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Resonances in Electron Impact on Atomic Oxygen

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The momentum-space coupled-channels-optical (CCO) method is used to study the resonances in electron–oxygen collision in the energy region of 9–12 eV. Present results have shown agreement with the available experimental and theoretical results, and new positions of resonances are found by the comparison of total cross sections.

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The study of resonance in electron–atom collisions has been an interesting subject for the several decades. The research field has rapidly advanced during the past 20–30 years due to the developments in experimental techniques, theoretical understanding and the computer power. However, there are only a few works which have been carried out in studies of resonances phenomena in electron–atomic oxygen collisions, compared with lots of works on calculations of various scattering cross sections for electron scattering by atomic oxygen, probably it owes to the open shell complicated structure of atomic oxygen. The investigations of resonances in e–O system is of great challenge.

The first experimental evidence for autodetaching states of O− was obtained by Edwards et al.[1] in keV collision of O− with He, H2, Ne, N2, and Edwards and Cunningham[2] obtained the peaks at 9.50, 10.11, 10.87, 12.12 and 13.71 eV in electron spectrum from O-He collisions in their subsequent work. Later, Spence[3,4] measured several resonances in total cross section of electron scattering by atomic oxygen, which verified three resonant states at 10.90, 12.10 and 13.71 eV, and found several new resonances states. Theoretical studies of resonances in electron–oxygen collision were performed by Rountree and Henry[5] using unitarized Born, the nonexchange, and two-state close-coupling approximations. They calculated the cross section for 2p3 3P− 2p3s 3S0 excitation and found resonances in the 2P and 4P channels at impact energies of 9.67 eV and 9.94 eV, respectively. Chase and Kelly[6] calculated the photo detachment cross section of O− 2p3 2P0 in many-body perturbation theory, and they found two resonances caused by the degeneracy of s− 2p and 2p− ks or kd transitions. Matese et al.[7,8] predicted 12 Feshbach resonances in oxygen in their configuration interaction calculations. Ormonde performed close-coupling of electron scattering by oxygen and predicted 2 resonances at 10.38 eV and 11.36 eV. Recently, Buckman and Clark[9] have performed MCHF calculations for resonances of oxygen ion, and the given resonances are similar to those of Matese et al.[7] Detailed information can be found in Ref. [9]. The latest work involved in studies of resonances in electron–oxygen system was carried out by Zatsarinny et al.[10] They investigated the low-energy elastic electron scattering by atomic oxygen by employing the B-spline R-matrix method, presented a detailed investigation of the low-energy electron scattering from oxygen atom, and found a Feshbach resonance at 8.763 eV with a width of 15.5 meV, which is in good agreement with experiment of Ref. [4]. Although the known resonances have been well documented for the electron–oxygen system, previous studies predicted there should be many resonances in the electron–oxygen system, which have not yet been observed or calculated.[9]

In this Letter, we employ the coupled channels optical (CCO) method[11–20] to study the energy dependence of electron–oxygen scattering at low energies. A distinct feature of the CCO method is that it uses an \textit{ab initio} equivalent local optical potential to describing continuum of targets. The real part of this polarization potential present polarization of the target, and the imaginary part of the potential describes excitation continuum of the target. This allows us to take long-range polarization and some short-range electron correlation accounted in the calculations, and the effects are expected to be very important in electron–oxygen scattering.[10]

The coupled integral equations are represented in momentum spaces:

\begin{equation}
\langle k|T_S|0\rangle = \langle k|V_S^{(Q)}|0\rangle + \sum_{j\in P} \int d^3q \frac{\langle k|V_S^{(Q)}|j\rangle \langle q\rangle S |T_S|0\rangle}{(E^+ - \varepsilon_j - q^2/2)}
\end{equation}
where \( i, j \) represent target states, \( P \) projects a finite set of target states including the ground state 0, and \( Q \) projects the continuum and the remaining discrete states. The subscript \( S \) indicates the total spin. \( V_S^{(Q)} \) has two parts, the electron–target potential \( V_S \) and the complex, nonlocal polarization potential \( W_S^{(Q)} \),

\[
V_S^{(Q)} = V_S + W_S^{(Q)},
\]

where the basic approximation for the matrix element of \( W_S^{(Q)} \) is

\[
\langle k'|W_S^{(Q)}|j\rangle = \sum_{l\in Q} \int d^3 q \frac{(k'|V_S|q)(q|V_S|j)}{E^{(+)} - \varepsilon_l - q^2/2} \]

\[
+ \int d^3 q' \int d^3 q \quad \frac{(k'|V_S|\psi^{(-)}(q_<)|q_>\psi^{(-)}(q_<)|V_S|j)}{E^{(+-)} - q^2/2 - \varepsilon_j/2}
\]

where \( q_< \) and \( q_> \) represent the less \( q \) and greater \( q' \), respectively, and \( \psi^{(-)}(q) \) is a Coulomb wave orthogonalized to the \( P \) space target orbital involved in the same matrix element. For computational feasibility it is necessary to use the equivalent local exchange amplitude in Eq. (3) and to make the angular momentum projection approximation

\[
\langle k'|W_S^{(Q)}|j\rangle = \sum_{l', m'} \int^+ C_{l', m', l} U_{l', m', j}(K) Y_{m', m}(\hat{\mathbf{k}}),
\]

where \( l m l' \) and \( l' m' \) are the orbital angular momentum quantum numbers of the states \( i \) and \( j \), respectively, and

\[
K = k - k'.
\]

The half-on-shell approximation

\[
\frac{1}{2} k^2 = E - \varepsilon_j
\]

is made for the amplitudes (3), reducing the computation of the optical potential to the function \( U_{l', m', j}(K) \) obtained by inverting (4). Details of the calculation are given in Ref. [16] and references therein.

The present calculation was carried out by using the same quadrature points for solving the integral equation (1) over a range of energies, thus making the off-shell potential matrices energy independent. We calculate the slowly varying optical potentials at a few energy points instead of the whole energy range. For computation we make a partial-wave expansion of the \( T_S \) and \( V_S^{(Q)} \) matrix elements, defining the partial matrix elements

\[
\langle k'n'l'|T_S|l\rangle
\]

for total orbital angular momentum quantum number \( J \) by

\[
\langle k'n'l'|T_S^{(Q)}|l\rangle
\]

\[
= \sum_{L,M,L',M',J,K} \langle k'|L'M'\rangle C_{L'J,J,K}^{M'MK}\]

\[
\cdot \langle k'n'l'|T_S|l\rangle\rangle C_{L,J,J,K}^{MLMK}\langle LM|\hat{\mathbf{k}}\rangle,
\]

where \( \langle k|LM\rangle \equiv Y_{LM}(\hat{\mathbf{k}}) \)

and \( C_{L,J,J,K}^{MLMK} \) is a Clebsch–Gordan coefficient. The definition of

\[
\langle k'n'l'|V_S^{(Q)}|l\rangle\rangle
\]

\[
= \sum_{L,M,L',M',J,K} \langle k'|L'M'\rangle C_{L'J,J,K}^{M'MK}\]

\[
\cdot \langle k'n'l'|V_S^{(Q)}|l\rangle\rangle C_{L,J,J,K}^{MLMK}\langle LM|\hat{\mathbf{k}}\rangle,
\]
is analogous to Eq. (7) with $V^{(Q)}_S$ substituted for $T_S$.

In the present calculation, 10 lowest lying discrete states of oxygen are included in P space. They are $2p^4\;^3P$, $2p^33s\;^3S^o$, $2p^33p\;^3P$, $2p^34s\;^3S^o$, $2p^33d\;^3D^o$, $2p^34p\;^3P$, $2p^53s\;^3S^o$, $2p^43d\;^3D^o$, $2p^35p\;^3P$, $2p^36s\;^3S^o$.

We have calculated total cross sections and partial wave cross sections of the $e$–O system at energies from 9 to 12 eV. The intervals are 0.005 eV and 0.002 eV partly. Figure 1 shows the curve of total cross sections. The resonances found in the present calculation are compared with earlier calculations and experiments.

The resonances of earlier researches at 9.5 eV,

- $10.63 \text{ eV}$
- $10.88 \text{ eV}$

and $10.90 \text{ eV}$ can be also found in the present result. They are located at 9.504 eV, 10.65 eV and 10.88 eV, respectively. Especially near 10.88 eV, there are two more peaks at 10.85 eV and 10.898 eV, which probably agree with the early results of 10.87 eV[2] and 10.90 eV[4] respectively. Except for these long-lived and narrow-wide resonances we have discussed above, there is another type of resonance in Fig. 1, which is short-lived and is wider than the former type in width. These possible resonances, which have not been reported before, have been found at 9.4, 9.96, 11.24 and 11.878 eV. They need the confirmation of further theoretical calculations and experiments.

In summary, we have reported the calculated results of the resonances in electron impact on atomic oxygen in the energy region of 9–12 eV. The present results have shown agreement with the available experimental and theoretical results, and new positions of resonances have been found. However, a further calculation of partial wave cross sections by CCO is needed to compare with total cross sections to confirm these resonances. Meanwhile, more data of experimental and theoretical works are needed.

References