCS for e^+-He ionization given by Griffith *et al.*[4] and Willis and McDowell,[5] the first quantum-mechanical calculation for the process was carried out by Basu *et al.*[6] They represented the incident positron by a distorted wave and used two models of final-state wave function. They also reported the first Born results for the process. The most elaborate theoretical calculations for e^+-He ionization were performed by Campeanu *et al.*[7] They studied in detail the effect of initial- and final-channel distortions and also the effect of screening in the final state of the ionizing system on the TCS. They found that although the effect of initial-channel distortion on the cross section is marginal the effects of final-channel distortion and screening are very pronounced.

Khan and Ghosh[8] used a distorted-wave polarized-orbital method to study the positronium formation cross section in e^+-He scattering and their results are in fairly good agreement with the experimental results of Diana *et al.*[9] They found the effect of the matrix elements arising from the distorted part of the target wave function (Temkin[10]) to be very important. But Basu *et al.* have not considered the matrix elements arising from the distorted part of the target wave function. In the present calculation we have employed the distorted-wave polarized-orbital method of Khan and Ghosh[8] to study the positron-impact ionization of helium in the energy range 30–150 eV of the incident positron. The wave function of the incident positron contains the effect of the dipole polarization potential and has the exact polarizability. We have also taken into account the effect of final-channel distortion, which was not considered by Basu *et al.*[6] In the present calculation we have used an analytical Hartree-Fock helium ground-state wave function (Byron and Joachain[11]) which is more accurate than the simple one-parameter wave function used by Basu *et al.*[6] In order to study the effect of screening in the final state of the ionizing system we have used two models of final-state wave functions. In the first model (M1) we have represented the wave function of the scattered positron by a plane-wave distorted in the field of the helium atom and that of the ejected electron is obtained by the method of polarized orbitals (Sloan[12]). In order that the full-screening model is consistent (Campeanu *et al.*[7]) we have taken the maximum value of the energy E_e of the ejected electron as $(E_i - V_{\text{ion}})/2$, where E_i is the energy of the incident positron and V_{ion} is the ionization potential of the target. In our second model (M2) for $E_e < E_F$ (E_f is the energy of the scattered positron), our final-state wave function is the same as that of model M1, but for $E_e > E_f$ we have represented the ejected electron as an attractive Coulomb wave in the field of double positive charge (e^+ and He^+) and the scattered positron as a repulsive Coulomb wave in the field of unit positive charge, since in this case the slowly moving positron screens the residual He^+ ion (Campeanu *et al.*[7]).

II. THEORY

Let $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ be the position vectors of the incident positron and the bound electrons with respect to the nucleus. The polarized-orbital wave function for the system of the incident positron and the helium atom is given by[8]

$$\psi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=[u(\mathbf{r}_2)+\Phi_{\text{pol}}(\mathbf{r}_1,\mathbf{r}_2)] \times[u(\mathbf{r}_3)+\Phi_{\text{pol}}(\mathbf{r}_1,\mathbf{r}_3)]F(\mathbf{r}_1)\ , \tag{1}$$

where $F(\mathbf{r}_1)$ is the wave function of the incident positron. $\Phi_{\text{pol}}(\mathbf{r}_1,\mathbf{r}_2)$ is the distorted part of the target wave function. In the framework of the dipole approximation it takes the form[8,13]

$$\Phi_{\text{pol}}(\mathbf{r}_1,\mathbf{r}_2)=-\pi^{-1/2}\frac{\epsilon(r_1,r_2)}{r_1^2}\frac{u_{1s\to p}(r_2)}{r_2} \times\cos(\hat{r}_1\cdot\hat{r}_2)\ , \tag{2}$$

where

$$\epsilon(r_1,r_2)=\begin{cases}1, & r_1>r_2\\ 0, & r_1<r_2\end{cases} \tag{3}$$

and

$$u_{1s\to p}(r)=(Z_p)^{1/2}\exp(-z_p r)(\tfrac{1}{2}Z_p r^3+r^2)\ , \qquad (4)$$

with $Z_p=1.594$. The value of Z_p is chosen so that it gives the exact polarizability. A number of authors (Srivastava and Kumar,[14] Srivastava *et al.*,[15,16] and Khan and Ghosh[8]) have used the Φ_{pol} calculated in the dipole approximation to calculate the polarization potential and have obtained results which are in fair agreement with the experimental results and rigorous theoretical results in the case of electron- and positron-impact excitation of helium and positronium formation in positron-helium scattering. $\Phi_{He}(\mathbf{r}_2,\mathbf{r}_3)$ is the wave function of the helium atom, which we have taken as the analytic wave function of Byron and Joachain,[11]

$$\Phi_{He}(r_2,r_3)=u(\mathbf{r}_2)u(\mathbf{r}_3)\ , \qquad (5)$$

$$u(\mathbf{r})=N[\exp(-\alpha r)+\delta\exp(-\beta r)]Y_{00}(\hat{\mathbf{r}})\ , \qquad (6)$$

with $N=2.6049754$, $\alpha=1.41$, $\beta=2.61$, and $\delta=0.79$. Now returning only the first-order terms in (1), we get

$$\psi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=[\Phi_{He}(\mathbf{r}_2,\mathbf{r}_3)+u(\mathbf{r}_2)\Phi_{pol}(\mathbf{r}_1,\mathbf{r}_3)+u(\mathbf{r}_3)\Phi_{pol}(\mathbf{r}_1,\mathbf{r}_2)]F(\mathbf{r}_1)\ . \qquad (7)$$

The total cross section for e^+-He ionization is given by

$$Q=\int\int d\hat{\mathbf{k}}_f\, d\mathbf{k}_e (k_f/k_i)/f_{ion}|^2\ , \qquad (8)$$

where $\mathbf{k}_i$, $\mathbf{k}_f$ and $\mathbf{k}_e$ are the momenta of the incident positron, scattered positron, and ejected electron, respectively. The ionization amplitude f_{ion} is given by

$$f_{ion}=(2\pi)^{-5/2}\times\langle\chi_{\mathbf{k}_f}(Z_f,\mathbf{r}_1)\psi_f(\mathbf{r}_2,\mathbf{r}_3)|V(r_1,r_2,r_3)|\psi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\rangle\ . \qquad (9)$$

$V(r_1,r_2,r_3)$ is the interaction potential between the incident positron and the helium atom,

$$V(r_1,r_2,r_3)=\frac{2}{r_1}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_3|}\ . \qquad (10)$$

$\chi_{\mathbf{k}_f}(Z_f,\mathbf{r}_1)$ is the wave function of the scattered positron. Z_f is the effective charge around the scattered positron. $\psi_f(r_2,r_3)$ represents the wave function of the final state of the e^--He^+ subsystem. It is made orthogonal to $\Phi_{He}(\mathbf{r}_2,\mathbf{r}_3)$:

$$\psi_f(\mathbf{r}_2,\mathbf{r}_3)=2^{-1/2}\{u(\mathbf{r}_2)[\chi_{\mathbf{k}_e}(Z_e,\mathbf{r}_3)-\langle\chi_{\mathbf{k}_e}(Z_e,\mathbf{r}')|u(\mathbf{r}')\rangle u(\mathbf{r}_3)]+(\mathbf{r}_2\gtrless\mathbf{r}_3)\}\ . \qquad (11)$$

$\chi_{\mathbf{k}_e}(Z_e,\mathbf{r})$ is the wave function of the ejected electron, Z_e is the effective charge around the ejected electron, and

$$u(\mathbf{r})=4\sqrt{2}\exp(-2r)Y_{00}(\hat{\mathbf{r}}) \qquad (12)$$

is the wave function of the He^+ ion. The wave function $F(r_1)$ of the incident positron is decomposed into partial waves as

$$F(\mathbf{r}_1)=k_i^{-1/2}\sum_{l_i=0}^{\infty}(2l_i+1)i^{l_i}\exp(i\delta_{l_i})\frac{u_{l_i}(k_i,r_1)}{r_1}P_{l_i}(\cos(\hat{k}_i\cdot\hat{r}_1))\ , \qquad (13)$$

where l_i is the orbital angular momentum quantum number of the incident positron. The radial part $u_{l_i}(k_i,r_1)$ of the wave function of the incident positron is obtained by solving the differential equation

$$\left[\frac{d^2}{dr_1^2}-\frac{l_i(l_i+1)}{r_1^2}-2V_i(r_1)\right]u_{l_i}(k_i,r_1)=E_i u_{l_i}(k_i,r_1)\ , \qquad (14)$$

with

$$V_i(r)=V_1=V_{st}(e^+\text{-He})+V_{pol}\ . \qquad (15)$$

$V_{st}(e^+\text{-He})$ is the static potential of the e^+-He system and V_{pol} is the dipole component of the polarization potential,

$$V_{st}(r)=\frac{2}{r}-\left\langle u(\mathbf{r}')\left|\frac{2}{|\mathbf{r}-\mathbf{r}'|}\right|u(\mathbf{r}')\right\rangle\ , \qquad (16)$$

$$V_{pol}(r)=\left\langle u(\mathbf{r}')\left|\frac{2}{|\mathbf{r}-\mathbf{r}'|}\right|\Phi_{pol}(\mathbf{r},\mathbf{r}')\right\rangle\ . \qquad (17)$$

We have decomposed $\chi_{\mathbf{k}_\lambda}(Z_\lambda,\mathbf{r})$ ($\lambda=f$ or e) into partial waves as

$$\chi_{\mathbf{k}_\lambda}(Z_\lambda,\mathbf{r})=\frac{4\pi}{k_\lambda}\sum_{l_\lambda=0}^{\infty}\sum_{m_\lambda=-l_\lambda}^{l_\lambda}i^{l_\lambda}\frac{G_{l_\lambda}(k_\lambda,Z_\lambda,r)}{r}Y_{l_\lambda m_\lambda}(\hat{\mathbf{r}})Y^*_{l_\lambda m_\lambda}(\hat{\mathbf{k}}_\lambda)\exp(-in_{l_\lambda})\ , \qquad (18)$$

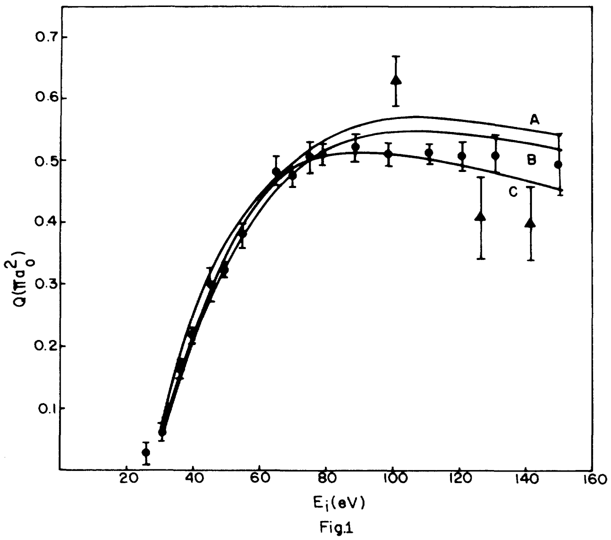

FIG. 1. Total cross section Q in units of πa_0^2 for positron-impact ionization of helium. The curves are the following: curve A, present model M2 results; curve B, present model M1 results; curve C, DW2 results of Basu *et al.* (Ref. 6); ●, experimental results of Fromme *et al.* (Ref. 3); ▲, experimental results of Diana *et al.* (Ref. 2).

where n_{l_λ} is the corresponding phase shift. For $E_e < E_f$ in models M1 and M2 the radial wave functions $G_{l_e}(k_e, Z_e, r)$ for the ejected electron are singlet exchange polarization functions for the scattering of electrons by the singly ionized helium obtained by the method of polarized orbitals (Sloan[12]). For $E_e < E_f$, in both models M1 and M2, the wave function of the scattered positron is calculated in the same manner as the wave function of the incident positron because we have assumed full screening of the residual He^+ ion by the ejected electron. In model M1, E_e is always less than E_f and the maximum value of E_e is $\frac{1}{2}(E_i - V_{ion})$.

In model M2 for $E_e > E_f$ the radial part $G_{l_\lambda}(k_\lambda, Z_\lambda, r)$ of $\chi_{\mathbf{k}_\lambda}(Z_\lambda, \mathbf{r})$ satisfies the differential equation

$$\left[\frac{d^2}{dr^2} - \frac{l_\lambda(l_\lambda+1)}{r^2} - 2V_\lambda(r)\right] G_{l_\lambda}(k_\lambda, Z_\lambda, r) = E_\lambda G_{l_\lambda}(k_\lambda, Z_\lambda, r) \ . \quad (19)$$

$E_\lambda = \frac{1}{2}k_\lambda^2$ is the corresponding energy and V_λ is the potential acting upon the particle. We have taken $Z_e = 2$, $Z_f = 1$, $V_e = -2/r$, and $V_f = 1/r$ for $E_e > E_f$ in model M2.

III. RESULTS AND DISCUSSIONS

In order to calculate Q we have taken adequate care regarding the convergence of Q with respect to the angular momentum quantum numbers l_i, l_f, and l_e of the incident positron, scattered positron, and the ejected electron, respectively. The maximum value of l_e was taken to be 5. The maximum value of l_i was varied from $l_i = 8$ for $E_i = 30$ eV to $l_i = 20$ for $E_i = 150$ eV. As a check of our program we have reproduced the CCA, CPT, and CPE results of Campeanu *et al.*[7]

In Fig. 1 we have plotted Q calculated in the two models M1 and M2. We have shown in Fig. 1 the experimental results of Fromme *et al.*[3] and Diana *et al.*[2] together with the DW2 results of Basu *et al.*[6] Our results using model M1 are very close to the DCPT3 results of Campeanu *et al.* and those corresponding to model M2 are close to the DCPE3 results of Campeanu *et al.*[7] and cannot be distinguished in the scale of Fig. 1. This is expected because the final-state wave function used in model M1 is very similar to that of the DCPT3 model of Campeanu *et al.*,[7] and that of model M2 is very close to the model DCPE3 of Campeanu *et al.* In Table I we have tabulated our present sets of results together with DCPT3, DCPE3, and DW2 results. Diana and coworkers are refining their method of measurement of Q and will repeat their work on positron-impact ionization of helium.[17] The apparent agreement of the results of Basu *et al.*[6] with the experimental results of Fromme *et al.*[3] is rather accidental. They have used a very simple helium atom wave function, and as they themselves have mentioned, the use of the analytic Hartree-Fock wave function for helium results in a variation of 4–16% in their results. Moreover, they have not taken into account the matrix elements arising from the distorted part of the target wave function. Our present results agree with more elaborate theoretical results and are in fair agreement with experimental results of Fromme *et al.*[3] This agreement is not accidental and it shows that, as in the case of positronium formation in e^+-He scattering, in

TABLE I. Total cross sections Q for positron-impact ionization of helium in different approximations. The results are given in units of πa_0^2. E_i is the energy of the incident positron.

	Q (units of πa_0^2)				
	Present results				
	Model	Model	Results of Ref. 7		Results of Ref. 6
E_i (eV)	M1	M2	DCPT3	DCPE3	DW2
30	0.0580	0.0604	0.0578	0.0585	0.0797
40	0.2104	0.2127	0.2100	0.2113	0.2522
60	0.4274	0.4372	0.4246	0.4337	0.4464
80	0.5205	0.5375	0.5130	0.5298	0.5067
100	0.5453	0.5669	0.5356	0.5569	0.5067
120	0.5344	0.5576	0.5296	0.5506	0.4903
150	0.5182	0.5425	0.5105	0.5315	0.4545

positron-impact ionization also the matrix elements arising from the distorted part of the target wave function play a crucial role. We also note that with the increase of the incident positron energy the present results tend to overestimate the experimental results. This feature of the distorted-wave polarized-orbital method has also been observed in electron-atom scattering.[18] This is due to the fact that with increase in energy of the incident positron, the adiabatic approximation becomes inaccurate.

ACKNOWLEDGMENTS

The authors are thankful to Professor R. P. McEachran for sending us Ref. 7 prior to publication. Thanks are due to Professor W. Raith and Professor L. M. Diana for sending the numerical value of their experimental results and to Professor H. N. K. Sarma and to Professor C. Amuba Singh for their keen interest in the present problem.

[1]O. Suekoa, J. Phys. Soc. Jpn. **51**, 2381 (1982).

[2]L. M. Diana, L. S. Fornari, S. C. Sharma, P. K. Pendlton, and P. G. Coleman, in *Proceedings of the 7th International Conference on Positron Annihilation, New Delhi, 1985,* edited by P. C. Jain, R. M. Singru, and K. P. Gopinathan (World Scientific, Singapore, 1985), p. 342.

[3]D. Fromme, G. Kruse, W. Raith, and G. Sinapus, Phys. Rev. Lett. **57**, 3031 (1986).

[4]T. C. Griffith, G. R. Heyland, K. S. Lines, and T. R. Twomey, J. Phys. B **12**, 1747 (1979).

[5]S. L. Willis and M. R. C. McDowell, J. Phys. B **15**, L31 (1982).

[6]M. Basu, P. S. Mazumdar, and A. S. Ghosh, J. Phys. B **18**, 369 (1985).

[7]R. I. Campeanu, R. P. McEachran, and A. D. Stauffer, J. Phys. B **20**, 1635 (1987).

[8]P. Khan and A. S. Ghosh, Phys. Rev. A **28**, 2181 (1983).

[9]L. M. Diana, P. G. Coleman, D. L. Brookes, P. K. Pendleton, and D. M. Norman, Phys. Rev. A **34**, 2731 (1986).

[10]A. Temkin, Phys. Rev. **116**, 368 (1959).

[11]F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. **146**, 1 (1966).

[12]I. H. Sloan, Proc. R. Soc. London, Ser. A **281**, 151 (1964).

[13]R. J. Drachman and A. Temkin, in *Case Studies in Atomic Collision Physics,* edited by E. W. McDaniel and M. R. C. McDowell (North-Holland, Amsterdam, 1972), Vol. 2.

[14]R. Srivastava and M. Kumar, Phys. Rev. A **31**, 3639 (1985).

[15]R. Srivastava, M. Kumar, and A. N. Tripathi, J. Chem. Phys. **82**, 1818 (1985).

[16]R. Srivastava, M. Kumar, and A. N. Tripathi, J. Chem. Phys. **84**, 4715 (1986).

[17]L. M. Diana (private communications).

[18]B. H. Brandsden and M. R. C. McDowell, Phys. Rep. **30C**, 207 (1977).