$n\,^1S$ and $n\,^1P$ excitations of heliumlike ions by electrons: A precise distorted-wave polarized-orbital approach

Rajesh Srivastava* and A. K. Katiyar
Department of Physics, University of Roorkee, Roorkee, India
(Received 16 June 1986)

Total-cross-section results for excitations of $n\,^1S$ and $n\,^1P$ ($n=2$–6) states of several heliumlike ions from the $1\,^1S$ ground state are reported in this paper for energies near threshold to above five times the threshold energy. These results are obtained using a reliable distorted-wave polarized-orbital approach where distortions are included due to static, polarization, and exchange effects appropriately as desired in both the initial and final channels of the distorted waves. Sensitivity of the results with respect to different choices of ion-target wave functions (such as hydrogenic, Hartree-Fock, and configuration-interaction types) in the present model is also examined. The results are compared with other available theoretical estimates.

I. INTRODUCTION

We do not wish here in this paper to reemphasize the undoubtedly well-known applications in plasma, fusion, and astrophysical researches of the various electron-impact-excitation cross-section data for heliumlike ions. We stress rather the reliable theoretical evaluations of these cross sections as the obvious experimental difficulties[1] preclude experimentalists from measuring these data accurately and demand a proper theoretical description of the collision process. There has many calculations available for heliumlike ions using various approaches; see, for example, a few reviews[2–4] and some recent papers and references therein.[5–7] It can be seen from the literature that the results reported so far are greatly different from each other and a reliable report of these results is desirable.

There are two major sources of uncertainties in the theoretical evaluation of cross sections in general in any collisional study. First, one adopts some approximation for treating the scattering process, e.g., first Born approximation, the distorted-wave approximation, or close-coupling approximations. Second, explicit calculations with any of these approximations uses input eigenfunctions of an ion (or atom) in the initial state and in the final state at least, and possibly also in intermediate states. For the precise evaluation of cross-section data, therefore, both these uncertainties should be minimized. In view, recently, Christensen and Norcross[5] have examined the sensitivity of results of scattering approximation, target wave functions, and resonance effects using mainly a five-state close-coupling (CC) method as well as the distorted-wave (DW) model of Eissner and Seaton[8] in the near-threshold energy region for $2\,^1S$ and $2\,^1P$ excitations of the Li^+ ion only. However, for intermediate and high energies a similar study would be worth doing for electron-impact excitation of various heliumlike ions considering other transitions also.

The DW approximation method[9–15] has proved to be a great success and a quite useful model in electron (or positron) scattering with an atom in the intermediate-energy range and provides (if sensibly applied) results equally as reliable as those obtained by close-coupling methods in low energies and at the same time is quite less expensive computationally. Presently, therefore, we aim in this paper to report the cross-section data for electron-impact excitation of several heliumlike ions for $n\,^1S$ and $n\,^1P$ excitations ($n=2$, 3, 4, 5, and 6) from the ground $1\,^1S$ state using a consistent distorted-wave-approximation method[9–13] as well as examining the results with the use of accurate ion-target wave functions. Our method will not consider the resonance effects which are usually confined in the near-threshold region of the incident electron energies[5] and where any DW method is not supposed to give reliable results. We shall report results in the region of near threshold to above five times threshold energies of electron impact.

There are, however, already a few DW approaches in various forms[6,8,16–19] which have been used to calculate the $n=2$ sublevel excitations of many heliumlike ions by electron impact and it is important to see how one can improve upon these DW methods. Before we describe the DW model we used here in this paper for our calculation, it would be necessary first to briefly mention the other most often used DW methods. Eissner and Seaton[8] have developed a DW method which used a single-distortion potential (the Thomas-Fermi type) both for initial and final distorted waves and also utilized this potential to get bound states of target ions. The DW method of Peek and Mann[16] used in both initial and final channels a spherically averaged electrostatic potential of the target ion and took also approximate account of exchange in the distortion potential. Bhatia and Temkin[17] as well as McDowell *et al.*[18] used a much better DW method where they took distortion due to polarization, static, and exchange potentials systematically in the initial channel while utilizing a simple Coulomb wave in the final channel. Singh, Srivastava, and Rai[19] used a variable-charge Coulomb-projected (VCCP) -type distorted-wave method. Recently, Itikawa and Sakimoto[6] performed calculations using the same

ground-state static-potential-generated distorted waves for initial and final distorted waves. In all the above-mentioned distorted-wave methods, in addition to the evaluation of the direct excitation T matrix, the exchange T matrix is also evaluated in the calculations. For the target-ion wave functions mostly the hydrogenic (H-type) (Ref. 20) or the Hartree-Fock (HF) type[17,21] wave functions have been used. However, Itikawa and Sakimoto[6] have used recently in their simple DW model the configuration-interaction (CI) -type wave function to represent the target ion.[22,23] For $n\,^1S$ and $n\,^1P$ ($n \geq 3$) excitations there are no distorted-wave calculations, only a few other calculations.[24–27] Among these Tully[24] and Nakazaki[25] reported results for some transitions in few ions using a Coulomb-Born approximation (CBA). Tayal and Kingston,[26] using an R-matrix method, have calculated the effective collision strengths for $3\,^1P$ excitation which are, however, not directly comparable to cross sections. However, Sampson, Parks, and Clarks[27] reported scaled cross sections for various transitions in several ions.

The DW method we use here for calculation consists of obtaining initial and final distorted waves in the field of same ground-state static and polarization potentials while in addition, the initial-state distorted wave, the exchange effect is incorporated accurately.[9,12,13] The exchange T matrix is also calculated using the Bonham-Ochkur approximation.[9] In fact, this type of DW approach has proved to be quite successful in reproducing experimental results (see our recent paper[9–13]) for electron (or positron) -impact excitation of $2\,^1S$ and $2\,^1P$ as well as a few doubly excited states of the neutral helium atom and encouraged us to extend the method for calculation of electron-impact excitation of heliumlike ions. Not only do we presently use an improved DW method but we also utilized simpler (H- or HF-type) or more accurate (CI-type) wave functions for the target ion to test the sensitivity of the results in our DW method.

A full account of our present DW method as applied to helium (or, one can say in general, a two-electron system) has already been given[9,12] and its extension to heliumlike ions is straightforward. However, it may be desirable to stress the points where the theoretical treatment for ions departs from one for a neutral helium atom. We present, therefore, in Sec. II, a brief account of our DW method.

II. THEORY

The differential and total cross sections for a transition from an an initial $1\,^1S$ state (say i) to a final $n\,^1S$ (or $n\,^1P$) state (say f) of any heliumlike ion target of nuclear charge Z, due to collision of an electron of initial energy k_i^2 (Ry) may be written as (atomic units are used throughout)

$$I(\theta,\phi)=\frac{1}{4\pi^2}\frac{k_f}{k_i}\sum_m |T_{if}^m|^2 \quad (a_0^2/\mathrm{sr}) \tag{1}$$

and

$$\sigma_{if}(k_i^2)=\frac{1}{2\pi^2}\frac{k_f}{k_i}\int_{-1}^{+1}\sum_m |T_{if}^m|^2 d(\cos\theta) \quad (\pi a_0^2)\,, \tag{2}$$

where k_i and k_f are the initial and final momentum of the incoming and outgoing electrons, respectively, and are related through excitation threshold energy ΔE and scattering angle θ by

$$k_i^2=k_f^2+\Delta E \quad \text{and} \quad \hat{\mathbf{k}}_i\cdot\hat{\mathbf{k}}_f=\cos\theta\,.$$

T_{if}^m is the T matrix for the excitation of the mth degenerate final state of the target ion from the initial state and is given by

$$T_{if}^m=\langle \Phi_{fm} \mid V \mid \Psi_i^+ \rangle\,, \tag{3}$$

where Φ_{fm} is the final unperturbed wave function in the final channel, V is the interaction potential between the incident projectile electron and the target heliumlike ion, and Ψ_i^+ represents the exact wave function describing the total system in the initial channel. These are expressed in the following way in our distorted-wave polarized-orbital approximation.[9,12] If we choose the center of mass to be fixed at the nucleus and let $\mathbf{r}_3$ be the position vector of the incident electron with respect to this point and the bound electrons have position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, then

$$\Phi_{fm}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=[\phi_{fm}(\mathbf{r}_1,\mathbf{r}_2)+\phi_f^{\mathrm{pol}}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]F^-(\mathbf{k}_f,\mathbf{r}_3)\,, \tag{4}$$

$$V(r_1,r_2,r_3)=-\frac{Z}{r_3}+\frac{1}{r_{13}}+\frac{1}{r_{23}}\,, \tag{5}$$

and

$$\psi_i^+(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=[\phi_i(\mathbf{r}_1,\mathbf{r}_2)+\phi_i^{\mathrm{pol}}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]F^+(\mathbf{k}_i,\mathbf{r}_3) -\phi_i(\mathbf{r}_2,\mathbf{r}_3)F_i^+(\mathbf{k}_i,\mathbf{r}_1)\,. \tag{6}$$

ϕ_i and ϕ_{fm} are unperturbed ground and excited wave functions of the target ion, respectively, while ϕ_i^{pol} and ϕ_f^{pol} are the polarized-orbital wave functions of the target ion in the initial and final state, respectively. $F^+(\mathbf{k}_i,\mathbf{r})$ and $F^-(\mathbf{k}_f,\mathbf{r})$ are the ingoing and outgoing distorted waves to be obtained after solving the following two equations separately:

$$H_i\psi_i^+=E_i\psi_i^+ \tag{7}$$

and

$$H_f\Phi_{fm}=E_f\Phi_{fm}\,. \tag{8}$$

H_i and H_f are the Hamiltonians corresponding to the initial and final channel of the system, respectively, and E_i and E_f are the corresponding energies. In writing Eq. (6) we have neglected for the sake of simplicity the exchange-polarization term as the polarization contribution will be small at distances where exchange is important.

We expand the $F^{\pm}(\mathbf{k},\mathbf{r})$ in general in the following way in terms of spherical harmonic expansion:

$$F^{\pm}(\mathbf{k},\mathbf{r})=\frac{1}{\sqrt{k}}\sum_{l=0}^{\infty}(2l+1)i^l e^{\pm i[\delta_l(k^2)+\eta_l(k^2)]} \times\frac{u_l(k,r)}{r}P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})\,, \tag{9}$$

where δ_l is the scattering phase shift for the lth partial wave while η_l is the Coulomb phase shift due to residual

TABLE I. The total excitation cross section for $1\,^1S \rightarrow 2\,^1S$ in units of πa_0^2. The numbers in square brackets are powers of ten by which the quantities are to be multiplied.

Ions	Incident energy (Ry)	HF-type wave function	CI-type wave function	H-type wave function
		$\Delta E = 4.48$	$\Delta E = 4.465$	$\Delta E = 4.48$
Li^+	5.000	0.1467[−1]	0.2890[−1]	0.9465[−2]
$Z = 3$	8.956	0.3623[−2]	0.3569[−2]	0.3088[−2]
	13.434	0.2645[−2]	0.1591[−2]	0.2495[−2]
	17.912	0.2265[−2]	0.7772[−3]	0.2165[−2]
	22.390	0.1983[−2]	0.5976[−3]	0.1896[−2]
		$\Delta E = 22.7$	$\Delta E = 22.368$	$\Delta E = 22.7$
C^{4+}	22.500	0.1046[−2]	0.1357[−2]	0.8899[−3]
$Z = 6$	44.736	0.2362[−3]	0.1355[−3]	0.2231[−3]
	67.104	0.1834[−2]	0.7214[−4]	0.1779[−3]
	89.472	0.1574[−3]	0.3247[−4]	0.1531[−3]
	111.840	0.1374[−3]	0.9750[−4]	0.1336[−3]
		$\Delta E = 41.79$	$\Delta E = 41.7801$	$\Delta E = 41.79$
O^{6+}	42.000	0.3077[−3]	0.3118[−3]	0.2758[−3]
$Z = 8$	83.592	0.7427[−4]	0.3089[−4]	0.7139[−4]
	125.388	0.5824[−4]	0.2005[−4]	0.5690[−4]
	167.184	0.4994[−4]	0.2191[−4]	0.4889[−4]
	208.980	0.4356[−4]	0.3072[−4]	0.4264[−4]
		$\Delta E = 136.0$	$\Delta E = 136.071$	$\Delta E = 136.0$
Si^{12+}	136.2	0.2747[−4]	0.2936[−4]	0.2598[−4]
$Z = 14$	272.0	0.7622[−5]	0.4042[−5]	0.7600[−5]
	408.0	0.6059[−5]	0.2602[−5]	0.6108[−5]
	544.0	0.5188[−5]	0.1691[−5]	0.5238[−5]
	680.0	0.4510[−5]	0.1351[−5]	0.4554[−5]
	816.0	0.3966[−5]	0.1130[−5]	0.4004[−5]
	952.0	0.3521[−5]	0.2068[−5]	0.3554[−5]
	1088.0	0.3149[−5]	0.2106[−5]	0.3178[−5]
		$\Delta E = 8.94$		
Be^{2+}	9.000	0.6047[−2]		
$Z = 4$	17.882	0.1193[−2]		
	26.823	0.9042[−3]		
	35.764	0.7757[−3]		
	44.705	0.6781[−3]		
		$\Delta E = 14.9$		
B^{3+}	15.000	0.2284[−2]		
$Z = 5$	29.810	0.4887[−3]		
	44.715	0.3761[−3]		
	59.620	0.3227[−3]		
	74.525	0.2818[−3]		
		$\Delta E = 31.32$		
N^{5+}	32.000	0.5137[−3]		
$Z = 7$	62.664	0.1270[−3]		
	93.996	0.9913[−4]		
	125.328	0.8500[−4]		
	156.660	0.7416[−4]		
		$\Delta E = 284.389$		
Ca^{18+}	285.0	0.4058[−5]		
$Z = 20$	568.778	0.1769[−5]		
	853.167	0.1447[−5]		
	1137.556	0.1220[−5]		
	1421.945	0.1027[−5]		

TABLE I. (*Continued*).

		$\Delta E=486.609$
Fe^{24+}	487.0	0.9571[−6]
$Z=36$	973.218	0.6444[−6]
	1459.827	0.5242[−6]
	1946.436	0.4106[−6]
	2433.045	0.3111[−6]

ionic charge $(Z-2)$ of the target heliumlike ion given by

$$\eta_l=\arg\left[l+1-i\frac{(Z-2)}{k}\right]. \tag{10}$$

With the help of the above expansion [Eq. (9)] and using Eqs. (4)—(6), Eqs. (6) and (8), respectively, can be written as

$$\left[\frac{d^2}{dr^2}+k_i^2-\frac{l(l+1)}{r^2}-2V_{ii}^{\rm st}(r)-V_l^{\rm pol}(r)\right]u_l^{+}(k_i,r)=A(r) \tag{11}$$

and

$$\left[\frac{d^2}{dr^2}+k_f^2-\frac{l(l+1)}{r^2}-2V_{ff}^{\rm st}(r)-V_f^{\rm pol}(r)\right]u_l^{-}(k_f,r)=0\,. \tag{12}$$

In both Eqs. (11) and (12) above, in general $V_{nn}^{\rm st}(r)$ and $V_n^{\rm pol}(r)$ are, respectively, the static and polarization potential of the heliumlike ion in its nth state and are given by

$$V_{nn}^{\rm st}(r_3)=\langle\phi_n(\mathbf{r}_1,\mathbf{r}_2)\,|\,V(r_1,r_2,r_3)\,|\,\phi_n(\mathbf{r}_1,\mathbf{r}_2)\rangle \tag{13}$$

and

$$V_n^{\rm pol}(r_3)=\langle\phi_n(\mathbf{r}_1,\mathbf{r}_2)\,|\,V(r_1,r_2,r_3)\,|\,\phi_n^{\rm pol}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\rangle\,. \tag{14}$$

In Eq. (11) $A(r)$ is the nonhomogeneous term (cf. Srivastava, Kumar, and Tripathi[9]) due to the exchange term in Eq. (6) and involves the integral over $u_l(k_i,r)$, which means Eq. (11) is in fact an integro-differential equation while in Eq. (12) for the outgoing wave there is no such term due to exchange. Further, in our calculation, we have taken as an approximation $V_{ff}^{\rm st}(r)=V_{ii}^{\rm st}(r)$ and $V_f^{\rm pol}(r)=V_i^{\rm pol}(r)$; thus the distortion effects in both the channels are taken by the same ground state of the heliumlike ion. This choice is found to be very adequate and has also been used in the past with success.[6,9,28–30] For $\phi_{\rm pol}$ in Eq. (14) we take as prevalent the dipole term only of the following expansion:[31]

$$\phi_i^{\rm pol}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\phi_i(\mathbf{r}_1,\mathbf{r}_2)\sum_{j=1}^{\infty}\frac{1}{r_3^{j+1}}\left[\frac{r_1^{j+1}}{j+1}+\frac{r_1^j}{j}\right]\times P_j(\hat{\mathbf{r}}_1\cdot\hat{\mathbf{r}}_3)\,. \tag{15}$$

We believe the dipole term of the above expression would sufficiently take into account the polarization contribution appropriately[28,33] as we have considered the exchange term in Eq. (9) accurately, not empirically.[30]

The two equations [viz., (11) and (12)] are solved for $u_l(k,r)$ in general using the following boundary conditions:

$$u_l(k,r)=0 \quad \text{as } r\to 0 \tag{16}$$

and

$$u_l(k,r)=k^{-1/2}\sin\left[kr-\frac{l\pi}{2}+\frac{(Z-2)\ln(2kr)}{k}+\eta_l(k)+\delta_l\right] \quad \text{as } r\to\infty \tag{17}$$

and adopting the noniterative approach of Marriot.[34] Further, the normalization of $u_l(k,r)$ and evaluation of δ_l are done by matching the JWKB solution as suggested by Burgess.[35]

For describing the target we have used (where available) the following different type of wave functions to represent ϕ_i and ϕ_{fm}: (i) hydrogenic orbitals[13,22] (H type), (ii) Hartree-Fock type as used by Bhatia and Temkin[17] (HF type), and (iii) configuration-interaction type[22] as used by van Wyngaarden, Bhadra, and Henry[23] and Itikawa and Sakimoto[6] (CI type).

After we have known the wave functions for the target ion as well as distorted waves, the evaluation of the T matrix [Eq. (3)] and consequently differential and total cross-section results [Eqs. (1) and (2)] can be obtained in a conventional and straightforward manner although the analysis is quite cumbersome and lengthy.[9,12] We should also mention that the convergence over the partial waves of scattered electrons in the case of $1\,^1S\to n\,^1S$ transitions was found within $l\le 10$ for all ions at all energies of impact of the incident electron. In contrast, for $1\,^1S\to n\,^1P$ transitions the summation of partial waves involved over matrix elements was slowly coverging and to overcome this numerical problem we carried out the summation over partial waves exactly up to a value ($l_{\max}\le 25$) for which the matrix element becomes nearly equal to the corresponding first Coulomb Born matrix element, and thereafter for higher partial waves the estimate by the Coulomb Born approximation is made (see, for example, Ref. 10). In Sec. III we shall display and discuss our different results and the comparison of these results with those obtained from other theories.

TABLE II. The total excitation cross section for $1\,^1S \rightarrow 2\,^1P$ in units of πa_0^2. The numbers in square brackets are powers of ten by which the quantities are to be multiplied.

Ions	Incident energy (Ry)	HF-type wave function	CI-type wave function	H-type wave function
		$\Delta E = 4.465$	$\Delta E = 4.572$	$\Delta E = 4.465$
Li^+	7.0	0.1948[−1]	0.2353[−1]	0.2491[−1]
$Z = 3$	9.0	0.2459[−1]	0.3065[−1]	0.3119[−1]
	13.41	0.2729[−1]	0.3506[−1]	0.3439[−1]
	20.00	0.2359[−1]	0.3129[−1]	0.3011[−1]
		$\Delta E = 22.523$	$\Delta E = 22.627$	$\Delta E = 22.523$
C^{4+}	25.0	0.8887[−3]	0.9723[−3]	0.9791[−1]
$Z = 6$	27.0	0.1068[−2]	0.1170[−2]	0.1169[−2]
	36.0	0.1719[−2]	0.1918[−2]	0.1875[−2]
	50.0	0.1744[−2]	0.1956[−2]	0.1900[−2]
	60.0	0.1708[−2]	0.1917[−2]	0.1860[−2]
	80.0	0.1546[−2]	0.1741[−2]	0.1682[−2]
	100.0	0.1337[−2]	0.1506[−2]	0.1455[−2]
		$\Delta E = 42.062$	$\Delta E = 42.175$	$\Delta E = 42.062$
O^{6+}	50.0	0.3703[−3]	0.3752[−3]	0.3950[−3]
$Z = 8$	64.0	0.5000[−3]	0.5143[−3]	0.5317[−3]
	75.0	0.5279[−3]	0.5421[−3]	0.5610[−3]
	90.0	0.5611[−3]	0.5786[−3]	0.5956[−3]
	105.0	0.5488[−3]	0.5665[−3]	0.5824[−3]
	126.0	0.5228[−3]	0.5405[−3]	0.5546[−3]
		$\Delta E = 136.051$	$\Delta E = 136.792$	$\Delta E = 136.051$
Si^{12+}	138.0	0.2993[−4]	0.2946[−4]	0.3016[−4]
$Z = 14.01$	196.0	0.5264[−5]	0.5303[−4]	0.5300[−4]
	400.0	0.5753[−4]	0.5872[−4]	0.5790[−4]
		$\Delta E = 8.983$		
Be^2	10.0	0.3756[−2]		
$Z = 4$	12.0	0.5677[−2]		
	15.0	0.7699[−2]		
	20.0	0.9313[−2]		
	25.0	0.9229[−2]		
		$\Delta E = 15.003$		
B^{3+}	18.0	0.2074[−2]		
$Z = 5$	27.0	0.3718[−2]		
	50.0	0.3282[−2]		
		$\Delta E = 31.543$		
N^{5+}	36.0	0.5396[−3]		
$Z = 7$	49.0	0.9086[−3]		
	75.0	0.9534[−3]		
		$\Delta E = 54.081$		
F^{7+}	60.0	0.1992[−3]		
$Z = 9$	81.0	0.2974[−3]		
	160.0	0.3265[−3]		
		$\Delta E = 67.600$		
Ne^{8+}	75.0	0.1366[−3]		
$Z = 10$	100.0	0.1960[−3]		
	200.0	0.2147[−3]		

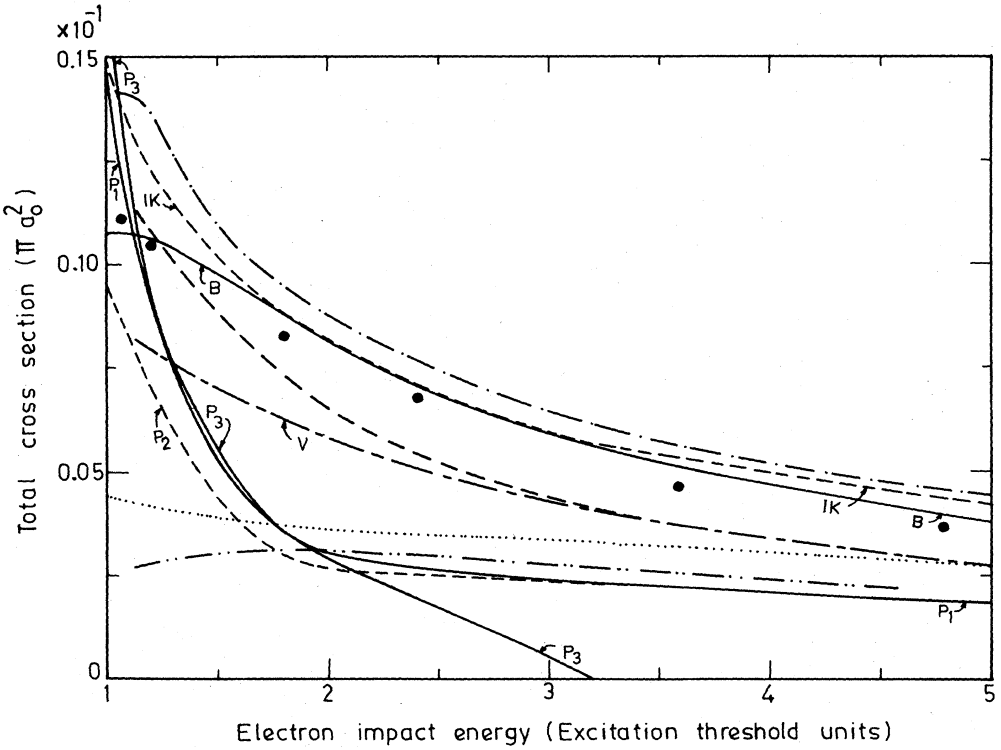

FIG. 1. Theoretical results for the $1\,^1S \rightarrow 2\,^1S$ excitation of Li^+. P_1 solid curve, present results (with HF-type wave function); P_2 broken curve, present result (with H-type wave function); P_3 solid curve, present results (with CI-type wave function); IK broken curve, DW results of Itikawa and Sakimoto (Ref. 6); B solid curve, five-state results of Badnell (Ref. 7); dot-dashed curve, CC results of van Wyngaarden, Bhadra, and Henry (Ref. 21); double-dot—dashed curve, DW results of Bhatia and Temkin (Ref. 17); dotted curve, DWPO results of McDowell *et al.* (Ref. 18); V small- and large-dashed curve, VCCPB results of Singh, Srivastava, and Rai (Ref. 19); broken curve, CB results of Bhatia and Temkin (Ref, 17); solid circle, scaled results of Sampson, Parks, and Clarks (Ref. 27).

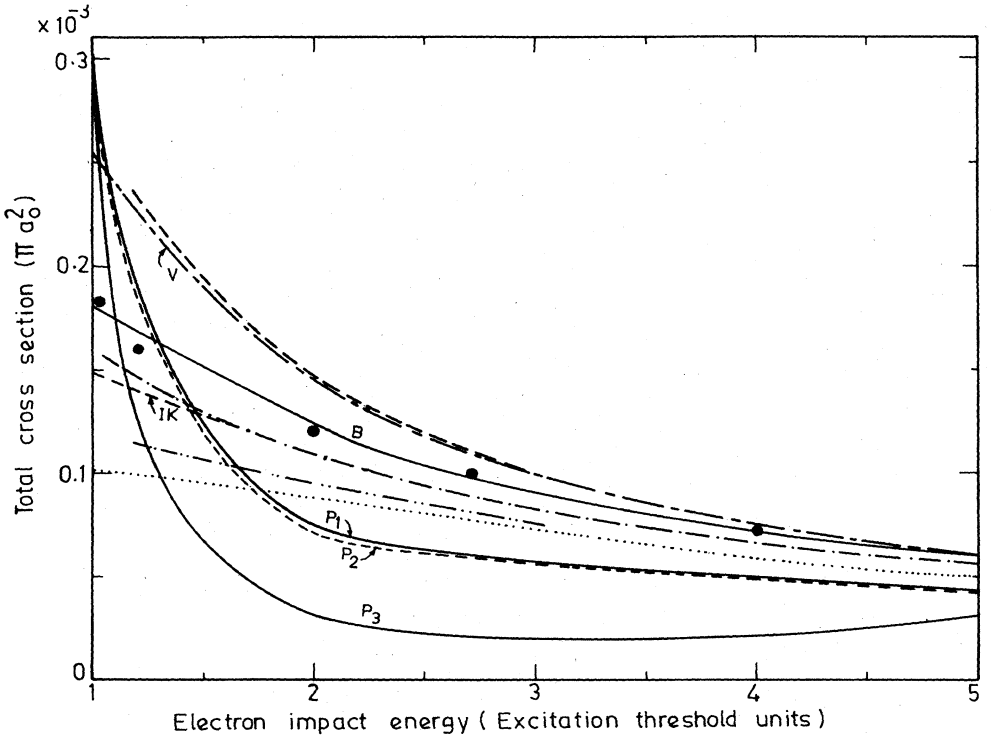

FIG. 2. Theoretical results for the $1\,^1S \rightarrow 2\,^1S$ excitation of O^{6+}, with notation the same as in Fig. 1.

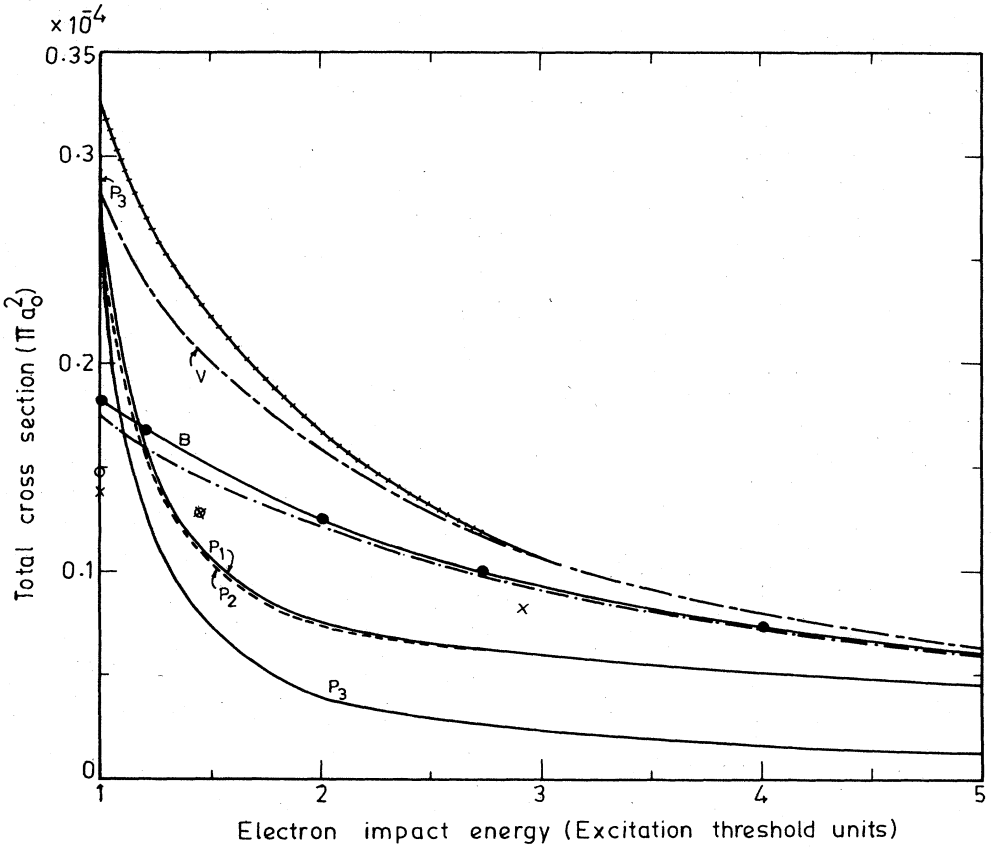

FIG. 3. Theoretical results for the $1\,^1S \rightarrow 2\,^1S$ excitation of Si^{12+}, with notation the same as in Fig. 1 except that now CB results of Bhatia and Temkin (Ref. 17) are represented as ——, DW results of Bhatia and Temkin (Ref. 17) by ×, and DWPO results (Ref. 18) by ○.

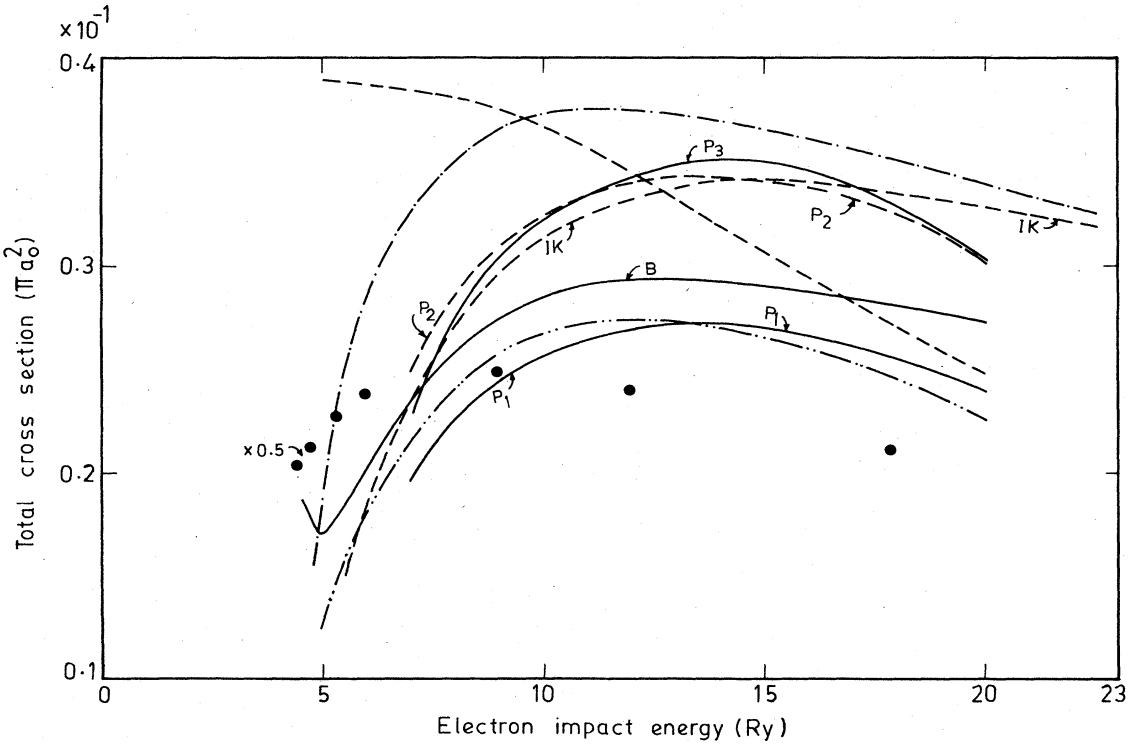

FIG. 4. Theoretical results for the $1\,^1S \rightarrow 2\,^1P$ excitation of Li^+, with notation the same as in Fig. 1.

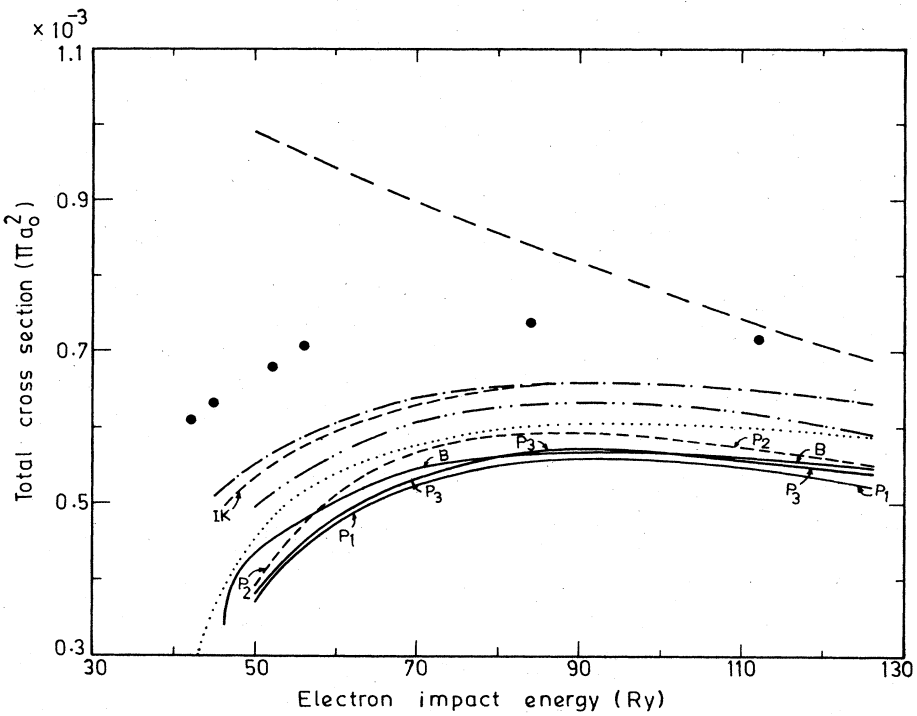

FIG. 5. Theoretical results for the $1\,^1S \rightarrow 2\,^1P$ excitation of O^{6+}, with notation the same as in Fig. 1.

III. RESULTS AND DISCUSSION

Total-cross-section results in general for exciting $n\,^1S$ and $n\,^1P$ ($n \leq 6$) states in various heliumlike ions from their ground $1\,^1S$ state are calculated for those ions only where other results are available for comparison. Results for $2\,^1S$ and $2\,^1P$ excitations in Li^+, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, C^{6+}, F^{7+}, Ne^{8+}, Si^{12+}, Ca^{18+}, and Fe^{24+} heliumlike ions are reported separately in Tables I and II for each transition. In addition to these two tables we have compared and shown our cross-section estimates for $2\,^1S$ excitation in Li^+, O^{6+}, and Si^{12+} in Figs. 1—3 separately as well as for the $2\,^1P$ transition of Li^+ and O^{6+} in Figs. 4 and 5, respectively. Finally, in Fig. 6, a display of differential cross-section results for $2\,^1S$ excitation in O^{6+} only is also done. Our choice of presenting only selective results graphically is based on the fact that for such cases only other largely theoretical calculations are available for meaningful comparison. For $n\,^1S$ and $n\,^1P$ ($n = 3$, 4, 5, and 6) excitations, the calculations are performed in Li^+, Be^{2+}, and O^{6+} ions only and the results are compiled in Tables III and IV for $n\,^1S$ and $n\,^1P$ states, respectively. Since not many other results were available for $n \geq 3$ excitations, we preferred to present the comparison of our DW results with others available for $3\,^1S$ and $3\,^1P$ states of the O^{6+} ion only in Table V.

To examine variation of the cross section with respect to choice of wave function, we have chosen only four ions, namely, Li^+, C^{4+}, O^{6+}, and Si^{12+} for which all the three types (viz., H type, HF type, and CI type) of wave functions for $2\,^1S$ and $2\,^1P$ states are found available. Therefore calculations are performed using all these three types

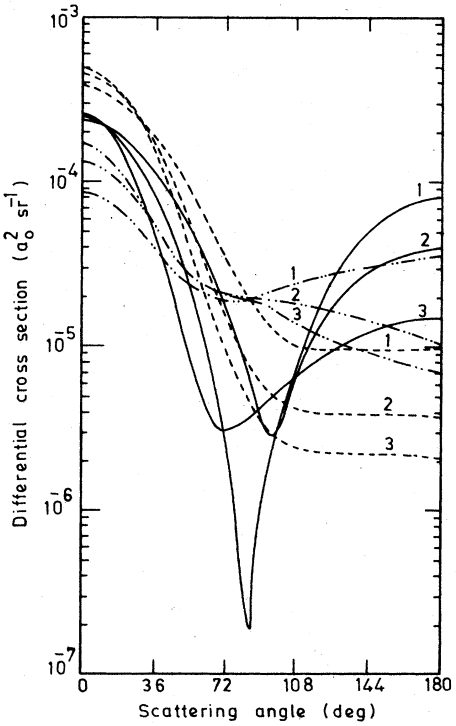

FIG. 6. $2\,^1S$ differential excitation cross section in O^{6+} (curves 1—3 refer to incident electron energies of 50, 60, and 75 Ry, respectively). Solid curve, present results (with HF-type wave function); dashed curve, VCCPB results of Singh, Srivistava, and Rai (Ref. 19); double-dot—dashed curve, DW results of Bhatia and Temkin (Ref. 17).

TABLE III. The total excitation cross section for $1\,^1S \rightarrow n\,^1S$ in units of πa_0^2. ΔE is the excitation threshold energy. The numbers in square brackets are powers of ten by which the quantities are to be multiplied.

Ions	Electron impact energy (in units of ΔE)	$n=3$	$n=4$	$n=5$	$n=6$
		$\Delta E=5.022$	$\Delta E=5.229$	$\Delta E=5.3226$	$\Delta E=5.3739$
Li^+	1[a]	0.1532[−2]	0.5946[−3]	0.2937[−3]	0.1666[−3]
$Z=3$	2	0.5265[−3]	0.2066[−3]	0.1024[−3]	0.5818[−4]
	3	0.4547[−3]	0.1793[−3]	0.8899[−4]	0.5064[−4]
	4	0.3968[−3]	0.1565[−3]	0.7768[−4]	0.4421[−4]
	5	0.3470[−3]	0.1368[−3]	0.6791[−4]	0.3865[−4]
	6	0.3062[−3]	0.1207[−3]	0.5991[−4]	0.3409[−4]
	7	0.2729[−3]	0.1076[−3]	0.5341[−4]	0.3039[−4]
	8	0.2458[−3]	0.9689[−4]	0.4809[−4]	0.2737[−4]
		$\Delta E=10.2032$	$\Delta E=10.6576$	$\Delta E=10.8672$	$\Delta E=10.9792$
Be^{2+}	1[a]	0.6407[−3]	0.2403[−3]	0.1166[−3]	0.6559[−4]
$Z=4$	2	0.1913[−3]	0.7274[−4]	0.3554[−4]	0.2006[−4]
	3	0.1609[−3]	0.6158[−4]	0.3016[−4]	0.1705[−4]
	4	0.1397[−3]	0.5350[−4]	0.2622[−4]	0.482[−4]
	5	0.1220[−3]	0.4674[−4]	0.2290[−4]	0.1294[−4]
	6	0.1077[−3]	0.4123[−4]	0.2021[−4]	0.1142[−4]
	7	0.9603[−4]	0.3678[−4]	0.1802[−4]	0.1018[−4]
	8	0.8652[−4]	0.3313[−4]	0.1623[−4]	0.9174[−5]
		$\Delta E=48.7104$	$\Delta E=51.1296$	$\Delta E=52.2496$	$\Delta E=52.8576$
O^{6+}	1[a]	0.4369[−4]	0.1568[−4]	0.7466[−5]	0.4156[−5]
$Z=8$	2	0.1248[−4]	0.4545[−5]	0.2178[−5]	0.1217[−5]
	3	0.1028[−4]	0.3768[−5]	0.1812[−5]	0.1013[−5]
	4	0.8876[−5]	0.3258[−5]	0.1567[−5]	0.8766[−6]
	5	0.7745[−5]	0.2843[−5]	0.1367[−5]	0.7650[−6]
	6	0.6832[−5]	0.2509[−5]	0.1206[−5]	0.6750[−6]
	7	0.6095[−5]	0.2238[−5]	0.1076[−5]	0.6021[−6]
	8	0.5492[−5]	0.2016[−5]	0.9693[−6]	0.5424[−6]

[a]Here incident energy is $\Delta E+0.2$ instead of ΔE.

of wave functions for these four ions. For the rest of the ions, only prevalent HF-type wave functions[17] for $1\,^1S$ ground and $2\,^1S$ ($2\,^1P$) excited states are used. For excited-state wave functions in transitions $n \geq 3$, the hydrogenic wave functions are used. The CI-type wave functions are those due to Hibbert[22] and have been used earlier by van Wyngaarden[23] and Itikawa and Sakimoto[6] also.

In Fig. 1, where various results for $2\,^1S$ excitation in Li^+ are shown, we find that among our different results obtained using three different type of wave functions, the results with use of the CI-type wave function are substantially reduced as compared to that obtained using HF- and H-type wave functions. These latter two, however, differ at low energies ($\leq 2\Delta E$). All these three results seem to merge with the increase of energies of electron impact (see also Table I). A little difference between H- and HF-type results as compared to CI type may be due to not much difference in their wave functions as compared to much different CI wave functions. Comparison of our DW results with that of Bhatia and Temkin[17] and McDowell *et al.*[18] suggest that the inclusion of polarization and static distortion effects, also in the final channel, reduces the cross section slightly at higher energies ($\geq 2\Delta E$) while it increases it below this energy range. CC results of van Wyngaarden, Bhadra, and Henry[23] are in general very high—it is probably (as noted by authors themselves) an outcome of nonconvergence of the close-coupling series. The close agreement of the variable-charge Coulomb-projected Born (VCCPB) (Ref. 19) results with that of Coulomb Born (CB) (Ref. 17) results is obvious because of the similarity of the two models, as VCCPB differs from CB by taking account by distortion in the final channel by static potential only. Further, the DW results of Itikawa and Sakimoto[6] using the CI wave function are in close agreement with the scaled-cross-section results of Sampson *et al.*[27] and of Badnell[7] who used a different type of approach. Comparison of our DW results using CI with that of Itikawa and Sakimoto[6] using the same CI wave function but using ground-state static potential in both the channels suggest the contribution of exchange and polarization effects in distorted waves, although the situation is not very clear at high energies where these effects should not be very strong. Overall observation of the entire curves reflects that all the curves tend to approach each other (as expected) at very high energies of electron

TABLE IV. The total excitation cross section for $1\,^1S \rightarrow n\,^1P$ in units of πa_0^2. ΔE is the excitation threshold energy. Numbers in square brackets are powers of ten by which the quantities are to be multiplied.

Ions	Electron impact energy (in units of ΔE)	$n=3$	$n=4$	$n=5$	$n=6$
		$\Delta E=5.049$	$\Delta E=5.2398$	$\Delta E=5.328$	$\Delta E=5.3766$
Li^+	1[a]	0.2617[−2]	0.9789[−3]	0.4747[−3]	0.2665[−3]
$Z=3$	2	0.5538[−2]	0.2106[−2]	0.1029[−2]	0.5806[−3]
	3	0.6133[−2]	0.2327[−2]	0.1135[−2]	0.6399[−3]
	4	0.5698[−2]	0.2163[−2]	0.1055[−2]	0.5947[−3]
	5	0.5055[−2]	0.1917[−2]	0.9346[−3]	0.5269[−3]
	6	0.4513[−2]	0.1709[−2]	0.8325[−3]	0.4692[−3]
	7	0.4032[−2]	0.1527[−2]	0.7445[−3]	0.4195[−3]
		$\Delta E=10.2448$	$\Delta E=10.6752$	$\Delta E=10.8752$	$\Delta E=10.984$
Be^{2+}	1[a]	0.7436[−3]	0.2729[−3]	0.1491[−3]	0.8332[−4]
$Z=4$	2	0.1838[−2]	0.6823[−3]	0.3293[−3]	0.1846[−3]
	3	0.1854[−2]	0.6879[−3]	0.3319[−3]	0.1861[−3]
	4	0.1576[−2]	0.5846[−3]	0.2824[−3]	0.1583[−3]
	5	0.1358[−2]	0.5037[−3]	0.2433[−3]	0.1365[−3]
	6	0.1203[−2]	0.4451[−3]	0.2147[−3]	0.1203[−3]
	7	0.1083[−2]	0.4004[−3]	0.1930[−3]	0.1082[−3]
	8	0.9789[−3]	0.3619[−3]	0.1745[−3]	0.9777[−4]
		$\Delta E=48.8128$	$\Delta E=51.1808$	$\Delta E=52.2752$	$\Delta E=52.8704$
O^{6+}	1[b]	0.4632[−4]	0.1647[−4]	0.7810[−5]	0.4338[−5]
$Z=8$	2	0.1015[−3]	0.3641[−4]	0.1733[−4]	0.9647[−5]
	3	0.9526[−4]	0.3420[−4]	0.1628[−4]	0.9061[−5]
	4	0.8055[−4]	0.2893[−4]	0.1378[−4]	0.7666[−5]
	5	0.6770[−4]	0.2430[−4]	0.1157[−4]	0.6441[−5]
	6	0.5745[−4]	0.2061[−4]	0.9810[−5]	0.5459[−5]
	7	0.4965[−4]	0.1778[−4]	0.8455[−5]	0.4704[−5]
	8	0.4356[−4]	0.1558[−4]	0.7410[−5]	0.4121[−5]

[a]Here incident energy is $\Delta E+1.0$ instead of ΔE.
[b]Here incident energy is $\Delta E+2.0$ instead of ΔE.

impact where compared to these high energies the effects of distortions are negligibly small. As observed by Christensen and Norcross[5] we also see that all the DW results have (except that of Itikawa and Sakimoto) different asymptotic high-energy behavior as compared to close-coupling results in that they fall more steeply and merge to CBA results. Similar features are also seen in $2\,^1S$ excitation of helium by electrons and positrons.[9,11] It can be concluded that for $2\,^1S$ excitation in Li^+ the choice of model is a more important issue then the choice of wave functions, while is relatively less effective.

In Figs. 2 and 3, respectively, we have displayed our results and compared these with others for $2\,^1S$ excitation in O^{6+} and Si^{12+}. In case of O^{6+} a calculation has been made recently with the use of R-matrix theory by Tayal and Kingston[26] for $2\,^1S$ and $2\,^1P$ excitations in O^{6+}. Except in the resonance region near threshold, the results of their calculation is very similar to the close-coupling results[23] and hence are not shown in Fig. 2 for comparison; only CC results are included. One finds in both these figures that most of the features of the comparison of our results with others are similar to those in Fig. 1, except that

TABLE V. The total excitation cross section for $1\,^1S \rightarrow 3\,^1S$, $3\,^1P$ of O^{6+} in units of πa_0^2. The numbers in square brackets are powers of ten by which the quantities are to be multiplied.

Energy in threshold units	$3\,^1S$ Present	$3\,^1S$ Ref. 24	$3\,^1S$ Ref. 27	$3\,^1P$ Present	$3\,^1P$ Ref. 24	$3\,^1P$ Ref. 27
1	0.437[−4]	0.556[−4]	0.400[−4]	0.463[−4]	0.197[−3]	0.895[−4]
2	0.125[−4]	0.297[−4]	0.286[−4][a]	0.102[−3]	0.160[−3]	0.121[−3][a]
3	0.103[−4]	0.200[−4]		0.953[−4]	0.134[−3]	
4	0.888[−4]		0.171[−4]	0.806[−4]		0.102[−3]

[a]These results are at 1.9 threshold units.

the close-coupling results[23] now compare with all DW results in a better manner. Also the differences in the various three types of our calculations as well as in the results obtained from different theories go on decreasing with the increase of ionic charge (i.e., going from O^{6+} to heavier ions; see also Table I) and with the increase of the incident energy of the electron. This feature is not very surprising because with the increase of incident energy of the electron or target ionic charge or both, the other effects (such as distorting due to static polarization and exchange effects) do not make as significant a contribution to the collision process as does the Coulomb field of the target ion or the incident high energy of the electron.

Figure 4 presents the comparison of our three different results among themselves as well as with other calculations from different theories for $2\,^1P$ excitation in Li^+. The situation in this figure for $2\,^1P$ excitation as compared to Fig. 1 for $2\,^1S$ is much different. We find that our DW results using CI- and H-type wave functions are now in closer agreement (which may be merely a coincidence) while the results with HF-type wave functions[17] are much lower, showing that use of CI wave function for the $2\,^1P$ state increases the cross sections in most of the energies. Comparing our DW results, using the HF-wave function as used by Bhatia and Temkin[17] and McDowell *et al.*,[18] with their DW results suggests that polarization contribution is not very effective for $2\,^1P$ excitation in Li^+ but is rather sensitive to the choice of wave functions used for the calculation. Again the CC results[21] are larger than all others and also have (along with results of Itikawa and Sakimoto) different asymptotic behavior. CBA, as usual, gives large results at low energies and merges with DW results at higher energies. Good agreement of our results with that of Itikawa and Sakimoto[6] again suggest that for $2\,^1P$ excitation, the choice of wave function is more effective rather than improvement of the DW model. It is also seen that scaled-cross-section results of $2\,^1P$ excitation predicted by Sampson, Parks, and Clarks[27] overestimate the cross section by nearly a factor of 1.5 to 2, although the agreement with others gets improved for heavier ions as we will see in Fig. 5 (for example). In Fig. 5 for $2\,^1P$ excitation in O^{6+}, the situation is the same as in Fig. 4 and the trend is similar to that of going from Fig. 1 to Fig. 2 or 3 for $2\,^1S$ excitation. Here again the overall agreement of the various results get improved, except the CBA results, for which the reverse is true.

We have calculated for all the transitions in various ions, in addition to total-cross-section results, the differential cross sections (DCS) also. Our DCS results can be obtained from us on request. Although the DW methods are better known to be useful in reproducing experimental DCS results in electron-atom scattering, there are not many reports of its use in electron-ion scattering because of the unavailability of experimental data. However, as a test case, in Fig. 6 we have displayed our different DCS results along with others at three electron incident energies of $2\,^1S$ excitation in O^{6+} only, where a few other theoretical results are also available. From Fig. 6 it is seen that all the three DW methods show similar variations of cross sections with scattering angles in near forward and backward directions except that their magnitudes are different because of differences in the models. Also the same can be said for predictions of minima at intermediate scattering angles and their disappearance with an increase of incident electron energy. These features are very similar to e-He scattering for $2\,^1S$ excitation.[9]

Our intention of reporting the results for higher $n\,^1S$ and $n\,^1P$ ($n \geq 3$) excitations in Tables III and IV is mainly to make available more reliable results, as these results are especially useful in various applications. No other results except those of Tully[24] who obtained results using the single Coulomb Born approach and that of Sampson, Parks, and Clarks[27] are available. All these results[24,27] compare with ours (although not shown here) much as our DW results compared with theirs for $2\,^1S$ and $2\,^1P$ excitations. CBA results, though, at that time were of Bhatia and Temkin.[17] However, as an example, in Table V we have displayed and compared for $3\,^1S$ and $3\,^1P$ excitation in O^{6+}. There are also available results for $3\,^1P$ excitation in O^{6+} of Nakazaki[25] using the CBA method and using slightly different wave functions than those used by Tully,[24] but the results were found to be hardly different and are therefore not included in the table. It can be seen that the results due to Sampson, Parks, and Clarks lie in between our DW results and those CBA results of Tully.

ACKNOWLEDGMENTS

We are grateful to Professor Y. Itikawa for his fruitful discussions with us. The authors are also thankful to the Council for Scientific and Industrial Research, New Delhi, for financial assistance to this work.

*Present address: Department of Physics and Astronomy, University of Toledo, Toledo, OH 43606 (for Spring 1986).

[1]K. T. Dolder and B. Peart, Rep. Prog. Phys. **39**, 693 (1976).
[2]M. J. Seaton, Adv. Atom. Mol. Phy. **11**, 83 (1975).
[3]R. J. W. Henry, Phys. Rep. **68**, 1 (1981).
[4]Y. Itikawa, K. Takayanagi, and T. Iwai, Atom. Data Nucl. Data Tables **31**, 215 (1984).
[5]R. B. Christensen and D. W. Norcross, Phys. Rev. A **31**, 142 (1985).
[6]Y. Itikawa and K. Sakimoto, Phys. Rev. A **31**, 1319 (1985).
[7]N. R. Badnell, J. Phys. B **18**, 955 (1985).
[8]W. Eissner and M. J. Seaton, J. Phys. B **5**, 2187 (1972).
[9]R. Srivastava, M. Kumar, and A. N. Tripathi, J. Chem. Phys. **82**, 1818 (1985).
[10]R. Srivastava, A. K. Katiyar, and I. Khurana, J. Phys. B (to be published).
[11]R. Srivastava, M. Kumar, and A. N. Tripathi, J. Chem. Phys. **84**, 4715 (1986).
[12]R. Srivastava and A. K. Katiyar (unpublished).
[13]R. Srivastava and M. Kumar, Phys. Rev. A **31**, 3639 (1985).
[14]L. A. Parcell, R. P. McEachran, and A. D. Stauffer, J. Phys. B **16**, 4249 (1983).

[15]D. H. Madison and K. H. Winter, J. Phys. B **16**, 4437 (1983).
[16]J. M. Peek and J. B. Mann, Phys. Rev. A **25**, 749 (1982).
[17]A. K. Bhatia and A. Temkin, J. Phys. B **10**, 2893 (1977).
[18]M. R. C. McDowell, L. A. Morgan, V. P. Myerscough, and T. Scott, J. Phys. B **10**, 2727 (1977).
[19]C. S. Singh, R. Srivastava, and D. K. Rai, Can. J. Phys. **61**, 981 (1983).
[20]C. A. Coulson, *Valence* (Oxford University, London, 1961).
[21]P. M. Morse, L. A. Young, and E. S. Haurwitz, Phys. Rev. A **48**, 948 (1935).
[22]A. Hibbert, Comput. Phys. Commun. **9**, 141 (1975).
[23]W. L. van Wyngaarden, K. Bhardra, R. J. W. Henry, Phys. Rev. A **20**, 1409 (1979).
[24]J. A. Tully, J. Phys. B **7**, 386 (1974).
[25]S. Nakazaki, J. Phys. Soc. Jpn. **41**, 2084 (1976).
[26]S. Tayal and A. E. Kingston, J. Phys. B **17**, 1383 (1984).
[27]D. H. Sampson, A. D. Parks, and R. E. H. Clarks, Phys. Rev. A **17**, 1616 (1978).
[28]L. D. Thomas, G. Y. Csanak, H. S. Tylor, and B. S. Yarlagaddee, J. Phys. B **7**, 1719 (1974).
[29]D. H. Madison and W. N. Shelton, Phys. Rev. A **7**, 499 (1977).
[30]M. E. Stewart and D. H. Madison, Phys. Rev. A **23**, 647 (1981).
[31]A. K. Bhatia, A. Temkin, and A. Silver, Phys. Rev. A **12**, 2044 (1975), and references therein.
[32]R. P. McEachran and A.D. Stauffer, J. Phys. B **16**, 255 (1983).
[33]R. P. McEachran and A.D. Stauffer, J. Phys. B **16**, 4023 (1983).
[34]R. A. Marriot, Proc. Phys. Soc. London **72**, 121 (1958).
[35]A. Burgess, Proc. Phys. Soc. London **81**, 442 (1963).