Double excitation of helium by electron impact: A distorted-wave polarized-orbital approach

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A distorted-wave model in its modified form (where distortion, polarization, and exchange effects as desired are appropriately implemented in both the channels) is used to calculate the differential and total cross sections for excitation of $2p^2\,^3P_g$, $2p3p\,^1P_g$, and $2p3d\,^{1,3}D_u$ states of neutral helium atom from the ground state $1s^2\,^1S_g$. The results are compared with the available theoretical and experimental results.

I. INTRODUCTION

All doubly excited states of helium lie embedded in the He I continuum. Many of these states autoionize after a certain time (10^{-13}–10^{-14} s) through their interaction with the continuum. Despite the fact that their energies lay far above the ionization potential, certain of these doubly excited states are stable against autoionization. Such stable states are also known as being of the parity-unfavored type, and their decay via electron emission is forbidden. Examples of these states in helium have the configuration $nln'l'\,^{1,3}L$ with $l+l'-L$ odd (where nl and $n'l'$ are the principal and orbital angular momentum quantum number of the two excited electrons and $^{1,3}L$ denotes the total orbital angular momentum L and multiplicity of the doubly excited state). Most of these states can be excited from the ground state by electron impact but not by photoabsorption. The unique characteristics of this class of collision events have been studied by many authors.[1–9] Studies of the parity-unfavored-type transitions in helium in particular, as well as those in alkaline-earth atoms, have been made in which the process had been treated as bound-state excitation.

Becker and Dahler[2] were the first to investigate theoretically the excitation (from the ground state) of some of the doubly excited states in helium by electron impact. In their study they calculated differential and total cross sections using the Born-Oppenheimer (BO) approximation and, for only some excitations, using the distorted-wave and close-coupling approximations. Roy and Sil[4] calculated the excitation cross sections for ^1S-^3P transition in helium using the integral form of the close-coupling approximation. Hickerson *et al*[6,7] repeated the calculations for the same transitions as considered by Becker and Dahler[2] both in BO approximation and Born-Oppenheimer-Rudge (BOR) approximation methods. Their choice for ground-state wave function was, however, different as they[6,7] performed calculations separately using Hartree-Fock and correlated wave functions. The only experimental measurement, also merely for ^1S-^3P excitation in helium, has been recently reported by Westerveld *et al.*[10] On comparison of each theoretical result with the experimental data for ^1S-^3P excitation in He, one concludes that none of the theoretical evaluations reproduces the experimental data. The relative behavior of the measured excitation cross-section-energy curve is not even satisfactorily reproduced.

In view of the above fact, Williamson *et al.*[8] and Ellis *et al.*[9] have very recently made an attempt to improve the high-energy behavior of the theoretical results by performing the calculation for ^1S-^3P excitation in Glauber-Ochkur approximation.[11] However, the calculation performed by these authors[8,9] using the form of Glauber-exchange amplitude as suggested by Franco and Halpern[11] is not fully reliable. An error of phase in it has been pointed out,[12] and it would be better attempted along the lines suggested by Padhy *et al.*[13] In almost all earlier theoretical models, simple analytic radial wave functions[2] were used to describe both the ground and excited states of helium. In order to probe the possibility of further improving the agreement between experimental and theoretical results for ^1S-^3P excitation in helium, we reconsider this process in the present paper and perform calculations in the distored-wave polarized orbital (DWPO) model.[14] Our present attempt is the consequence of the success of our DWPO model[14] in obtaining excellent cross-section results for electron-impact excitation of 2^1S state in the helium atom. The distorted-wave model[14] we will be using includes the distortion, polarization, and exchange effects appropriately in both the ingoing and outgoing distorted waves (rather than in a single channel only[15]). We would have preferred to perform the present DWPO calculation using the configuration-interaction ground-state wave function,[6,7] but in order to avoid additional complexities only simple analytical wave functions[2] have been used. In addition, this choice of our wave function provides the real comparative suitability which as we know is possible only when similar wave functions are used in different models. Essentially, the wave functions we adopted are the same as in various earlier approaches (e.g., BO, close-coupling, and Glauber approximations[2,4,8]). In addition to $2p^2\,^3P$ excitation, the present calculations are further extended for sake of completeness to other parity-nonfavored doubly excited states of helium, viz., $2p3p\,^1P$ and $2p3d\,^{1,3}D$.

II. THEORY

We consider the case of electron-impact double electron excitation from the ground state of helium (viz., ^1S_g) in distorted-wave approximation. The T matrices for singlet and triplet excitations then can be given, respectively, as (on integration over spin functions)

$$T_s=\langle\psi_f^s(1,2)F^-(k_f,3)\,|\,V_f(1,2,3)\,|\,\psi_i^s(1,2)F^+(k_i,3)\rangle - \langle\psi_f^s(1,2)F^-(k_f,3)\,|\,V_f(1,2,3)\,|\,\psi_i^s(2,3)F^+(k_i,1)\rangle \tag{1}$$

and

$$T_T=\sqrt{3}\langle\psi_f^a(1,2)F^-(k_f,3)\,|\,V_f(1,2,3)\,|\,\psi_i^s(2,3)F^+(k_i,1)\rangle. \tag{2}$$

In the above two expressions $F^+(k_i,r)$ and $F^-(k_f,r)$ are the ingoing and outgoing distorted waves, respectively, with the associated $\mathbf{k}_i$ and $\mathbf{k}_f$ wave vectors. Through these waves only the different distortion effects such as their distortion by static potential, polarization of the target, and exchange effects are appropriately incorporated. $V_f=-2/r_3+1/r_{13}+1/r_{23}$ is the interaction of the scattered electron with target atom. ψ_i^s is the symmetrized wave function of the initial state of the target, while $\psi_f^{s(a)}$ is the symmetrized (or antisymmetrized) final-state wave function. These various wave functions needed for the different transitions are described through the following expressions (standard notations are used):

$$\psi^s(1,2;^1S_g)=R_{10}(1)R_{10}(2)Y_{00}(1)Y_{00}(2), \tag{3}$$

$$\psi_f^a(1,2;^3P_g)=\sum_{m_1,m_2}\langle 11m_1m_2\,|\,1M_L\rangle \times R_{21}(1)R_{21}(2)Y_{1m_1}(1)Y_{1m_2}(2)\,, \tag{4}$$

$$\psi_f^s(1,2;^1P_g) =\frac{1}{\sqrt{2}}\sum_{m_1,m_2}\langle 11m_1m_2\,|\,1M_L\rangle \times[R_{21}(1)R_{31}(2)Y_{1m_1}(1)Y_{1m_2}(2) +R_{21}(2)R_{31}(1)Y_{1m_1}(2)Y_{1m_2}(1)]\,, \tag{5}$$

and finally

$$\psi_f^{s(a)}(1,2;^{1(3)}D_u) =\frac{1}{\sqrt{2}}\sum_{m_1,m_2}\langle 12m_1m_2\,|\,2M_L\rangle \times[R_{21}(1)R_{32}(2)Y_{1m_1}(1)Y_{2m_2}(2) \pm R_{21}(2)R_{32}(1)Y_{1m_1}(2)Y_{2m_2}(1)]\,. \tag{6}$$

Here $+ve$ and $-ve$ refer to the symmetric and antisymmetric state, respectively. The radial wave functions $R_{nl}(r_i)$ are chosen to be the variationally optimized hydrogenic orbitals as constructed by Becker and Dahler.[2]

$F^{\pm}(k,r)$, the distorted waves, are expanded in partial waves as[16]

$$F^{\pm}(k,r)=\frac{1}{\sqrt{k}}\sum_l(2l+1)(\pm i)^l\frac{u_l^{\pm}(k,r)}{r} \times e^{\pm i\delta_l(k^2)}P_l(\cos\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})\,,$$

where $u_l(k,r)$ satisfies the equation

$$\left[\frac{d^2}{dr^2}+k^2-\frac{l(l+1)}{r^2}-2V_{\rm st}(r)-2V_{\rm pol}(r)\right]u_l^{\pm}(k,r)=A(r) \tag{7}$$

under the following boundary conditions:

$$u_l(k,r)\to 0 \quad \text{as} \quad r\to 0 \tag{8}$$

and

$$u_l(k,r)\sim k^{-1/2}\sin\left[kr-\frac{l\pi}{2}+\delta_l\right] \quad \text{as } r\to\infty\,. \tag{9}$$

Here, δ_l is the phase shift of the lth partial wave. $A(r)$ is the nonhomogeneous term involving an integral over $u_l(k,r)$ for the incoming wave [i.e., making Eq. (7) an integro-differential equation] and is zero for the outgoing wave. The potential terms $V_{\rm st}(r)$ and $V_{\rm pol}(r)$ are chosen, respectively, to be

$$V_{\rm st}(r)=-\frac{2}{r}+\left\langle R_{10}(t)Y_{00}(\hat{\mathbf{t}})\left|\frac{2}{|\mathbf{r}-\mathbf{t}|}\right|R_{10}(t)Y_{00}(\hat{\mathbf{t}})\right\rangle \tag{10}$$

and

$$V_{\rm pol}(r)=\left\langle R_{10}(t)Y_{00}(\hat{\mathbf{t}})\left|\frac{2}{|\mathbf{r}-\mathbf{t}|}\right|\phi_{\rm pol}(\mathbf{r},\mathbf{t})\right\rangle\,. \tag{11}$$

The dipole term of the following wave function is chosen as suggested by Temkin and Lamkin:[17]

$$\phi_{\rm pol}(\mathbf{r},\mathbf{t})=R_{10}(t)Y_{00}(\hat{\mathbf{t}}) \times\sum_{m=1}^{\infty}\frac{1}{r^{m+1}}\left[\frac{t^{m+1}}{m+1}+\frac{t^m}{m}\right]P_m(\cos\hat{\mathbf{r}}\cdot\hat{\mathbf{t}})\,. \tag{12}$$

Equation (7) as well as the expressions for $V_{\rm st}$ and $V_{\rm pol}$ [viz., Eqs. (10)–(12)] reveal that we have taken into account the distortion effects in both of the channels by the ground state of helium. This choice is justified by the fact that one can expect the passage time of the projectile electron in the vicinity of the target helium atom to be much smaller than that required for the helium atom to make its transition from ground state to final excited state. This fact, in other words, implies that the projectile is essentially always in the field of the ground state[18] of the

helium atom. The radial equation (7) is solved for $u_l^{\pm}(k,r)$ using the boundary conditions [Eqs. (8) and (9)] and exactly following the procedure as adopted by McDowell *et al.*,[16] Singh *et al.*,[19] and Srivastava *et al.*[14] In essence the procedure[14,16,19] consists of using the non-iterative method of Marriott[20] to obtain the solution $u_l^{\pm}(k,r)$ from Eq. (7). The normalization of radial wave function and phase shift δ_l being obtained by matching with the JWKB solution in the manner suggested by Burgess.[21] After obtaining $u_l^{\pm}(k,r)$ and carrying out some preliminary algebra for angular momentum along with the integrations over the various variables in a straightforward manner, the T matrices [Eq. (1) and/or Eq. (2)] can finally be put in the one-dimensional integral form. Integrals are then evaluated using Simpson's method. The T matrices for various transitions as well as the corresponding differential and total cross sections are obtained from them in the conventional manner.

III. RESULTS AND DISCUSSION

In Fig. 1, present total cross-section results for $1s^2\,{}^1S-2p^2\,{}^3P$ excitation in an energy range from threshold to nearly 150 eV are displayed. We also compare our results with almost all the theoretical calculations available along with the only reported relative experimental data (the figure, however, displays the normalized value at 120 eV, where most of the theoretical estimates nearly agree). Before comparing the results it would be worthwhile to mention that in almost all previous calculations[2-9] the ground as well as different doubly excited states were represented by the hydrogenic (H) wave functions. However, in a few of the attempts,[4,6,7] while the final doubly excited states wave function was changed and chosen to be either Hartree-Fock (HF) type or configuration-interaction (CI) type.[6,7] In the figure, curves $B1$, $B2$, and $B3$ represent various BO results using H-, HF-, and CI-type ground-state wave functions. Results are available[6,7] using both the 20- and 35-term CI wave functions, but in the figure we have shown only the 20-term results as there is no significant difference between the two. Curves $C1$ and $C2$ display the close-coupling results obtained using H and HF wave functions, respectively. Curve G is the Glauber approximation result[8,9] obtained utilizing a H-type wave function. The results obtained by Becker and Dahler[2] in different versions of distorted-wave approximations and that of Hickerson *et al.*[7] using BOR theory are not shown in the figure because of their large deviations from the experimental data.

First, we compare the experimental results with the different theoretical results obtained using H-type wave functions. These results are, in fact, curves $B1$, $C1$, G, and P (present calculation). We find that curve G behaves in a totally different manner as compared with other curves in the energy range below 100 eV. In this range, however, the rest of the curves (viz., $B1$, $C1$, and P), including experiment, display the occurrence of distinct maxima a little displaced from each other. Above an impact energy of 100 eV all the curves fall off rapidly (as compared to experiment) except that of the Glauber result which falls a little less steeply. This particular behavior is

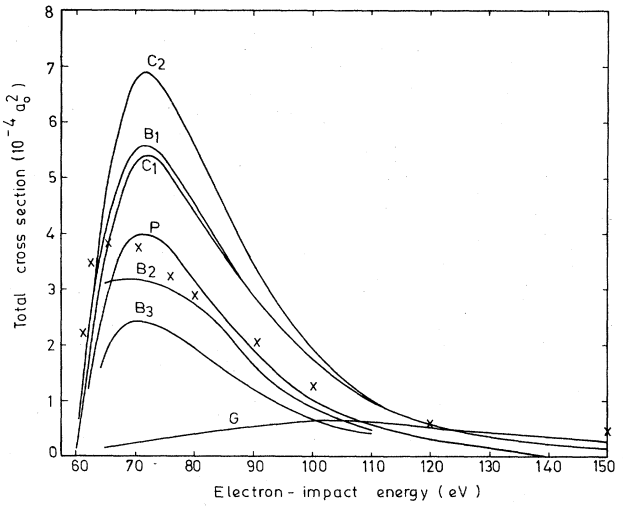

FIG. 1. Total electron-impact cross sections for $2p^2\,{}^3P_g$ excitation. Curve P, present results; curve $B1$, BO results with H-type functions (Ref. 2); curve $B2$, BO results with HF function (Ref. 2); curve $B3$, BO results with CI functions (Ref. 6); curve $C1$, close-coupling results with H-type function (Ref. 4); curve $C2$, close-coupling results with HF functions (Ref. 4); curve G, Glauber results (Ref. 8); $\times$, experimental results (Ref. 10).

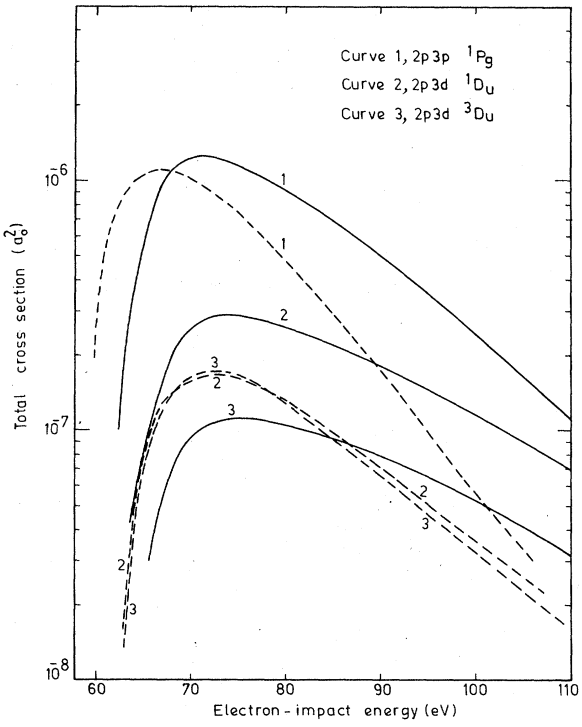

FIG. 2. Total electron-impact excitation cross sections for the (1) $2p3p\,{}^1P_g$, (2) $2p3d\,{}^1D_u$, and (3) $2p3d\,{}^3D_u$ doubly excited states of helium. Solid curves are BO-theory results with H-type wave functions (Ref. 2); dashed curves are present DWPO calculations.

well explained by Williamson *et al.*[8] Our present curve *P*, when compared with other theoretical results, suggests the importance of distortion and polarization effects. Let us compare now the various results in other aspects. We compare the close-coupling approximation curves *C*1 and *C*2 and, separately, the BO theory curves *B*1, *B*2, and *B*3. These are the results obtained using different wave functions (of ground state only) in the same model. The results in BO theory are so modified that the HF wave function reduces the cross sections which are further lessened with the use of CI wave function. In contrast to the BO model, the use of a HF function surprisingly increases the cross sections in the close-coupling approximation (see curves *C*1 and *C*2). One is therefore led to infer that the choice of the different ground-state wave functions in two separate models modifies the results in different manners. It is therefore desirable to perform the calculations in any reliable approximation method which at least properly describes the scattering process so that the uncertainties in the results are avoided. The present DWPO model can be considered to be a reliable model in this context.

Total cross-section results for excitation of $2p3p\ ^1P$, $2p3d\ ^1D$, and $2p3d\ ^3D$ states are shown in Fig. 2. We compare our present results with those of Becker and Dahler[2] using BO theory with identical H-type wave functions. However, the only other calculations for $2p3d\ ^{1,3}D$ states are those of Hickerson *et al.*[6] who used ground-state HF and CI functions in BO theory. These seem to compare with our results in a manner similar to that for $2p^2\ ^3P$ excitation. However, the differences in the results are less, and therefore are not displayed in Fig. 2 to avoid overlapping. From Fig. 2 we find that the present ^1D and ^3D results are not much different from each other. Such is not the case in the BO approximation where both these results substantially differ at all energies. In contrast to ^3P excitation, the BO and present DWPO models predict maxima at energies which are quite markedly displaced from one another. For all three transitions, the present DWPO curves of present calculation estimate cross sections which fall off a little more steeply than shown by BO theory. Again, the differences in the two sets of theoretical results presented in Fig. 2 suggest sufficient contribution due to distortion and polarization effects.

We find that in all four of these different excitations (viz., $2p^2\ ^3P$, $2p3d\ ^1D$, $2p3d\ ^3D$, and $2p3p\ ^1P$), the differential cross sections become zero in forward and backward directions. This fact is consistent with the predic-

TABLE I. Total cross sections (in units of a_0^2) of helium for different excitations. The number in parentheses denotes the power of ten by which the quantity should be multiplied.

Energy (eV)	$2p^2\ ^3P_g$	$2p3p\ ^1P_g$	$2p3d\ ^1D_u$	$2p3d\ ^3D_u$
60.00	6.719 789(−6)	2.946 810(−7)		
61.00	6.523 556(−5)	5.306 822(−7)		
62.00	1.2146(−4)	7.231 024(−7)		
63.00	1.777 875(−4)	8.7236(−7)	1.586 673(−8)	1.362 643(−8)
64.00	2.375 352(−4)	9.785 935(−7)	4.589 533(−8)	4.347 93(−8)
65.00	2.756 361(−4)	1.047 346(−6)	7.543 554(−8)	7.354 359(−8)
67.00	2.492 151(−4)	1.093 967(−6)	1.227 236(−7)	1.219 54(−7)
68.00	3.701 299(−4)	1.083 646(−6)	1.395 268(−7)	1.394 624(−7)
69.00	3.847 614(−4)	1.057 28(−6)	1.519 854(−7)	1.525 716(−7)
70.00	3.940 194(−4)	1.019 644(−6)	1.608 613(−7)	1.619 525(−7)
71.00	3.976 251(−4)	9.733 726(−7)	1.658 78(−7)	1.671 618(−7)
72.00	3.978 459(−4)	9.217 705(−7)	1.682 767(−7)	1.697 052(−7)
73.00	3.943 26(−4)	8.668 148(−7)	1.684 696(−7)	1.699 936(−7)
74.00	3.874 734(−4)	8.105 222(−7)	1.666 813(−7)	1.681 016(−7)
75.00	3.793 513(−4)	7.538 498(−7)	1.632 998(−7)	1.644 725(−7)
78.00	3.445 455(−4)	5.904 418(−7)	1.469 064(−7)	1.470 007(−7)
80.00	3.175 019(−4)	4.940 951(−7)	1.335 42(−7)	1.323 244(−7)
85.00	2.481 897(−4)	3.035 402(−7)	9.969 813(−8)	9.665 066(−8)
90.00	1.869 971(−4)	1.777 298(−7)	7.205 092(−8)	6.945 617(−8)
95.00	1.375 357(−4)	9.993 154(−8)	5.087 657(−8)	4.885 808(−8)
100.00	9.984 439(−5)	5.485 147(−8)	3.564 296(−8)	3.434 968(−8)
120.00	2.647 477(−5)	3.518 952(−9)	7.804 497(−9)	7.084 768(−9)
130.00	1.366 738(−5)	5.220 539(−10)	3.675 746(−9)	3.227 956(−9)
140.00	7.152 758(−6)	1.478 477(−11)	1.883 41(−9)	1.7424(−9)
150.00	3.811 183(−6)	3.572 407(−11)	9.065 473(−10)	7.934 248(−10)
170.00	1.140 439(−6)	1.548 145(−10)	2.308 488(−10)	1.891 586(−10)
190.00	3.649 925(−7)	1.379 844(−10)	6.165 591(−11)	4.506 948(−11)
230.00	4.544 139(−8)	5.500 865(−11)	5.753 103(−12)	3.718 247(−12)
250.00	1.722 042(−8)	3.139 094(−11)	1.692 605(−12)	8.035 683(−13)
300.00	1.892 534(−9)	7.528 468(−12)	1.052 001(−13)	2.217 77(−14)

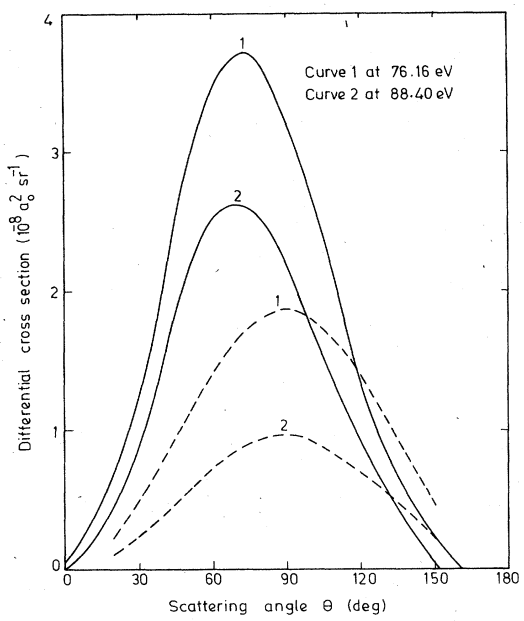

FIG. 3. Differential cross-section results for $2p3d\ ^1D$ excitation in helium. Same as in Fig. 2.

tion of Fano,[22] who has shown that for parity-unfavored transitions the cross sections vanish for scattering angles equal to zero and π. In Fig. 3, as a sample we present our theoretical prediction of differential cross sections for $2p3d\ ^1D$ state at two different energies. We also compare our results with the only available results of Becker and Dahler[2] using an H-type wave function in BO theory. On comparison, we find our results are distinctly different from their results at both the electron-impact energies displayed. In addition, the present calculation predicts the peak of the cross section shifted towards higher angles by almost 15°—20° as compared to that obtained from BO theory.[2] Finally, all the results for total cross sections for electron-impact energies up to 300 eV are collected in Table I. Various results for the differential cross sections for all four transitions can be obtained on request.

In conclusion, we feel in general that more perfect studies are desirable, theoretically and experimentally, for electron-impact excitation of various doubly excited states in helium—at least for ^1S-^3P excitation, where more theoretical studies are made, an absolute measurement is called for strongly, together with an accurate theoretical approach in which both initial- and final-state wave functions are described properly. Present study suggests the importance of polarization effect which therefore should also be incorporated.

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