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Elastic scattering from sodium at 20 to 150eV

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Coupled-channel optical calculation of electron-atom scattering: Elastic scattering from sodium at 20 to 150 eV

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A coupled-channel optical method for electron-atom scattering is applied to elastic electron-sodium scattering at energies of 20, 22.1, 54.4, 100, and 150 eV. It is demonstrated that the effect of all of the inelastic channels on elastic scattering may be well reproduced by the *ab initio* calculated complex non-local polarization potential. The results are found to be in good agreement with the recent experiments of Lorentz and Miller [*Proc. 16th ICPEAC*, New Yo k, 1989, abstracts p. 198]

I. INTRODUCTION

The coupled-channel optical (CCO) method is an *ab initio* approach to electron-atom scattering. It treats a finite set of scattering channels (P space) explicitly via the coupled-channel formalism, whilst the rest of the channels (Q space), including the target continuum, are taken into account indirectly through a complex nonlocal polarization potential. This potential is calculated from first principles by taking into account the main high order processes up to numerical convergence. This potential, together with the first order potential of the explicitly-treated channels, forms the optical potential.

We will use our usual notation nCC for a calculation that has the lowest n target states treated explicitly in P space (coupled-channel approach), and similarly for nCCO except that the Q space is not excluded but is treated via the polarization potential.

The philosophy of the CCO approach to electron-atom scattering is that the most important channels are explicitly coupled through P space whereas the less important channels are relegated to Q space. The CCO method is useful whenever an nCC calculation does not produce satisfactory (convergent) results even for relatively large n. This is often the case when scattering electrons have energies above the ionization threshold of the atom.

Our CCO approach has proved to be very successful in the description of electron-hydrogen elastic scattering at energies ranging from 0.5 to 30 eV[1] and from 30 to 400 eV[2]. Our current implementation of the CCO method[1] assumes a single valence electron in the target atom. We believe that as this method works well for hydrogen it should also work well for alkali atoms, which are well described by the Hartree-Fock model with one valence electron above a frozen core[3]. Furthermore, it has been found that the effects of core excitation and target electron correlation on scattering are

negligible[4].

The aim of this paper is to demonstrate the effect of the *ab initio* calculated polarization potential in electron scattering from sodium. To maximize this effect and therefore provide a most stringest test of the polarization potential, we do a series of 1CCO calculations, where P space contains only the ground state and Q space contains the complete set of the sodium excited states. Even though the $1s^22s^22p^63p\ ^2P$ excited state of sodium couples very strongly to the ground $1s^22s^22p^63s\ ^2S$ state, we leave this state in Q space to show that even this strong coupling may be reproduced by the polarization potential.

In Sec. II we present the formal theory of our CCO method. The complete derivation of the theory was done in McCarthy and Stelbovics[5] and Bray, Korovalov, and McCarthy[1]. Thus, we give only the final equations for electron scattering on alkali atoms.

In Sec. III we present the results of 1CCO calculations for projectile energies of 20, 22.1, 54.4, 100, and 150 eV (Table I). We compare these results (Fig. 1) with the measurements of elastic differential cross sections of Lorentz and Miller[6]. The agreement between this experiment and our theory is very good. To show the contribution of the polarization potential we also present the corresponding 1CC calculations (static exchange) which leave out this potential all together.

II. FORMAL THEORY OF THE CCO METHOD FOR ALKALI ATOMS

If the target atom can be described as one electron above the frozen core in the independent-particle model then the total nonrelativistic Hamiltonian for the electron-atom scattering problem can be reduced (see for example Ref. [5]) to

$$H = K_1 + K_2 + v_1 + v_2 + v_3, \tag{1}$$

where K_1 and K_2 are the kinetic energy operators of the projectile and the valence

electrons with the corresponding electron-core potentials v_1 and v_2. The electron-electron potential is v_3. For sodium we use the notation C for the frozen core $1s^22s^22p^6\ ^1S$ and A for the ground state of the atom $1s^22s^22p^63s\ ^2S$. As the mass of the nucleus is very much greater than that of the electrons, the center of mass frame is taken to be the nucleus. In coordinate space representation

$$v_\alpha\phi_i(\mathbf{r}_\alpha) = \left(-\frac{Z}{r_\alpha} + 2\sum_{\phi_j\in C}\int d^3r' \frac{|\,\phi_j(\mathbf{r}')\,|^2}{|\,\mathbf{r}_\alpha - \mathbf{r}'\,|}\right)\phi_i(\mathbf{r}_\alpha)$$
$$- \sum_{\phi_j\in C}\int d^3r' \frac{\phi_j^*(\mathbf{r}')\phi_i(\mathbf{r}')}{|\,\mathbf{r}_\alpha - \mathbf{r}'\,|}\phi_j(\mathbf{r}_\alpha), \qquad \alpha = 1,2, \tag{2}$$

and

$$v_3(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{|\,\mathbf{r}_1 - \mathbf{r}_2\,|}. \tag{3}$$

The $\phi_j(\mathbf{r}) \in C$ are the one electron core orbitals calculated via the self-consistent field Hartree-Fock method[7] for the ground state of the atom A,

$$\left(K_\alpha + v^{HF} - \epsilon_j\right)\phi_j(\mathbf{r}_\alpha) = 0, \qquad \alpha = 1,2, \quad j \in A, \tag{4}$$

where

$$v^{HF}\phi_j(\mathbf{r}) = \left(-\frac{Z}{r} + 2\sum_{\phi_{j'}\in A}\int d^3r' \frac{|\,\phi_{j'}(\mathbf{r}')\,|^2}{|\,\mathbf{r} - \mathbf{r}'\,|}\right)\phi_j(\mathbf{r})$$
$$- \sum_{\phi_{j'}\in A}\int d^3r' \frac{\phi_{j'}^*(\mathbf{r}')\phi_j(\mathbf{r}')}{|\,\mathbf{r} - \mathbf{r}'\,|}\phi_{j'}(\mathbf{r}). \tag{5}$$

The $\phi_i(\mathbf{r})$ in equation (2) are the one electron excited orbitals which are calculated in the frozen core Hartree-Fock approximation[8] i.e.,

$$\left(K_\alpha + v_\alpha - \epsilon_i\right)\phi_i(\mathbf{r}_\alpha) = 0, \qquad \alpha = 1,2, \quad i \notin C. \tag{6}$$

The solution of the above equation gives us all of the excited states as well as the continuum functions of the target atom in the frozen core approximation.

To get the polarization potential we first define symmetric P and Q using one-electron projection operators[1], P_α and Q_α, by

$$P_\alpha + Q_\alpha = I_\alpha, \quad P = P_1 I_2 + I_1 P_2 - P_1 P_2, \quad Q = Q_1 Q_2, \tag{7}$$

where

$$P_\alpha = \sum_{\phi_i \in P_\alpha} |\,\phi_i\rangle\langle\phi_i\,|, \qquad Q_\alpha = \sum_{\phi_i \in Q_\alpha} |\,\phi_i\rangle\langle\phi_i\,|, \tag{8}$$

and where now the I_α excludes core space. The sum over Q_α space indicates a sum over excited discrete states and an integral over the continuum states. The complex non-local polarization operator V_Q is then given by

$$PV_Q P = Pv_3 Q G_Q(E^{(+)}) Q v_3 P, \tag{9}$$

where the Q-projected Green's function G_Q satisfies

$$Q(E^{(+)} - H) Q G_Q(E^{(+)}) = Q. \tag{10}$$

The Lippman-Schwinger equation for the T matrix, which depends on the total spin S, is[1]

$$\begin{aligned}\langle \mathbf{k}\phi_i \mid T^S \mid \phi_{i_0}\mathbf{k}_0\rangle = {} & \langle \mathbf{k}\phi_i \mid V_Q^S \mid \phi_{i_0}\mathbf{k}_0\rangle \\ & + \sum_{\phi_{i'} \in P_2} \int d^3k' \frac{\langle \mathbf{k}\phi_i \mid V_Q^S \mid \phi_{i'}\mathbf{k}'\rangle}{(E^{(+)} - \epsilon_{i'} - k'^2/2)} \langle \mathbf{k}'\phi_{i'} \mid T^S \mid \phi_{i_0}\mathbf{k}_0\rangle,\end{aligned} \tag{11}$$

where the projectile with momentum $\mathbf{k}_0$ is incident on the target with the valence electron in state ϕ_{i_0} above the frozen core.

Writing the coordinate space-exchange operator as P_r the matrix elements of V_Q^S are given by[5]

$$\begin{aligned}\langle \mathbf{k}\phi_i \mid V_Q^S \mid \phi_{i'}\mathbf{k}'\rangle = {} & \langle \mathbf{k}\phi_i \mid v_1 + v_3 + (-1)^S v_3 P_r \mid \phi_{i'}\mathbf{k}'\rangle \\ & + (-1)^S \langle \mathbf{k}\phi_i \mid (\epsilon_i + \epsilon_{i'} - E) P_r \mid \phi_{i'}\mathbf{k}'\rangle \\ & - \delta_{ii'} \sum_{\phi_j \in C} \langle \mathbf{k}\phi_j \mid (2\epsilon_j - E) P_r \mid \phi_j \mathbf{k}'\rangle \\ & + \langle \mathbf{k}\phi_i \mid V_Q + (-1)^S V_Q P_r \mid \phi_{i'}\mathbf{k}'\rangle,\end{aligned} \tag{12}$$

The details of the calculation of the polarization potential matrix elements may be found in Ref.[1], however we would like to make explicit here the approximations used in its calculation.

All of the approximations in the calculation of V_Q are made in the evaluation of G_Q. The major approximation that enables us to perform the calculation is that of weak coupling in one of the Q_α spaces. This neglects non-diagonal matrix elements in that space.

If one of the electrons is in a discrete Q_α state then we assume that the potential in which the other electron moves is local and is created by the residual charge of the core, and the first electron. If, however, one of the electrons is in a continuum Q_α state, we assume that the other electron can be well approximated as a free particle.

These approximations in calculation of G_Q have been tested thoroughly for hydrogen and have been found to work extremely well[1].

III. RESULTS AND CONCLUSIONS

In Fig. 1 we present elastic differential cross sections for electron scattering on atomic sodium. The experimental data are due to Lorentz and Miller[6]. These data are relative and have been normalized to our total elastic cross sections σ_e (Table I), which agree with the absolute measurements of Srivastava and Vuskovic[9] (Table II). The solid line shows the 1CCO calculation, where P space contains only the ground state of the atom, and Q space contains all of the excited states including the target continuum. The dashed curve is due to the 1CC calculation (static exchange) which excludes Q space all together.

The 1CCO calculation gives good agreement with experiment at all presented energies. This indicates that the very large effect of the inelastic channels on the elastic scattering may be reproduced by the polarization potential. However, this effect di-

minishes with increasing energy for non-small angles. Already at 150 eV the simple static exchange calculation gives very good agreement with experiment.

In the calculation of the elastic differential cross section convergence to less than 1% was achieved by taking, in (8), excited bound states with angular momentum (L) up to 3 and principal quantum number up to 10. For continuum target states we took L up to 8 and used 25 points in the integration of equation (8).

There are a number of elastic differential cross section measurements of electron scattering on atomic sodium, see Ref. [6] and references therein. Whilst the experiments generally agree at small angles and therefore agree on the total elastic cross section, there is considerable discrepancy at intermediate and backward angles. Thus the choice of normalization does not resolve these discrepancies. Therefore, other nCCO calculations should be performed with lowest-lying excited states coupled explicitly through P space. These will check the stability of the current results, and furthermore will provide inelastic data, where there are also discrepancies between different experiments. These calculations are considerably more time consuming as the number of polarization potential matrix elements grows as the square of n. Such calculations are currently being undertaken.

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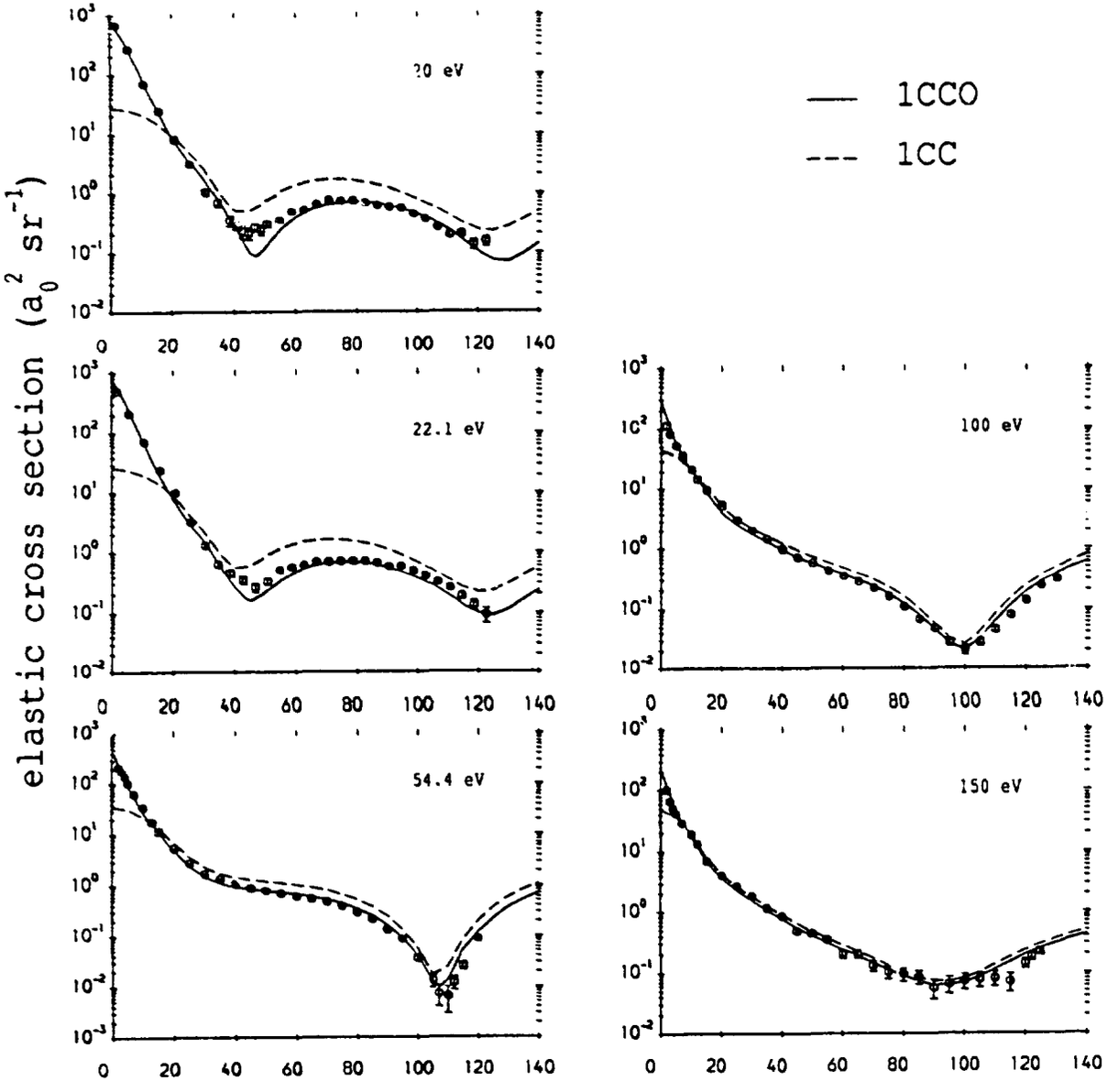
TABLE I. Elastic differential cross sections ($a_0^2\ sr^{-1}$) calculated using the 1CCO model at a range of energies (eV) at angles θ (deg.). The integrated elastic σ_e and the total σ_t cross sections are in πa_0^2. Square brackets denote powers of 10.

θ	20.0	22.1	54.4	100.0	150.0
0	8.00[2]	7.70[2]	4.66[2]	2.93[2]	2.25[2]
5	3.05[2]	2.73[2]	9.60[1]	5.80[1]	4.84[1]
10	8.69[1]	7.45[1]	2.80[1]	2.07[1]	1.73[1]
15	2.55[1]	2.22[1]	1.12[1]	8.76	6.93
20	8.59	7.86	4.93	4.25	3.67
25	3.55	3.33	2.42	2.53	2.27
30	1.66	1.52	1.49	1.75	1.50
35	7.18[-1]	6.31[-1]	1.11	1.27	1.06
40	2.64[-1]	2.53[-1]	9.37[-1]	9.61[-1]	7.65[-1]
50	1.20[-1]	2.19[-1]	7.79[-1]	5.85[-1]	4.09[-1]
60	3.88[-1]	4.90[-1]	6.69[-1]	3.76[-1]	2.38[-1]
70	6.35[-1]	6.80[-1]	5.20[-1]	2.33[-1]	1.42[-1]
80	7.11[-1]	6.95[-1]	3.39[-1]	1.22[-1]	9.10[-2]
90	6.20[-1]	5.65[-1]	1.65[-1]	4.70[-2]	6.29[-2]
100	4.32[-1]	3.69[-1]	4.10[-2]	2.08[-2]	6.96[-2]
110	2.36[-1]	1.92[-1]	1.37[-2]	6.38[-2]	1.12[-1]
120	1.03[-1]	9.73[-2]	1.17[-1]	1.87[-1]	1.93[-1]
130	7.21[-2]	1.12[-1]	3.56[-1]	3.85[-1]	3.01[-1]
140	1.39[-1]	2.28[-1]	6.95[-1]	6.32[-1]	4.31[-1]
150	2.70[-1]	4.02[-1]	1.07	8.90[-1]	5.60[-1]
160	4.16[-1]	5.82[-1]	1.41	1.11	6.67[-1]
170	5.30[-1]	7.21[-1]	1.66	1.27	7.54[-1]
180	5.79[-1]	7.81[-1]	1.78	1.35	7.44[-1]
σ_e	11.8	10.8	5.84	4.27	3.36
σ_t	68.4	64.9	35.9	21.3	15.4

TABLE II. Integrated elastic (σ_e) and total (σ_t) cross sections (πa_0^2) at 20 and 54.4 eV calculated using the 1CCO model. The experimental data σ^{exp} are due to Srivastava and Vuskovic[9].

Energy	σ_e	σ_e^{exp}	σ_t	σ_t^{exp}
20	11.8	15.9±4.8	68.4	60.7±18.0
54.4	5.84	6.14±1.8	35.9	34.3±10.3

FIG. 1. Elastic differential cross sections. The solid line is the 1CCO calculation and the dashed line is the static exchange (1CC) calculation. The experiments of Lorentz and Miller are denoted by o. The experimental data were obtained via a private communication. A preliminary publication of the 5-4.4 eV results may be found in Ref. [6].


20 eV
22.1 eV
54.4 eV
100 eV
150 eV
1CCO
1CC
elastic cross section (a_0^2 sr^{-1})
scattering angle (deg)