Low-energy electron scattering by atomic oxygen†

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A matrix variational calculation has been done for electron scattering by atomic O, which includes $2s^2 2p^4$, $2s2p^5$, and $2p^6$ target configurations and all possible single excitations of the $2p$ orbital. Integral and differential cross sections are reported for elastic and inelastic scattering for energies up to the first $n = 3$ excitation threshold. The full effects of long-range polarization and short-range correlation appear to be nearly completely accounted for. No low-lying resonances are observed.

I. INTRODUCTION

Matrix variational calculations for electron scattering by C, N, and O atoms have recently been reported[1] which augmented the ground configuration $2s^2 2p^m$ with configurations $2s2p^{m+1}$ and $2p^{m+2}$. That work is extended here for O to include all possible single excitations of the $2p$ orbital by a reasonably complete basis of s, p, d, and f orbitals. This appears to give a nearly complete account of the effects of short-range correlation and long-range polarization.

Integral cross sections for scattering from the ground configuration terms are reported for energies up to the first $n=3$ excitation threshold. Differential cross sections are also given for elastic and inelastic scattering. The ratio of forward to backward elastic scattering agrees well with the recent experiments of Dehmel *et al.*[2]

Narrow resonances just below the $n=3$ threshold are not represented in the present results.

II. BASIS SET

The one-electron basis functions were the same as those used in a previous calculation.[1] Slater-type orbitals were used with the number of s, p, d, and f orbitals being 8, 6, 4, and 1, respectively. The exponents were chosen in such a way as to give approximately stationary and converged results for the ^4P partial wave at $k=0.173$. This and the ^2P partial wave make the main contribution to the cross section at low energy.

The target-atom states were calculated using the Hartree-Fock ground configurations $2s^2 2p^4$ plus the near-degenerate $2s2p^5$ and $2p^6$ configurations. In the configuration-interaction (CI) calculation[1] the target-plus-electron system is represented by appending all unoccupied orbitals of the proper symmetry constructed from the orbital basis to these target configurations. In the present work the wave function of the CI representation is augmented by including all configurations arising from virtual excitation of the $2p$ orbital.

A systematic study showed the $2p$ virtual excitations to give the principal single-excitation effect on s-wave cross sections. Inclusion of $2s$ excitations beyond those in the CI target configurations gave negligible effects. Therefore, the effects of pair correlations of the scattered electron with those of the valence-shell target electrons have essentially been accounted for.

III. RESULTS

The results for total scattering from the ground state are shown in Table I and Fig. 1. The differential cross sections for elastic and inelastic scattering with excitation to the low-lying ground configuration terms ^1D and ^1S are shown in Figs. 2–4.

Experimental measurements of low-energy e-O scattering are difficult because of the need for molecular dissociation. No experiment of reason-

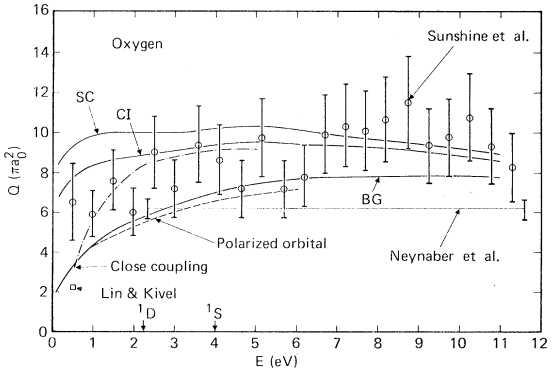

FIG. 1. Integral cross sections for total scattering from the ground (^3P) state of O.

TABLE I. Oxygen integral cross sections in units of πa_0^2 for total scattering from the ground ^3P state. Columns 5 and 6 give the non-s-wave contributions to the cross sections.

		Q (tot)		Q (tot) $-Q(^2P+^4P)$	
(1)	(2)	(3)	(4)	(5)	(6)
k	SC	CI	BG	SC	BG
0.10	8.43	6.84	2.07	0.43	0.52
0.20	9.46	7.87	3.45	1.24	0.54
0.30	9.95	8.53	4.74	2.26	0.94
0.40	10.03	8.92	5.75	2.48	1.40
0.50	10.03	9.19	6.59	3.18	1.87
0.60	10.27	9.59	7.39	4.00	2.68
0.70	9.90	9.40	•••		
0.75	•••	•••	7.80		
0.80	9.47	9.11	•••		
0.90	8.90	8.67	7.78		
1.00	8.25	8.11	•••		

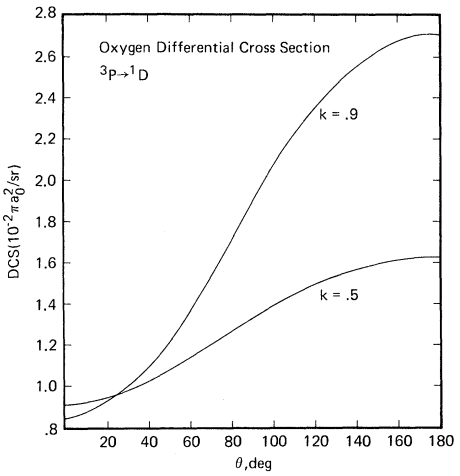

FIG. 3. Differential cross sections for the excitation $^3P \rightarrow {}^1D$ of O.

ably high precision has been performed, but data obtained by Neynaber *et al.*[3] and by Sunshine *et al.*[4] give the general trend of the total ground-state cross section. The present results (labeled BG in Fig. 1) follow the general trend of the lower limit of the ±20% error bars of the data of Sunshine *et al.*[4] and are in reasonable agreement with the shock-tube result of Lin and Kivel[5] and the least-squares value used by Neynaber *et al.*[3] to represent their data.

Dehmel *et al.*[2] have recently measured the ratio of the forward to backward scattering by separately collecting the scattered flux of electrons in the cones defined by the angles 20°–88° and 92°–160°. This ratio has been computed by integrating the elastic differential cross-section curves shown in Fig. 2 through the angles 20°–90° and 90°–160°.

Figure 5 shows excellent agreement with the experiment. The ratio approaches a small energy limit that differs from unity owing to the long-range electric-quadrupole potential of the ^3P target ground state. For short-range potentials the K-matrix elements $K^{LS}_{\gamma l,\gamma' l'}$ become proportional to $k^{l+l'+1}$.[6] The contributions to the cross section due to a short-range potential would approach a nonzero limit only for s waves and the scattering would be isotropic in the low-energy limit. However, the presence of a long-range quadrupole potential makes the K-matrix elements proportional to k in this limit as long as $1 < (l+l'+1)$.[6] Therefore, all partial waves can give nonzero contributions to the cross section and it will not

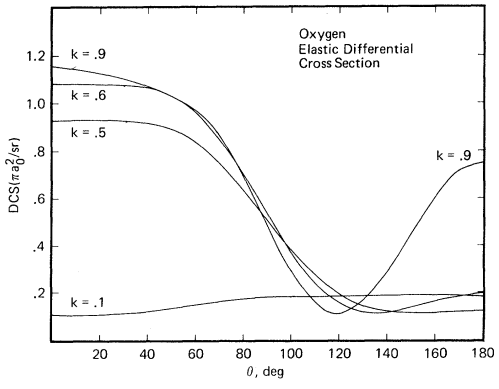

FIG. 2. Differential cross sections for elastic scattering from the ground (^3P) state of O.

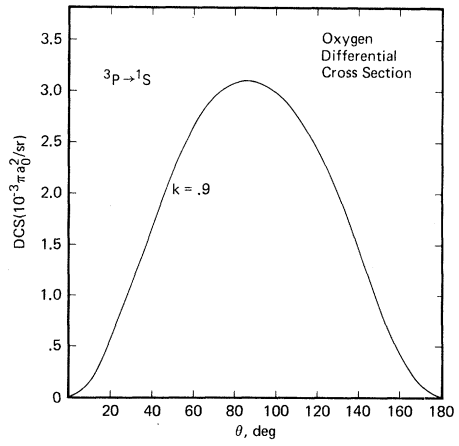

FIG. 4. Differential cross section for the excitation $^3P \rightarrow {}^1S$ of O.

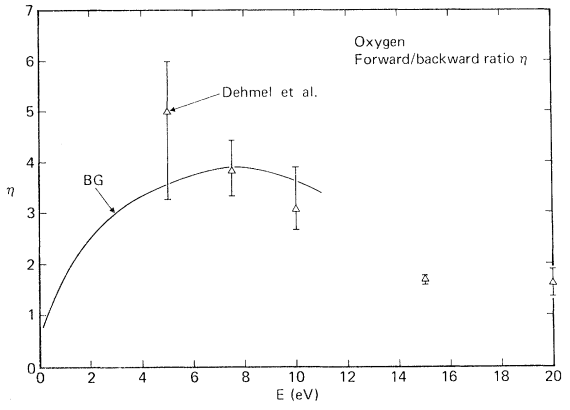

FIG. 5. Ratios of forward to backward elastic scattering from the ground (^3P) state of O.

in general be isotropic.

Of particular interest in the inelastic differential cross sections is the prominent backscattering for the ^3P-^1D transition (Fig. 3) and the selection rule forbidding forward and backward scattering for the ^3P-^1S transition (Fig. 4). This selection rule can be deduced from the symmetry properties of axial scattering.[7] More specifically, the transition from the $M=0$ magnetic sublevel is forbidden at all angles when the P and S states have the same parity.[8]

Threshold laws[6] predict that cusps are possible only at the ^1D threshold for elastic scattering from the ^3P state and at the ^1S threshold for elastic scattering from the ^1D state. No cusp behavior was found at either of these thresholds on a scale of $\Delta k = 0.002$. Therefore no cusps would be experimentally observed at these thresholds.

Also shown in Fig. 1 are the polarized-orbital results of Henry[9] and the close-coupling calculation of Rountree *et al.*[10] Comparison with the polarized-orbital result indicates that this BG calculation includes a good representation of the target-atom polarizability. Vo Ky Lan *et al.*[11] have augmented the single-configuration close-coupling equations with a multichannel dipole polarization potential. Figure 6 compares their results with the present calculation for elastic scattering from the ground ^3P state. The calculations agree reasonably well above 6 eV; however, the BG result falls off much faster at lower energies. This indicates that while there are no low-lying resonances in oxygen as there are in C and N,[1] short-range correlations are nevertheless an important effect. Table II gives the integral cross sections for inelastic scattering and Fig. 7 compares them with those of Vo Ky Lan *et al.*[11] Their energy scales were translated by +0.25 eV and −0.19 eV for the ^1D and ^1S excitations, respectively, so that the thresholds coincided with the BG results.

TABLE II. Elastic and inelastic integral cross sections in units of πa_0^2.

k	$^3P - {}^3P$	$^3P - {}^1D$	$^3P - {}^1S$	$^1D - {}^1S$
0.50	6.425	0.164	...	...
0.60	7.107	0.270	0.013	0.085
0.75	7.500	0.279	0.021	0.075
0.90	7.520	0.233	0.028	0.060

The close-coupling calculations of Rountree *et al.*[10] have shown the importance of including excitations of the $2p$ orbitals in computing the s-wave partial cross sections. Columns 5 and 6 of Table I show that $2p$ excitations are also important

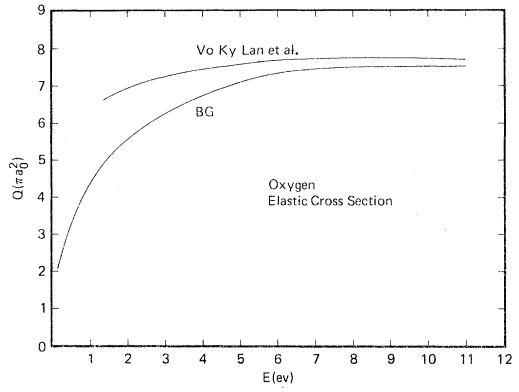

FIG. 6. Comparison of integral elastic cross sections with those of Vo Ky Lan *et al.*

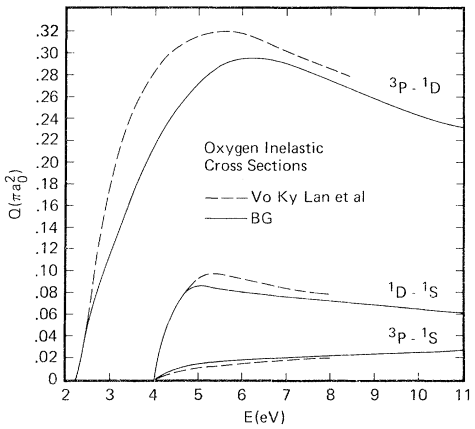

FIG. 7. Comparison of integral inelastic cross sections with those of Vo Ky Lan *et al.*

for the other partial waves. Adding the s-wave BG result to the SC results for the remaining partial waves (column 5 in Table I) gives a curve similar to the close-coupling curve in Fig. 1. Because pair correlations with the target electrons as well as the target polarizability seem to be well represented, the present BG calculations should be close to the true cross section.

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