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Calculations of elastic scattering cross sections at large angles between electrons and multiply charged ions in the distorted-wave approximation

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Abstract. The elastic differential cross sections of electrons scattered from one- and two-electron multiply charged ions are calculated within the first-order distorted-wave approximation. The exchange amplitude is found to be important for scattering at large angles. The results are compared with previous calculations and with experimental differential cross sections at 180° derived from analysing the binary-encounter electron spectrum from the collision of 19-30 MeV F^{7+} and F^{8+} ions with H_2 and He targets.

1. Introduction

The differential cross sections for elastic collisions between electrons and atoms often serve as a fundamental test of quantum mechanical scattering theories. Over the years many theoretical models have been developed. A good review of the various models has been given by Bransden and McDowell (1977). Most of the quantum mechanical models are based upon either the perturbation series method or the non-perturbative close-coupling method. The close-coupling method has been most useful for low energies and the perturbation series method has been successful for higher energies (Brandsen and McDowell 1977, 1978). The attraction of the perturbation series method lies in the fact that the first term is easy to calculate and it is now known that the first term in the Born series predicts reliable integrated cross sections at high energy but unreliable differential cross sections while the first term in the distorted wave series typically yields reasonable results for the differential cross sections as well. In the intermediate energy range, terms higher than first order become important and it has been only very recently that an exact calculation of the second-order term for the fundamental electron–hydrogen problem has been reported (Madison *et al* 1990, 1991). In this work, it was demonstrated that the distorted-wave series converge after two terms for incident electron energies greater than 30 eV for elastic scattering from hydrogen and that both the second-order direct and exchange terms were important in the intermediate energy range. While the theoretical models for electron–atom collisions could be applied to electron–ion collisions after suitable modifications, experimental data of this type are not available since they have to be obtained by merged-beam or cross-beam methods. While some total excitation cross sections have been reported recently (Wahlin *et al* 1991), no differential information is available so far and thus many theoretical models for electron–ion collisions remain untested.

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In a recent report Richard *et al* (1990) studied the production of binary encounter electrons (BEe) in 19–30 MeV F^{q+} collisions with He and H_2 gas targets. The electrons were observed at zero degrees with respect to the beam direction, which corresponds to $\theta = 180°$ in the projectile rest frame. Using the impulse approximation (Brandt 1983), the binary encounter electrons produced in fast collisions can be considered as resulting from the elastic scattering of 'quasi-free' electrons in the target from the projectile ions. Viewed in the projectile frame, the BEe come from the target gas and elastically scatter to 180°. The validity of such a model has been demonstrated in Lee *et al* (1990) where the BEe productions resulting from collisions between bare ions with He and H_2 targets have been shown to be explained by the Rutherford scattering cross sections convoluted with the Compton profile of the target atom. By studying the BEe production in the collision between F^{q+} ions with He or H_2, the elastic differential cross sections for the scattering between electrons and ions can be extracted.

In studying the BEe cross sections, Richard *et al* (1990) found an 'anomalous' q-dependence in that the double differential cross section (DDCS) at $\theta = 180°$ in the projectile frame increases with decreasing q. In other words, additional electrons in the F^{q+} ions appear to enhance the differential cross sections at 180° instead of reducing them as would be expected if the electrons totally screened the nuclear charge of the ion. Furthermore, the results of Richard *et al* (1990) are in contradiction with earlier experiments at $\theta \ll 180°$ (Stolterfoht *et al* 1974, Toburen and Wilsen 1979) where the DDCS were shown to decrease smoothly with increasing q.

In two previous letters (Shingal *et al* 1990, Reinhold *et al* 1990) the anomalous q-dependence of the DDCS in $F^{q+}(q = 3\text{–}8) + \text{He}$ and H_2 collisions has been interpreted as the elastic scattering of electrons from a screened static potential for the F^{q+} ion. The theoretical results were shown to be in qualitative agreement with experimental data. This is somewhat surprising since the equivalent incident electron energies are below or near the first excitation threshold of the target ion where exchange effects between the incident electron and the target electrons might be important, especially at large angles. In a recent letter, Taulbjerg (1990) examined the elastic scattering of electrons with F^{8+} using first-order perturbation theory. He showed that better agreement with experimental data can be achieved if the effect of electron exchange is considered.

The purpose of this paper is to apply the distorted-wave approximation which has been applied previously in electron–atom collisions to electron–ion collisions. Two models of the distorted-wave approximation are discussed in section 2 for elastic collisions of electrons from one- and two-electron target ions. The calculated results and the comparison with experimental data are discussed in section 3. A summary is given in section 4.

2. Theoretical models

2.1. Direct amplitude

For the calculation of the direct scattering amplitude, we use the standard method for scattering from a static potential. In this work we restrict our attention to one- and two-electron ions and for this case the static potential for a F^{q+} ion is given by

$$U(r) = -q/r + V_s(r) \tag{1}$$

where $V_s(r)$ is the short-range potential resulting from screening

$$V_s(r) = -N(Z+1/r)\,e^{-2Zr} \tag{2}$$

and where N is the number of electrons in the ion (1 or 2) and Z is the nuclear charge. The direct scattering amplitude for the potential (1) is given by

$$T_N^d = f_C(\theta) + f_s(\theta) \tag{3}$$

where $f_C(\theta)$ is the Coulomb scattering amplitude for charge q and

$$f_s(\theta) = (2ik)^{-1} \sum_l (2l+1)\exp(2i\sigma_l)[\exp(2i\delta_l)-1]P_l(\cos\theta) \tag{4}$$

is the scattering amplitude for the short-range potential where σ_l is the Coulomb phaseshift and P_l is the Legendre polynomial. By calculating the phaseshifts δ_l from the numerical solution of the differential equation one can show that only small l contribute to the summation in (4). The resulting differential cross sections, $d\sigma/d\Omega = |T_N^d|^2$, at $\theta = 180°$, as shown in Shingal *et al* were found to agree reasonably well with the experimental data of Richard *et al* (1990). It should also be noted that the same calculation predicts that at smaller angles ($\theta < 60°$) the differential cross section shows the expected screening effect, i.e. it decreases with increasing number of electrons in the ion.

2.2. Exchange amplitude

We have used the perturbation series approach to obtain the exchange amplitude. Consider the scattering of an electron from an N-electron target ion. In the two-potential approach (Madison *et al* 1991) the exact exchange amplitude is

$$T^{ex} = -2\pi^2 N\langle \chi_f^-(1)\psi_f(0,2,\ldots,N)|V - U_f(1)|\Psi_i^+\rangle \tag{5}$$

where V is the total interaction potential, Ψ_i^+ is the full initial state wavefunction satisfying the outgoing wave boundary condition, U_f is the final state distorting potential, ψ_f is the final state wavefunction of the target ion and χ_f^- is the final state distorted wave which is obtained from

$$(-\tfrac{1}{2}\nabla^2 + U_f - \tfrac{1}{2}k_f^2)\chi_f^- = 0 \tag{6}$$

where $\frac{1}{2}k_f^2$ is the kinetic energy of the continuum electron.

In the first-order distorted-wave approximation (DWB1) one assumes

$$\Psi_i^+ = \psi_i(1,\ldots,N)\chi_i^+(0) \tag{7}$$

where ψ_i is the initial state of an isolated N-electron ion and χ_i^+ is an initial state distorted wave which is obtained from

$$(-\tfrac{1}{2}\nabla^2 + U_i - \tfrac{1}{2}k_i^2)\chi_i^- = 0 \tag{8}$$

where U_i is the initial state distorting potential and $\frac{1}{2}k_i^2$ is the initial state kinetic energy of the incident electron. For elastic scattering, $U_i = U_f = U$ (of equation (1)), $\psi_i = \psi_f$ and $k_i = k_f$. As a result, the exchange amplitude in the distortion approximation for a one-electron ion is given by

$$T_1^{ex} = -2\pi^2\left\langle \chi_f^-(1)\psi_{1s}(0)\left|\frac{1}{r_{10}} - \frac{Z}{r_1} - U_f(r_1)\right|\psi_{1s}(1)\chi_i^+(0)\right\rangle. \tag{9}$$

For a two-electron ion, on the other hand, the exchange amplitude is given by

$$T_2^{\text{ex}} = -2\pi^2 \left\langle \chi_f^-(1)\psi_{1s}(0) \left| \frac{1}{r_{10}} - \frac{Z}{r_1} - \tfrac{1}{2}U_f(r_1) \right| \psi_{1s}(1)\chi_i^+(0) \right\rangle \tag{10}$$

where r_{10} is the distance between electrons 0 and 1. The differential cross section for a one-electron ion is given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \tfrac{1}{4}|T_1^{\mathrm{d}} + T_1^{\text{ex}}|^2 + \tfrac{3}{4}|T_1^{\mathrm{d}} - T_1^{\text{ex}}|^2. \tag{11}$$

The first term on the right-hand side of (11) is the contribution from singlet scattering and the second from triplet scattering. For two-electron ions, the differential cross section is obtained from

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |T_2^{\mathrm{d}} - T_2^{\text{ex}}|^2. \tag{12}$$

The present exchange amplitude for one-electron ions is similar to that used by Taulbjerg (1990), but there are two differences. (i) In Taulbjerg's calculation the distortion potential is the Coulomb potential for a charge $(Z-1)$ so the distorted wave is replaced by a Coulomb wave. This is not an important difference for high-Z target ions. (ii) Taulbjerg did not include the single particle terms $(-Z/r_1 - U(r_1))$ in the evaluation of the exchange amplitude.

The exchange amplitude resulting from the single particle terms for a one-electron ion is given by

$$T_1^{\text{sp}} = -2\pi^2 \langle \chi_f^-(1)| -Z/r_1 - U_f(r_1)|\psi_{1s}(1)\rangle\langle\psi_{1s}(0)|\chi_i^+(0)\rangle. \tag{13}$$

The distorting potential $U_f(r_1)$ for a one-electron ion is the sum of the interaction of electron 1 with the nucleus plus the interaction of this electron with another electron in the 1s orbital. Consequently in the expression $-Z/r_1 - U_f(r_1)$, the nuclear terms cancel and one is left with the interaction of electron 1 with an atomic electron. As a result, the exchange amplitude (13) may be interpreted as electron 0 being captured into the final atomic state not through an interaction but rather through a non-zero overlap of initial and final state wavefunctions, electron 1 is then ejected through its interaction with electron 0 in the 1s state. This process is analogous to a shakeoff process except that there is an exchange of particles in the present process. The significance of the single particle terms is further discussed in the next section.

3. Results and discussion

In figure 1 we show the ratio of the calculated elastic differential cross sections for $e^- + F^{8+}$ collisions with that for $e^- + F^{9+}$ collisions for incident energies at 40 and 60 Ryd. The curves are from three different theoretical models. (i) The full curves are calculated from the direct scattering amplitudes only. They are identical to those given by Shingal *et al* (1990). (ii) The dotted curves are from calculations in which both the direct and the exchange amplitudes are calculated but the latter are obtained without the single-particle terms, i.e. the terms $-Z/r_1 - U_f(r_1)$ in (9). These results are essentially identical to those given by Taulbjerg (1990) where he replaced the distorted waves by the Coulomb waves. (iii) The broken curves are from calculations where the full operators in (9) and (10) are used. We first note that all three curves merge at small scattering angles showing that exchange amplitude is important only at large scattering

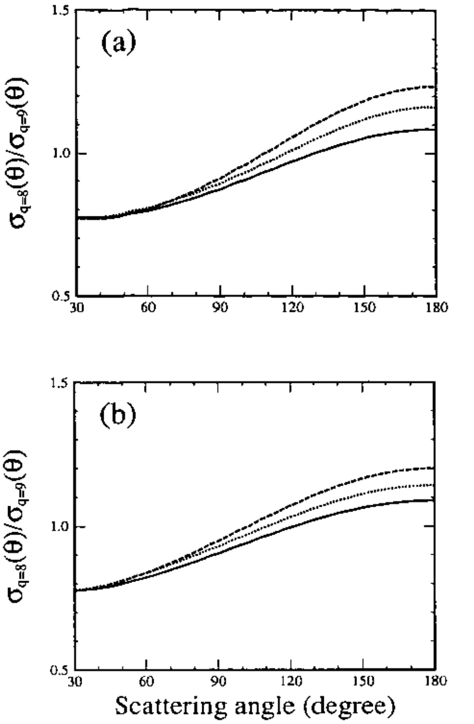

Figure 1. Variation of the calculated ratio of differential cross sections for $e^- + F^{8+}$ collisions compared with those for $e^- + F^{9+}$ collisions as a function of scattering angle. The incident energies are: (*a*) 40 Ryd, (*b*) 60 Ryd. The full curves are from the direct amplitudes only. The other two curves include both the direct and exchange amplitudes, see text.

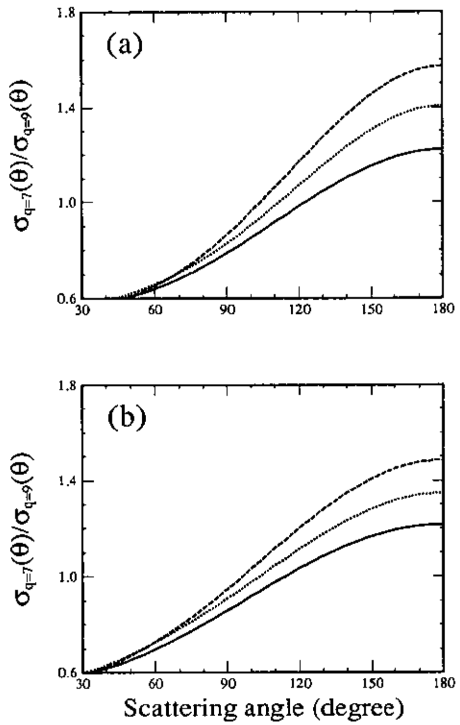

Figure 2. Variation of the calculated ratio of differential cross sections for $e^- + F^{7+}$ collisions compared with those for $e^- + F^{9+}$ collisions as a function of scattering angles. The incident energies are: (*a*) 40 Ryd, (*b*) 60 Ryd. The full curves are from the direct amplitudes only. The other two curves include both the direct and exchange amplitudes, see text.

angles, with the effect being largest at $\theta = 180°$. Note that the exchange enhances the differential cross sections at large angles. This has been traced (Taulbjerg 1990) to the fact that the exchange amplitude T_N^{ex} has opposite sign from the direct amplitude T_N^{d} and the enhancement comes mostly from the $|T_N^{d} - T_N^{ex}|^2$ term. A similar graph for the ratios for $e^- + F^{7+}$ collisions is given in figure 2, also at 40 and 60 Ryd. The effect of the exchange term is larger for the latter system.

The only experimental data available for comparison are those obtained from the doubly differential cross sections of the BEe peaks in $F^{q+} + He$ and H_2 collisions. According to the impulse approximation, the measured BEe electrons can be used to deduce the elastic differential cross sections at $\theta = 180°$. The derived data at the two energy points of 19 and 28.5 MeV (corresponding to an electron energy of 40 and 60 Ryd respectively) for $F^{q+} + H_2$ ($q = 7, 8$) collisions are plotted against the results from the three theoretical models in figure 3. For F^{8+} ions, the experimental results clearly indicate that the exchange amplitude contributes to bring the theoretical results into better agreement with data. Between the two versions of treating the exchange, the one without the single particle terms is in better agreement with experiment at 40 Ryd, but at 60 Ryd the one with single particle exchange terms is in better agreement with experiment. For F^{7+} ions, the experimental data appear to favour the inclusion

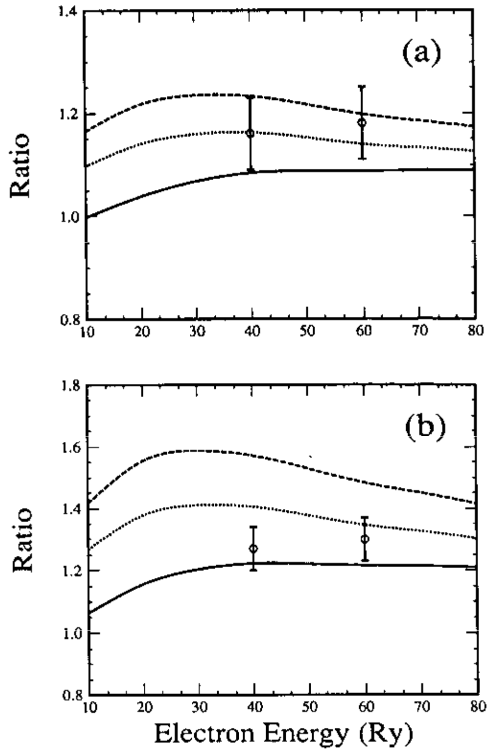

Figure 3. Variation of the ratio of differential cross sections for $e^- + F^{q+}$ with $e^- + F^{9+}$ at $\theta = 180°$ as a function of the incident energy of the electron: (*a*) for $q = 8$; (*b*) for $q = 7$. Experimental data are obtained from Richard *et al* (1990). The theoretical curves are identical to those given in figures 1 and 2.

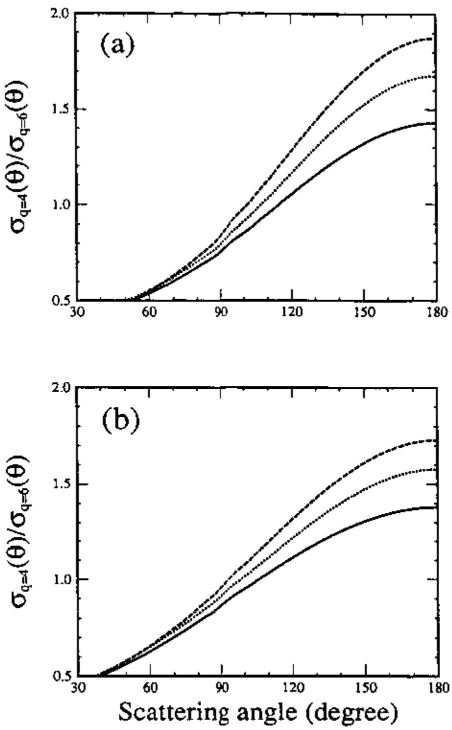

Figure 4. Variation of the calculated ratio of differential cross sections for $e^- + C^{4+}$ collisions compared with those for $e^- + C^{6+}$ collisions as a function of scattering angles. The incident energies are: (*a*) 17.78 Ryd, (*b*) 26.67 Ryd. The full curves are from the direct amplitudes only. The other two curves include both the direct and exchange amplitudes, see text.

of the exchange at the higher energy point but not at the lower energy point, in contradiction to what one would expect that exchange is more important at lower energies. Furthermore, the experimental results clearly differ from calculations where exchange amplitude is calculated with the inclusion of single particle terms.

The 'anomalous' enhancement of differential cross sections at large scattering angles becomes more pronounced as the nuclear charge of the ion is decreased. In figure 4 we show similar calculations for $e^- + C^{4+}$ collisions at two energies. The collision energies were selected by the Z^2 scaling, i.e. they are reduced by $(\frac{6}{9})^2 = \frac{4}{9}$ from the values used in $e^- + F^{8+}$ and $e^- + F^{7+}$ collisions. The enhancement with respect to the Rutherford scattering by bare ions at large angles is again quite transparent. At smaller angles ($\theta < 90°$), the three theoretical results merge. All these features are similar to those for $e^- + F^{q+}$ collisions except that the enhancement is larger.

The results shown above seem to favour calculating the exchange amplitude without the single particle terms. However, this cannot be justified from the formulation of the perturbation expansion series. The single particle terms would vanish if the initial distorted wave were orthogonal to the target 1s wavefunction. This overlap is small but non-zero since the distorted wave sees a screened charge at large distances while the 1s electron sees the whole nuclear charge. Physically one can interpret these terms as the target electron being ejected to the continuum due to the average interaction of the incident electron with the target electron while the incident electron becomes trapped in the ion in the process. These terms contribute only when the target electron and the incoming electron wavefunctions are not orthogonal (see equation (13)), and the contribution to the scattering amplitude has to be interpreted as a type of shakeoff process. While the degree of non-orthogonality is small, the single particle integral is sufficiently large that the net contribution from the single particle terms is about 20–75% of the integral involving the two-particle term.

While the comparison with experiment would tempt one to argue that the single particle terms should be dropped, it would seem inconsistent to selectively decide that one part of the first-order amplitude should be kept and another part should be dropped, particularly when they are of comparable size. Madison *et al* (1991) included the single particle terms in both the first- and second-order terms in their work for electron–hydrogen scattering and in this case the terms brought experiment and theory in better accord. The discrepancy from the experimental data seen here is probably an indication that second-order contributions to the scattering amplitude need to be examined. One may wish to speculate that the exchange due to overlap is cancelled when higher order terms are included, but such a statement can be supported only with actual calculations.

4. Summary

We have used the first-order distorted-wave approximation to study elastic scattering cross sections for electron–ion collisions. Electron exchange was found to play a significant role in determining the differential cross sections at large angles. In contrast, exchange has no effect at small angles. The theoretical results at $\theta = 180°$ for $e^- + F^{q+}$ ($q = 6, 8$) are compared with experimental data derived from binary encounter electrons in $F^{q+} + H_2$ collisions, assuming the validity of the impulse approximation.

Within the distorted-wave approximation, we have identified two terms that contribute to the exchange amplitude, one is the standard electron–electron interaction term, and the other is the single particle term. The latter can be neglected under the assumption that the initial target electron wavefunction is orthogonal to the wavefunction of the scattered electron. We have found that this term gives non-negligible contributions to the exchange amplitude. However, the experimental data deduced from the binary encounter electrons seem to favour results for which the exchange amplitude is calculated without the single particle term. On the other hand, there is no justification for dropping this term from the perturbation series expansion. The increasing deviations from experimental data which result when exchange is included suggest that second-order calculations need to be carried out. Calculations using the close-coupling method are also desirable since the collision energy is below or near the excitation threshold for the $n = 2$ states and the convergence of the close-coupling calculations is expected even when a few basis functions are used in the expansion.

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Note added in proof. A one-channel close-coupling calculation for the present collision systems has been carried out recently by Bhalla and Shingal (1991).

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