PHYSICAL REVIEW A VOLUME 15, NUMBER 1 JANUARY 1977

Electron-impact excitation of carbon and silicon in the distorted-wave approximation

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(Received 30 August 1976)

The $^3P \rightarrow {}^1D$ electron-impact excitation cross section within the ground configuration of both neutral carbon and silicon is calculated in the distorted-wave approximation of the two-state Hartree-Fock coupled equations. An essential element of the present treatment is that we do not assume orthogonality to core orbitals in deriving equations for the scattering orbitals. A local adiabatic polarization potential is also added to the distorted-wave equations. Both elements are necessary in getting good agreement with close-coupling results for carbon to low impacting energies. The agreement is sufficiently good that our predictions for silicon should be accurate to within a factor of 2.

I. INTRODUCTION

In recent years interest in the theoretical aspects of electron-impact excitation of atoms and ions has been stimulated by advances in observational astronomy[1] and laboratory plasma research.[2] In particular, considerable effort has been made in studying the electron excitation between spectral terms of the ground configuration $2p^q$ and $3p^q$ (where $q = 2, 3, 4$) of various atoms and ions.[3] Optical deexcitation of these levels gives rise to the forbidden lines found in gaseous nebulae and quasistellar objects. Opacity calculations for stellar atmospheres[4] also rely heavily on accurate values for these electron-impact excitation cross sections.

At incident electron energies within a few volts of threshold, the generalized Hartree-Fock or close-coupling method[5] has been applied quite successfully to the calculation of electron-impact cross sections of atoms and ions. In intermediate-energy regions for atoms where many channels are open or in energy regions for highly charged positive ions where many closed-channel resonances[6] are present, a full solution to the Hartree-Fock coupled equations becomes impractical. We believe the distorted-wave method is a reasonable approach to which additional modifications may be systematically included.

In this paper we calculate the $^3P - {}^1D$ excitation cross section within the ground configuration of both carbon and silicon using the distorted-wave method in the manner developed by Mott and Massey[7] (see Sec. II). In deriving the Hartree-Fock coupled equations from the Kohn variational principle, we do *not* assume orthogonality of the same symmetry core and free orbitals. This gives rise to specific exchange overlap potentials in the distorted-wave equations as well as important overlap terms in the distorted-wave S matrix. At energies near threshold it becomes important to include an adiabatic polarization potential in the distorted-wave equations. Results from this adiabatic-exchange approximation for carbon and silicon are given in Sec. III. Section IV contains a brief summary.

II. DISTORTED-WAVE METHOD

Although the general aspects of the distorted-wave method are well known, the specific techniques are multifarious. In this paper we shall use the approach of Mott and Massey[7] which is a very natural approximation of the close-coupling expansion. In the two-state approximation, the total wave function Ψ for the electron-atom system equals the sum of the initial state ψ_1 and the final state ψ_2. Both the initial and final states may then be expanded in a representation $(nL_nS_nk_nl_nsLSM_lM_s)$, in which the orbital and spin angular momenta of the scattered electron (k_nl_ns) and the atom (nL_nS_n) are coupled together. One assumes that the total and component orbital and spin angular momentum quantum numbers L, S, M_l, M_s, as well as the parity Π, are conserved during the collision.

The initial state $\Phi_1(L_1S_1)$ and the final state $\Phi_2(L_2S_2)$ of the atom or ion may be calculated in the Hartree-Fock self-consistent-field approximation.[8] The single-particle spin orbitals are assumed to have the form

$$\langle \vec{r} | nlm_lm_s \rangle = [P_{nl}(r)/r] Y_{lm}(\theta, \phi) X_s(m_s), \qquad (1)$$

where $Y_{lm}(\theta, \phi)$ is a spherical harmonic and $X_s(m_s)$ is the electron spin function. By taking suitable linear combinations of spin-orbital determinants, the free electron may be coupled to the atomic states to form eigenfunctions ψ_1 and ψ_2 of the L^2, M_l, S^2, and M_s operators.[8]

The generalized Hartree-Fock coupled equations for Ψ are derived[9] from the Kohn variational principle, which is equivalent to

$$\langle \delta\Psi | H - E | \Psi \rangle = 0, \qquad (2)$$

where the variation is made on the free electron radial function in both the initial and final states. No orthogonality restrictions are made on core and free orbitals of the same symmetry. In Eq. (2), H is the nonrelativistic Hamiltonian for the electron-atom system while the total energy $E = E_1 + k_1^2/2 = E_2 + k_2^2/2$, where E_i is the energy of the atom and k_i is the momentum of the scattered electron. We will use atomic units throughout this paper (1 a.u. = 27.21 eV).

For a fixed set of conserved quantum numbers $\Gamma = LS\Pi$, the radial coupled equations derived from Eq. (2) have the general form

$$[T_{l_1} - 2V_{11}^{\Gamma}(r) + k_1^2]F_{1i'}^{\Gamma}(r) = 2V_{12}^{\Gamma}(r)F_{2i'}^{\Gamma}(r)\,, \tag{3}$$

$$[T_{l_2} - 2V_{22}^{\Gamma}(r) + k_2^2]F_{2i'}^{\Gamma}(r) = 2V_{21}^{\Gamma}(r)F_{1i'}^{\Gamma}(r)\,, \tag{4}$$

where

$$T_{l_i} = \frac{d^2}{dr^2} - \frac{l_i(l_i+1)}{r^2} + \frac{2Z}{r}\,. \tag{5}$$

The potentials $V_{ij}^{\Gamma}(r)$ in Eqs. (3) and (4) contain both direct and exchange integrals, while Z in Eq. (5) is the atomic number. The S^{Γ} matrix asymptotic form of the $F_{ii'}^{\Gamma}(r)$, where i' specifies the initial conditions, may be written as[10]

$$F_{ii'}^{\Gamma}(r) \xrightarrow[r\to\infty]{} (1/\sqrt{k_i})\{\delta_{ii'}e^{-ix_i} - S_{ii'}^{\Gamma}e^{ix_i}\}\,, \tag{6}$$

where

$$x_i = k_i r - \tfrac{1}{2}l_i\pi + (q/k_i)\ln(2k_i r) + \sigma_i\,, \tag{7}$$

q is the residual charge on the atom, and σ_i is the Coulomb phase shift. For neutral atoms, $q = 0$ and $\sigma_i = 0$. The distorted-wave equations for the system of Eqs. (3) and (4) may be written as

$$[T_{l_i} - 2V_{ii}^{\Gamma}(r) + k_i^2]f_{k_i l_i}^{\Gamma}(r) = 0, \tag{8}$$

where the free orbitals $f_{k_i l_i}^{\Gamma}(r)$ are given the normalization

$$f_{k_i l_i}^{\Gamma}(r) \xrightarrow[r\to\infty]{} \sin(x_i + \delta_i), \tag{9}$$

and δ_i is the non-Coulomb phase shift.

The distorted-wave S^{Γ} matrix using the normalization given in Eqs. (6) and (9), takes the form[7]

$$S^{\Gamma} \cong \begin{pmatrix} e^{2i\delta_1} & S_{12}^{\Gamma} \\ S_{21}^{\Gamma} & e^{2i\delta_2} \end{pmatrix}, \tag{10}$$

where

$$S_{21}^{\Gamma} = \frac{4}{i\sqrt{k_1 k_2}}\, e^{i(\delta_1+\delta_2)} \int_0^{\infty} f_{k_2 l_2}^{\Gamma}(r)V_{21}^{\Gamma}(r)f_{k_1 l_1}^{\Gamma}(r)\,dr. \tag{11}$$

The various differential as well as total excitation cross sections are then found[10] using the form of the S matrix in Eqs. (10) and (11). The total excitation cross section σ (in units of πa_0^2) for the transition $nL_1S_1 \to n'L_2S_2$ is given by

$$\sigma = \sum_{LSl_1l_2} \sigma(\Gamma, l_1 \to l_2), \tag{12}$$

where

$$\sigma(\Gamma, l_1 \to l_2) = \frac{(2L+1)(2S+1)}{2k_1^2(2L_1+1)(2S_1+1)}\,|S_{21}^{\Gamma}|^2. \tag{13}$$

III. CALCULATIONS AND RESULTS

A. Carbon

In this subsection we apply the distorted-wave method of Sec. II to the calculation of the $^3P \to {}^1D$ electron excitation cross section of neutral carbon. The ground configuration $1s^22s^22p^2$ of carbon couples to give three spectral terms: the ^3P ground state, the ^1D excited state with a threshold for excitation of 1.264 eV, and the ^1S state with a threshold of 2.683 eV.[11] The single-particle core orbitals for the initial ground atomic state $\Phi_1(^3P)$ were calculated numerically in the Hartree-Fock approximation using only the single configuration $1s^22s^22p^2$.[12] The largest partial-wave contribution to the $^3P \to {}^1D$ excitation cross section for neutral carbon was found to be $\sigma(^2D^0, p \to p)$ of Eq. (12). Equation (8) for the initial $\mathrm{C}(^3P\ k_1p\ ^2D^0)$ scattering orbital is given by

$$\{T_p - 2[V_{\mathrm{core}}^{l=1} + 2J_{2p}^0 - \tfrac{1}{25}J_{2p}^2 + \tfrac{1}{2}K_{2p}^0 + \tfrac{2}{25}K_{2p}^2 + \tfrac{1}{2}(\epsilon_{2p} - \tfrac{1}{2}k_1^2)I_{2p}] + k_1^2\}\, f_{k_1p}(r) = 0, \tag{14}$$

where

$$V_{\mathrm{core}}^{l=1} = 2J_{1s}^0 - \tfrac{1}{3}K_{1s}^1 + 2J_{2s}^0 - \tfrac{1}{3}K_{2s}^1\,, \tag{15}$$

$$J_{nl'}^{\kappa} f_{kl}(r) = \int_0^{\infty} dr_1\, P_{nl'}^2(r_1)\frac{r_<^{\kappa}}{r_>^{\kappa+1}} f_{kl}(r), \tag{16}$$

and the integral terms, symbolized by K and I above, are explicitly

$$K_{nl'}^{\kappa} f_{kl}(r) = \int_0^{\infty} dr_1\, P_{nl'}(r_1)f_{kl}(r_1)\,\frac{r_<^{\kappa}}{r_>^{\kappa+1}}\, P_{nl'}(r), \tag{17}$$

$$I_{nl} f_{kl}(r) = \int_0^{\infty} dr_1\, P_{nl}(r_1)f_{kl}(r_1)P_{nl}(r), \tag{18}$$

and $r_< = \min(r_1, r)$ and $r_> = \max(r_1, r)$. The radial exchange overlap integral I_{2p} of Eq. (14) is a consequence of the nonorthogonality of the $2p$ core state and the k_1p scattering orbital. The Hartree-Fock equation for the $2p$ core state is used in attaining the form expressed in Eq. (14). For the single-particle core eigenenergy ϵ_{2p}, however, we used the experimental removal energy in order to have the threshold agree with experiment.

The $\overline{2p}$ core orbital for the final atomic state $\Phi_2({}^1D)$ was calculated in the Hartree-Fock approximation by using the $1s$ and $2s$ orbitals of $\Phi_1({}^3P)$ as a fixed core. Equation (8) for the final $\mathrm{C}({}^1D\ k_2p\,{}^2D^o)$ scattering orbital is then given by

$$\{T_p - 2[V_{\text{core}}^{l=1} + 2J_{\overline{2p}}^0 - \tfrac{7}{25}J_{\overline{2p}}^2 + \tfrac{1}{2}K_{\overline{2p}}^0 - \tfrac{4}{25}K_{\overline{2p}}^2 + \tfrac{1}{2}(\epsilon_{\overline{2p}} - \tfrac{1}{2}k_2^2)I_{\overline{2p}}] + k_2^2\} f_{k_2p}(r) = 0. \tag{19}$$

Using Eqs. (11) and (13), the $\sigma({}^2D^o, p\rightarrow p)$ partial-wave contribution to the ${}^3P\rightarrow{}^1D$ excitation cross section for carbon is written

$$\begin{aligned}\sigma({}^2D^o, p\rightarrow p) = (80/9k_1^3k_2)[&-\tfrac{3}{2}\langle k_2p\,\overline{2p}|\,v^0\,|2pk_1p\rangle\langle\overline{2p}|\,2p\rangle + \tfrac{3}{25}\langle k_2p\,\overline{2p}|\,v^2|2pk_1p\rangle\langle\overline{2p}|2p\rangle\\ &-\tfrac{3}{2}(\epsilon_{\overline{2p}} - \tfrac{1}{2}k_1^2)\langle\overline{2p}\,|\,k_1p\rangle\langle k_2p|\,2p\rangle\langle\overline{2p}|2p\rangle + \Delta(2p,\overline{2p})]^2,\end{aligned} \tag{20}$$

where

$$\langle k_2lnl|\,v^\kappa|\,mlk_1l\rangle = \int_0^\infty\int_0^\infty f_{k_2l}(r_1)P_{nl}(r_1)\frac{r_<^\kappa}{r_>^{\kappa+1}}P_{ml}(r_2)f_{k_1l}(r_2)\,dr_1\,dr_2, \tag{21}$$

$$\langle nl\,|\,k_1l\,\rangle = \int_0^\infty P_{nl}(r_1)f_{k_1l}(r_1)\,dr_1, \tag{22}$$

and $\Delta(2p,\overline{2p})$ is discussed below. The various Coulomb matrix elements found in Eq. (20) follow from the form of the coupling potential $V_{21}^{2D^o}$ derived using Eq. (2). One should note that the matrix elements are exchange integrals due to the spin forbidden nature of the ${}^3P\rightarrow{}^1D$ transition. Convergence of the partial-wave expansion should thus be rapid. At incident energies from 0 → 20 eV the first and third matrix elements are the largest terms. The third term arises from the nonorthogonality of the scattering orbitals with the core orbitals. Since at low energies the first and third terms are of opposite sign, neglecting the orthogonality term would lead to a quite large $\sigma({}^2D^o, p\rightarrow p)$ partial cross section near threshold. In fact, at an incident energy of 3 eV, the partial cross section goes to zero due to the cancellation. With the addition of an adiabatic polarization potential, which will be discussed below, this minimum in the $\sigma({}^2D^o, p\rightarrow p)$ cross section disappears.

The $\Delta(2p,\overline{2p})$ in Eq. (20) is symbolic of a series of terms which only fail to vanish because $2p$ and $\overline{2p}$ are not identical. If the $1s$ and $2s$ orbitals were allowed to vary in the exit channel, there would be additional Δ terms. Since $\langle\overline{2p}|2p\rangle = 0.9995$ for carbon, we expect $\Delta(2p,\overline{2p})$ to be quite small for all energies and thus have neglected its contribution in subsequent cross-section results. In fact at an incident energy of 5 eV the contribution of the $\Delta(2p,\overline{2p})$ terms is 0.6% relative to the first matrix element in Eq. (20).

Hartree-Fock phase shifts obtained from Eq. (14) are given for ten values of the incident energy in column three of Table I. The $\sigma({}^2D^o, p\rightarrow p)$ partial cross-section results in the Hartree-Fock distorted-wave approximation are listed in column four of Table II.

At low incident energies it is known that induced

TABLE I. Phase shifts (in radians) for carbon ${}^3P$ ground-state scattering orbitals.

Partial wave	$\delta(kp\,{}^2D^o)$			$\delta(kp\,{}^2P^o)$		$\delta(ks\,{}^2P^e)$		$\delta(kd\,{}^2F^e)$	
E(eV)	H[a]	HF[b]	AE[c]	HF	AE	HF	AE	HF	AE
2.0	0.204	1.584	2.193	0.645	1.482	5.369	5.537	0.012	0.068
3.5	0.468	1.775	2.107	1.187	1.686	5.111	5.278	0.016	0.106
5.0	0.766	1.781	2.034	1.365	1.700	4.922	5.087	0.020	0.138
7.5	1.150	1.745	1.948	1.438	1.673	4.687	4.847	0.032	0.187
10.0	1.357	1.711	1.892	1.449	1.645	4.510	4.665	0.050	0.231
15.0	1.520	1.666	1.826	1.446	1.610	4.252	4.397	0.101	0.309
20.0	1.568	1.642	1.789	1.445	1.594	4.066	4.202	0.161	0.376
30.0	1.579	1.616	1.745	1.451	1.581	3.804	3.925	0.281	0.480
40.0	1.562	1.596	1.713	1.454	1.571	3.619	3.729	0.382	0.554
50.0	1.539	1.578	1.685	1.452	1.559	3.476	3.577	0.459	0.608

[a] Hartree approximation.
[b] Hartree-Fock.
[c] Adiabatic-exchange.

TABLE II. Partial cross sections (in πa_0^2) for ${}^3P \rightarrow {}^1D$ electron excitation of neutral carbon.

Partial wave	$\sigma({}^2D^o, p \rightarrow p)$				$\sigma({}^2P^o, p \rightarrow p)$		$\sigma({}^2F^e, d \rightarrow d)$		$\sigma({}^2P^e, s \rightarrow d)$	
E(eV)	B[a]	HO[b]	HF[c]	AE[d]	HF	AE	HF	AE	HF	AE
2.0	1.341	1.912	7.298	0.754	2.399	1.274	0.000	0.001	0.000	0.000
3.5	4.996	2.609	0.035	1.215	1.657	1.048	0.006	0.011	0.002	0.003
5.0	7.316	0.333	0.428	1.192	0.067	0.834	0.020	0.037	0.003	0.005
7.5	8.393	0.000	0.635	0.953	0.329	0.575	0.053	0.091	0.004	0.005
10.0	7.765	0.020	0.586	0.712	0.317	0.406	0.083	0.131	0.004	0.004
15.0	5.493	0.102	0.367	0.383	0.203	0.215	0.114	0.152	0.002	0.002
20.0	3.654	0.104	0.215	0.210	0.122	0.121	0.113	0.129	0.001	0.001
30.0	1.651	0.055	0.078	0.072	0.047	0.044	0.075	0.073	0.000	0.000
40.0	0.807	0.026	0.032	0.029	0.021	0.019	0.043	0.039	0.000	0.000
50.0	0.425	0.013	0.015	0.014	0.010	0.009	0.025	0.022	0.000	0.000

[a] Born approximation.
[b] Hartree-orthogonalized.
[c] Hartree-Fock.
[d] Adiabatic-exchange.

polarization effects are important in electron scattering from neutral atomic systems.[13] Within the diagrammatic perturbation theory for atoms as developed by Kelly[14] we have calculated a local adiabatic polarization potential $V_{\text{pol}}(r)$ for the ground ${}^3P$ state of carbon. Only the dipole $2s \rightarrow 2p$ and $2p \rightarrow n, kd$ excitations were used to evaluate the lowest-order expression, given by

$$V_{\text{pol}}(r) = \frac{4}{9}\left(\frac{\left[\int_0^r P_{2p}(r')(r'/r^2)P_{2s}(r')\,dr'\right]^2}{\epsilon_{2s} - \epsilon_{2p}} + \sum\!\!\!\!\!\!\int_{n,k} \frac{\left[\int_0^r P_{n,kd}(r')(r'/r^2)P_{2p}(r')\,dr'\right]^2}{\epsilon_{2p} - \epsilon_{n,kd}} \right), \tag{23}$$

where $\sum\!\!\!\!\!\!\int_{n,k}$ represents a sum over bound states and integration over continuum states, while the factor $\frac{4}{9}$ comes from averaging the angular integrations. The bound and continuum n, kd states were calculated numerically as fixed-core Hartree-Fock $1s^2 2s^2 2p\, kd\, {}^3D$ functions. For $\epsilon_{2s} - \epsilon_{2p}$ we used -0.3300 a.u. which is an average over the experimental values[11] for the various final-state couplings. One should note that $V_{\text{pol}}(r)$ of Eq. (23) neglects contributions obtained when the perturbing charge distance is less than the core electron radius. This is in the same spirit as the Callaway-Temkin potential as opposed to the Bethe-Reeh potential.[15] Monopole terms in $V_{\text{pol}}(r)$ were omitted since they tend to be cancelled by short-range nonadiabatic effects.[15] Since as $r \rightarrow \infty$, $V_{\text{pol}}(r) \rightarrow -\alpha_d/2r^4$, the dipole polarizability α_d can be extracted. Equation (23) yields $\alpha_d = 12.7a_0^3$ for carbon. This lowest-order result compares favorably, for our purposes, with the more sophisticated many-body $(10.4a_0^3)$[16] and polarized pseudostate close-coupling $(11.03\,a_0^3)$[17] results. The polarization potential of Eq. (23) was used to calculate new carbon scattering orbitals in both the initial and final states. The adiabatic-exchange phase shifts for the $\mathrm{C}({}^3P\; kp\, {}^2D^o)$ state, calculated by adding $V_{\text{pol}}(r)$ to the potentials in Eq. (14), are compared in Table I with the Hartree-Fock values (see columns three and four). The $\sigma({}^2D^o, p \rightarrow p)$ partial cross section in the adiabatic-exchange approximation is given in column five of Table II at ten incident energies.

Other formulations of the distorted-wave method of electron excitation of atoms have also been made.[18-21] One possible method is to ignore exchange terms completely in the distorted-wave equations [Eq. (8)] and then orthogonalize free and core orbitals of the same symmetry by either the addition of Lagrange multipliers or a simple Schmidt orthogonalization. In column two of Table I we present the Hartree phase shifts for $\mathrm{C}({}^3P\; kp\, {}^2D^o)$ orbitals, obtained from Eq. (14) by ignoring all exchange terms. The difference between the Hartree and Hartree-Fock phase shifts is an indication of the importance of potential terms representing the capture of the colliding electron into the unfilled $2p$ shell of carbon. After Schmidt-orthogonalizing the incoming and outgoing Hartree kp orbitals to the $2p$ and $\overline{2p}$ orbitals, respectively, the cross section using Eq. (20) is computed and given in column three of Table II. The Hartree orthogonalized $\sigma({}^2D^o, p \rightarrow p)$ partial cross section is found to differ in both magnitude and energy variation from the Hartree-Fock and adiabatic-exchange results. This result emphasizes the need of including bound channel correlation terms[5,21] in the calculation when using any type of same symmetry orthogonalized distorted waves. Also presented in column two of Table II are Born cross section results for $\sigma({}^2D^o, p \rightarrow p)$.

Radial equations similar to Eqs. (14) and (19) were also obtained for the distorted waves needed to calculate the $\sigma(^2P^o, p\rightarrow p)$, $\sigma(^2F^e, d\rightarrow d)$ and $\sigma(^2P^e, s\rightarrow d)$ partial cross sections for the $^3P\rightarrow{}^1D$ excitation in carbon. Phase shifts for various ground-state scattering orbitals are given in Table I while partial cross-section results in both the Hartree-Fock and adiabatic-exchange distorted-wave approximation are given in Table II. As found in previous close-coupling work[22] the $\sigma(^2D^o, p\rightarrow p)$ and $\sigma(^2P^o, p\rightarrow p)$ partial cross sections make the largest contributions at low energies. As noted before, the partial-wave convergence is extremely rapid for the $^3P\rightarrow{}^1D$ transition in carbon. $\sigma(^2F^e, d\rightarrow d)$ is the largest of the $d\rightarrow d$ type. The quite small $\sigma(^2P^e, s\rightarrow d)$ contribution is typical of the $\Delta l=2$ transitions for carbon, such as $p\rightarrow f$, $d\rightarrow s$, and $d\rightarrow g$.

The total Hartree-Fock and adiabatic-exchange distorted-wave cross sections for the $^3P\rightarrow{}^1D$ ground configuration transition in carbon are shown in Fig. 1. The Hartree-Fock cross section has not been extended below 5 eV incident energy. From Table II one can easily see that the Hartree-Fock cross section would go to a minimum at low energy and then rise at lower energy. This is completely out of keeping with more elaborate calculations. Specifically, a single-ground-configuration close-coupling calculation[22] is shown in Fig. 1. The height of the shape resonance is about the same for the close-coupling and adiabatic-exchange distorted-wave cross sections, although the latter is about 1.7 times the former at 8 eV. A recent matrix variational calculation[23] is also shown in Fig. 1. The matrix variational results augment the ground configuration with configurations $1s^22s2p^3$ and $1s^22p^4$ as well as certain virtual excitations of the $2p$ orbital. The height of the shape resonance is reduced by a factor of 2 in the matrix variational cross section. The differences at low energies in the four curves shown in Fig. 1 indicate that slight changes in the exchange and polarization potentials have a quite large effect on the $^3P\rightarrow{}^1D$ excitation cross section in carbon.

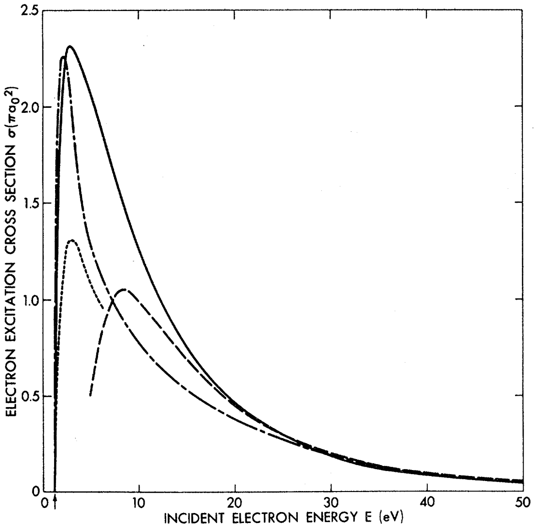

FIG. 1. Total cross section for the $^3P\rightarrow{}^1D$ electron excitation of neutral carbon: ——, adiabatic-exchange distorted-wave method; ----, Hartree-Fock distorted-wave method; ——•——, single-configuration close-coupling method (Ref. 22); • • • • •, matrix variational method (Ref. 23). The arrow indicates the threshold for excitation.

Also shown for carbon in Fig. 2 are differential cross-section results at 5, 10, and 20 eV in the adiabatic-exchange approximation and a matrix variational result at 6.67 eV.

B. Silicon

In this subsection we present results for the $^3P\rightarrow{}^1D$ electron excitation cross section of neutral silicon. The distorted-wave method applied to carbon in Sec. IIIA can be immediately extended to silicon since both atoms possess two $l=1$ electrons in their outer shell. The ^1D excited state of the ground configuration $1s^22s^22p^63s^23p^2$ of silicon has a threshold at 0.7807 eV. The entrance- and exit-channel core orbitals were calculated in the Hartree-Fock approximation using the single ground configuration of silicon.[12] Again the $1s$, $2s$, $2p$, and $3s$ orbitals were fixed for calculation of the $\overline{3p}$ orbital in the exit channel. Explicit equations for the silicon distorted waves, as well as the partial cross sections, are similar to carbon due to the angular symmetry. For ex-

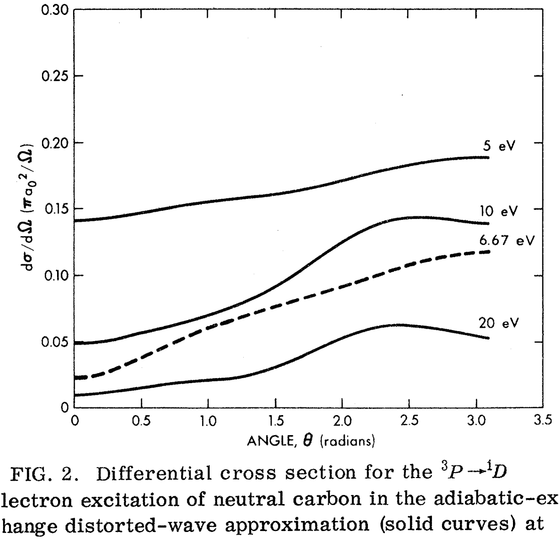

FIG. 2. Differential cross section for the $^3P\rightarrow{}^1D$ electron excitation of neutral carbon in the adiabatic-exchange distorted-wave approximation (solid curves) at three different incident energies. A matrix variational result (Ref. 23) is also shown (dashed curve) at 6.67 eV.

TABLE III. Phase shifts (in radians) for silicon ^3P ground-state scattering orbitals.

Partial wave / E(eV)	$\delta(kp\,^2D^o)$		$\delta(kp\,^2P^o)$		$\delta(ks\,^2P^e)$		$\delta(kd\,^2F^e)$	
	HF[a]	AE[b]	HF	AE	HF	AE	HF	AE
2.0	5.074	5.424	4.502	5.040	8.250	8.569	0.024	0.231
3.5	4.888	5.183	4.512	4.859	7.934	8.228	0.035	0.343
5.0	4.756	5.027	4.441	4.734	7.707	7.982	0.064	0.440
7.5	4.602	4.851	4.334	4.589	7.429	7.680	0.157	0.594
10.0	4.494	4.726	4.252	4.487	7.221	7.453	0.297	0.741
15.0	4.339	4.544	4.132	4.340	6.915	7.119	0.628	0.990
20.0	4.222	4.407	4.041	4.228	6.692	6.875	0.899	1.165
30.0	4.042	4.199	3.895	4.053	6.368	6.523	1.195	1.369
40.0	3.901	4.039	3.775	3.914	6.132	6.268	1.330	1.473
50.0	3.784	3.908	3.672	3.798	5.944	6.067	1.404	1.533

[a] Hartree-Fock approximation.
[b] Adiabatic-exchange.

ample, the initial Si($^3P\ k_1p\,^2D^o$) scattering orbital is obtained by replacing $2p$ with $3p$ in Eq. (4) and substituting for $V_{\text{core}}^{l=1}$ as follows:

$$V_{\text{core}}^{l=1}=2J_{1s}^{0}-\tfrac{1}{3}K_{1s}^{1}+2J_{2s}^{0}-\tfrac{1}{3}K_{2s}^{1}+6J_{2p}^{0}-K_{2p}^{0}-\tfrac{2}{5}K_{2p}^{2}+2J_{3s}^{0}-\tfrac{1}{3}K_{3s}^{1}\,. \qquad (24)$$

It should be noted that it is a good approximation to allow same symmetry free and core orbitals to be orthogonal when the core orbitals occupy a closed shell.[22] Thus there are no exchange overlap terms arising from the $2p$ shell in Eq. (24).

At energies near threshold an adiabatic polarization potential was added to the distorted-wave equations for silicon. The construction of the polarization potential was similar to Eq. (23) with the $3s\rightarrow 3p$ and $3p\rightarrow nd$, kd excitations replacing the carbon outer-shell transitions. For $\epsilon_{3s}-\epsilon_{3p}$ we used -0.2517 a.u. which is again an average over experimental values.[11] The dipole polarizability was found to be $48.8a_0^3$, which is in acceptable agreement with an uncoupled Hartree-Fock $(46.0a_0^3)$[24] result and a finite perturbation calculation $(36.3a_0^3)$.[25]

Because of the lower threshold energy, the partial-wave convergence in scattering from silicon is slightly slower than carbon and thus the d waves are found to be more prominent.[21] Phase shifts for various ground-state scattering orbitals of silicon are given in Table III. Results for six different partial-wave cross sections in both the Hartree-Fock and adiabatic-exchange distorted-wave approximation are given in Table IV. Cancellation effects due to orthogonality terms are again found to be very important in the $p\rightarrow p$ transitions. The total cross sections in the Hartree-Fock and adiabatic-exchange approximation are shown in Fig. 3. The Hartree-Fock cross section has not been extended below 3.5 eV. The

TABLE IV. Partial cross sections (in πa_0^2) for $^3P\rightarrow{}^1D$ electron excitation of neutral silicon.

Partial wave / E(eV)	$\sigma(^2D^o, p\rightarrow p)$		$\sigma(^2P^o, p\rightarrow p)$		$\sigma(^2F^e, d\rightarrow d)$		$\sigma(^2P^e, d\rightarrow d)$		$\sigma(^2P^e, s\rightarrow d)$		$\sigma(^2D^e, d\rightarrow s)$	
	HF[a]	AE[b]	HF	AE	HF	AE	HF	AE	HF	AE	HF	AE
2.0	0.381	2.262	1.427	1.433	0.053	0.211	0.008	0.036	0.025	0.052	0.067	0.130
3.5	0.907	1.720	0.308	1.015	0.343	1.193	0.065	0.237	0.068	0.121	0.088	0.133
5.0	0.847	1.160	0.433	0.682	0.767	1.965	0.158	0.398	0.085	0.122	0.084	0.108
7.5	0.549	0.594	0.319	0.363	1.314	1.955	0.264	0.353	0.071	0.064	0.064	0.064
10.0	0.328	0.319	0.204	0.206	1.357	1.347	0.241	0.214	0.040	0.024	0.042	0.034
15.0	0.122	0.109	0.084	0.077	0.662	0.469	0.097	0.069	0.006	0.002	0.012	0.006
20.0	0.051	0.045	0.038	0.034	0.214	0.154	0.032	0.024	0.000	0.000	0.001	0.000
30.0	0.013	0.011	0.010	0.009	0.024	0.021	0.005	0.004	0.001	0.001	0.000	0.000
40.0	0.004	0.004	0.004	0.003	0.005	0.004	0.001	0.001	0.001	0.001	0.000	0.000
50.0	0.002	0.002	0.002	0.002	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000

[a] Hartree-Fock approximation.
[b] Adiabatic-exchange.

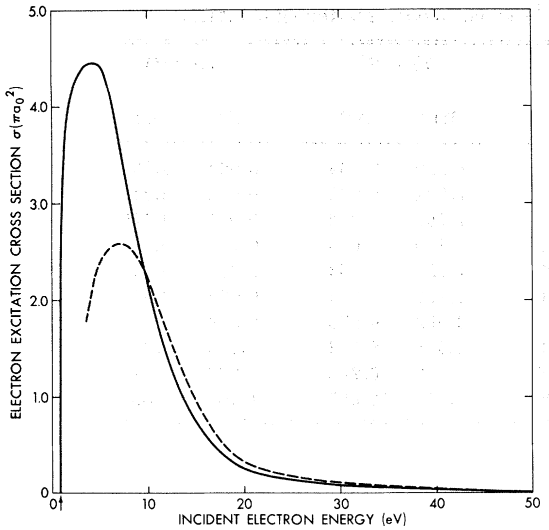

FIG. 3. $^3P\rightarrow{}^1D$ electron excitation cross section for the neutral silicon atom: ——, adiabatic-exchange distorted-wave method; ----, Hartree-Fock distorted-wave method. The arrow indicates the threshold for excitation.

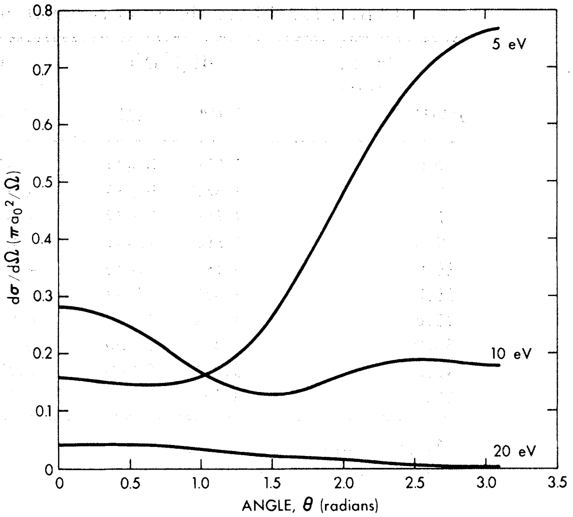

FIG. 4. Differential cross section for the $^3P\rightarrow{}^1D$ electron excitation of neutral silicon in the adiabatic-exchange distorted-wave approximation at three different incident energies.

energy variation of the cross sections is similar to the carbon results, although the peak height has increased. The magnitude of the $^3P\rightarrow{}^1D$ total cross section for silicon at low energies agrees fairly well with a rough isoelectronic extrapolation made of the same cross section for various 14-electron ions.[26] From our previous calculation on carbon in Sec. III A, we feel that our prediction for the $^3P\rightarrow{}^1D$ total cross section of silicon should be accurate to within a factor of 2 at low energies. Also shown for silicon in Fig. 4 are differential cross-section results at 5, 10, and 20 eV in the adiabatic-exchange approximation.

IV. SUMMARY

It has been shown above that the distorted-wave method can be used quite effectively in calculating electron excitation cross sections of complex neutral atoms to quite low incident energies. Exchange and polarization effects were found to be extremely important for the $^3P\rightarrow{}^1D$ excitation in carbon and silicon. Non-orthogonality effects between scattering and core orbitals of the same symmetry were shown to play a critical role.

Fairly good agreement was obtained between the adiabatic-exchange distorted-wave results for carbon and the very sophisticated close-coupling and correlation methods. It is hoped that with more accurate target functions and a more incisive distorted-wave function that the agreement would improve even further.

The numerical simplicity and relatively small computing cost of the distorted-wave method makes it quite attractive for the compiling of atomic data needed for astrophysical and laboratory plasma research. In the future we hope to apply the distorted-wave method to the calculation of electron excitation cross sections for positive ions. Closed-channel resonance effects should increase in importance relative to exchange and polarization as the charge on the target ion is increased.

ACKNOWLEDGMENTS

One of us (M. S. P.) would like to thank the National Research Council for its financial support and Dr. R. J. Drachman and Dr. K. Omidvar for helpful discussions. We would also like to thank Dr. M. A. J. Snijders for pointing out the astrophysical need for reliable silicon cross sections.

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