Direct and indirect relativistic effect on electron scattering from cesium and gold atoms

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The differential cross section (DCS), Stokes parameters, and the STU parameters for electron scattering from a cesium atom are calculated by two kinds of distorted-wave methods, each including different relativistic effects. Comparing our results with those from the relativistic distorted-wave method of the Toronto group, we find that, at an incident electron energy of 50 eV, the direct relativistic effect is more important than the indirect relativistic effect for cesium. Further the direct relativistic effect leads to the invalidity of the ''fine-structure approximation'' for the case of cesium. We also calculated the DCS and the Stokes parameters for an electron-gold collision at incident electron energy of 50 eV. Unlike the cesium case, the indirect relativistic effect is more important for gold. [S1050-2947(99)02408-7]

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It is well known that with increasing atomic number the relativistic effect in atomic structure becomes more and more important. Cesium is the heaviest alkali-metal atom and often serves as a prototype atom in the study of the relativistic effect. Since atomic cesium is easy to prepare experimentally and since its theoretical model is fairly simple, much attention has been given to the relativistic effect in electron-cesium scattering [1–5]. A gold atom is very similar to an alkali-metal atom in that their ground states both consist of the core of closed-shell orbitals and one valence electron in a $(ns)^2S_{1/2}$ orbital. So a gold atom can be treated like an alkali-metal atom [6].

According to Lam and Baylis [7] the relativistic effect in electron scattering by atoms can be divided into a direct and an indirect relativistic effect. The direct relativistic effect arises from the relativistic motion of incident electrons in the atomic field, while the indirect relativistic effect is due to the relativistic motion of the bound electrons in the target atom. A fully relativistic treatment of both incident and target electrons will give a complete description of these effects [3]. However, it is useful to explore these effects at different levels in order to understand their importance in scattering processes. We have carried out detailed numerical calculations, based on the distorted-wave method (DWM), at two levels: (i) nonrelativistic treatment for both projectile and target electrons, and (ii) relativistic treatment for target electrons only. The results are compared with the fully relativistic approach [3,6].

The DWM is widely used in electron-atom collision calculations in the intermediate energy range [8]. The relativistic version of the method was recently developed by the Toronto group [3,9–13] and applied to calculations of electron-impact on atoms of cesium, ytterbium, silver, gold, and noble gases. In their relativistic distorted-wave (RDW) treatment, both the continuum and bound electrons are described by the Dirac equation. One of the advantages of the DWM is that it is unique in dealing with the continuum electrons and bound electrons separately. Therefore, the DWM allows the direct and indirect relativistic effects to be studied individually within various models and including different levels of relativistic effects.

Our first approach is based on the ordinary distorted-wave (ODW) method, which is purely nonrelativistic. The Schrödinger equation is used to describe the continuum electron and the Roothaan-Hatree-Fock wave function is used to describe the bound electrons. Throughout this work, the static potential is used as the distortion potential. The electron charge distribution of the target atom and the static potential are nonrelativistic in this case. We use the same calculation outlines as the Toronto group so that our results can be compared with their results. The intrarelativistic distorted-wave (IDW) method, our second approach, includes relativistic effects of the target electron only. The Dirac-Slater method is used to describe the bound electrons, while the continuum electron is treated nonrelativistically as in the first model. As a result, the relativistic effect is included in the electron density of the target atom and the distorted potential. The indirect relativistic effect (actually the intra-atom relativistic effect [14]) is thus fully included in the IDW. By comparing the DCS, Stokes, and STU parameters of the IDW method with those of the ODW method, the indirect relativistic effect can be extracted. We can also compare our IDW results with those from RDW treatment. The direct relativistic effect can thus be found. Nuclear depolarization is taken into account in the calculations of the Stokes parameters. The perturbation coefficients of fine and hyperfine structure for the Stokes parameters are calculated by the program ACFF [15].

Detailed descriptions of the STU parameters and the Stokes parameters can be found in the paper by Bartschat and Andersen [16,17]. The differential Stokes parameters calculated in this work are for the case of unpolarized electrons scattered from unpolarized atoms. The ''fine-structure approximation'' is used in the calculation of STU parameters in the ODW model. In this case, the STU parameters satisfy the following equations:

$$S_p \equiv S_p^{1/2} = -2S_p^{3/2}, \tag{1}$$

$$T \equiv T_x^{1/2} = T_y^{1/2} = T_z^{1/2} = T_x^{3/2} = T_y^{3/2} = T_z^{3/2}, \tag{2}$$

$$U_{xz} \equiv U_{zx}^{1/2} = U_{xz}^{1/2} = -2U_{zx}^{3/2} = -2U_{xz}^{3/2}. \tag{3}$$

Our results, along with those of RDW [3,6] are shown in Figs. 1–5. In the ODW model, the excited state is spin av-

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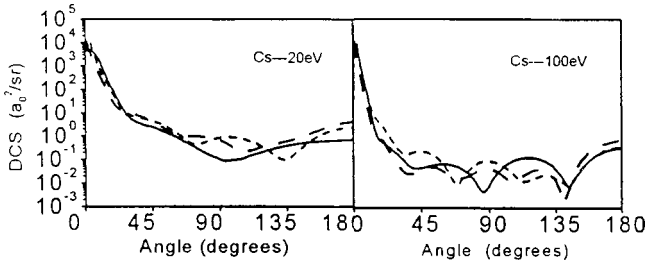

FIG. 1. Differential cross section for electron scattering from cesium. Solid line stands for the results of the IDW, dashed line for the RDW, short dashed line for the ODW methods.

eraged while in both IDW and RDW calculations the excited state is $(6p)^2P_{3/2}$. Figure 1 shows the DCS for cesium at two different incident electron energies using the ODW, IDW, and RDW methods. In Fig. 2 we have presented the differential Stokes parameters P_i $(i=1,2,3)$ for cesium and gold at incident electron energy of 50 eV. Figure 3 shows both the theoretical and experimental DCS of gold and T parameters of cesium at incident in electron energy of 50 eV. The S_P and S_A parameters for cesium obtained from the three methods usually agree within 10%. We give the S_P only in Fig. 4, at incident electron energies of 20 and 100 eV. Figure 5 shows the U_{xz} parameters for cesium at energies of 20 and 100 eV. Because the fine-structure approximation was used in the calculation of the ODW model the three T parameters reduce to 1 and the two U parameters reduced to 1 as well. As was the case for the S parameters, the magnitudes of U_{xz} and U_{zx} parameters usually agree within 10% and therefore the U_{ZX} are not shown. To data there has not been any experimental data published for the differential cross section of cesium, the differential Stokes parameters, and the STU parameters of cesium and gold in the intermediate energy range. We hope to have some experimental data for comparison.

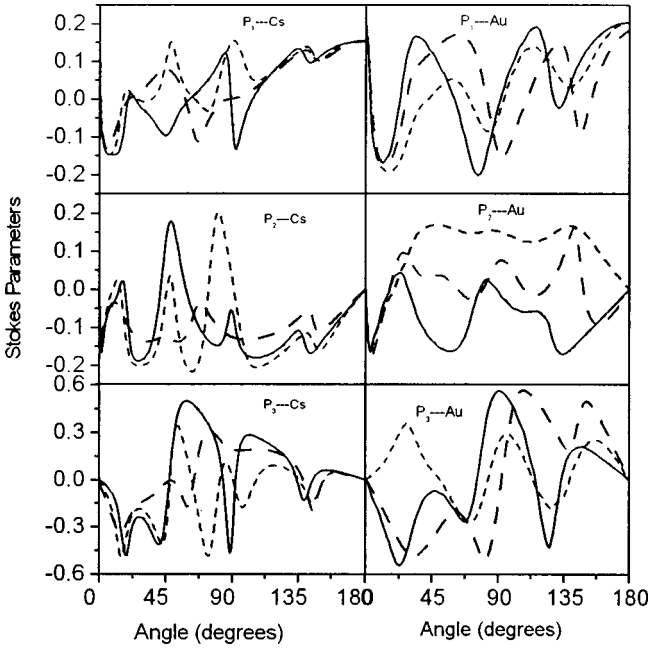

FIG. 2. Stokes parameters P_1, P_2, and P_3 for cesium and gold are shown at 50 eV incident electron energy. Line style as in Fig. 1.

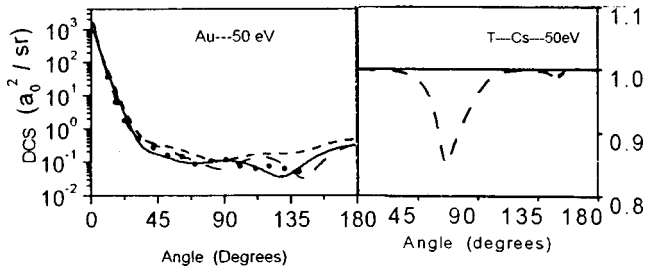

FIG. 3. DCS for Au and T parameter for Cs are shown at incident electron energy of 50 eV. Line style as in Fig. 1. ● stands for the experimental results [22].

According to Bartschat the measurement of DCS is a ''classical'' experiment in scattering physics [18]. So the DCS is a ''classical'' standard by which to test the validity of scattering theories, too. By comparing the DCS in Figs. 1 and 3, we can see differences in the results from the ODW, IDW, and RDW models. When the angle is less than 26°, results from three approaches in Fig. 1 are almost the same. This implies that there is little difference in the total cross section in the three models. At large angles, however, differences appear. From the data of the IDW and RDW model is seen that the direct relativistic effect exists not only for high-energy incident electrons but also for low energy incident electrons (20 or 100 eV). This is also supported by the DCS of gold in Fig. 3. A slow incoming electron is accelerated by the strong Coulomb field of the nucleus and thus becomes relativistic near the target [19]. Comparing the ODW with the method IDW, the indirect relativistic effect is obtained. This is also shown for cesium in Fig. 1 and for gold in Fig. 3. At the same time, Fig. 3 shows the reliability of DWM with the experimental results.

Stokes parameters for cesium and gold each using 50 eV incident electrons are shown in Fig. 2. For cesium both the magnitude and shape of P_i $(i=1,2,3)$ in the IDW and ODW models are close to each other. Especially in P_2-Cs the IDW results are similar to the ODW results over the whole range. They are different from the RDW results. In P_3-Cs at small and large angles ($\leqslant 53°$ and $\geqslant 140°$) the results of IDW and ODW agree with each other very well. But the RDW results differ the IDW and ODW results. For gold, to our surprise, the situation is reversed. In P_1-Au the line structure is almost the same for all three methods. However, considering the magnitude, the difference between the IDW line and the RDW line is less than the difference between IDW line and ODW line. In P_2-Au the ODW results differ greatly from those from RDW; however, the IDW results are

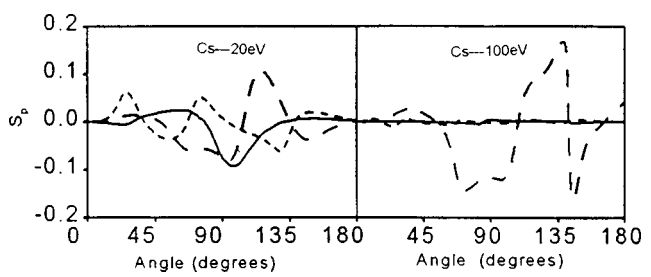

FIG. 4. Polarization function S_p of 20 and 100 eV. Line style as in Fig. 1.

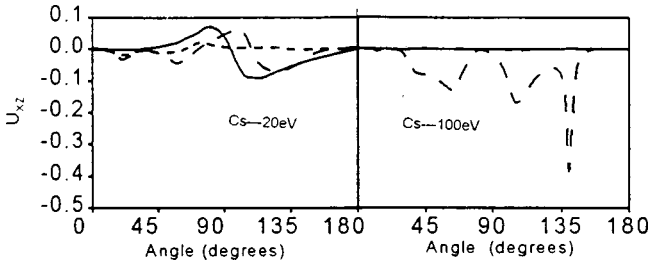

FIG. 5. Rotation parameter U_{XZ} of 20 and 100 eV. Line style as in Fig. 1.

close to those of the RDW. In P_3-Au the results from the IDW roughly agree with those from the RDW both in magnitude and structure, but the ODW results differ from the RDW results especially at small angles ($\leqslant 45°$). These comparisons tell us that for gold atom with 50 eV incident electron energy the indirect relativistic effect is more important than the direct one. Because a gold is heavier than a cesium, it can be visualized that the indirect relativistic effect in gold is more important than in cesium.

Because the fine-structure approximation has been used in the calculation of STU parameters in the ODW and IDW methods, a comparison of the three methods does not allow us to draw conclusions like those above for Stokes parameters. But the reason of invalidity of the fine-structure approximation can be inferred from the comparison. The fine-structure approximation was discussed in detail by Hanne [20], who shows that excitation amplitudes to different fine-structure levels are not independent of each other. This approximation is expected to work very well for alkali-metal-like atoms, where the spin-dependent effect is less important than the electron exchange effect during the excitation process. But recently, many authors [3,4,21] have found that this approximation fails for electron-cesium scattering. From our results on the STU parameters for electron cesium scattering, we conclude that this invalidity is mainly due to the direct relativistic effect of continuum wave functions. It is shown in Fig. 3 that both the magnitude and structure of T parameters calculated by the RDW method are very different from those calculated by the IDW and the ODW methods. In Fig. 4 the $S_p/(-2)$ of the ODW model and $S_p^{3/2}$ of the IDW and the RDW models are shown. By the fine-structure approximation the three kinds of results should be the same. In fact the three kinds of results do not agree very well. When the incident electron energy is 20 eV, the direct and indirect relativistic effect may compete with each other in the scattering process. When the incident electron energy is 100 eV, the RDW results differ greatly from those of the IDW and ODW. It can be inferred that it is the direct relativistic effect which causes such a discrepancy. In other words, because of the direct relativistic effect the fine-structure approximation fails. A similar argument for the U_{XZ} in Fig. 5 gives the same conclusion. The STU parameters for gold are very similar to those for cesium. We do not list them. The fine-structure approximation holds in the calculation of the STU parameters at small angles, but becomes invalid as the angle increases. In other words the exchange scattering is dominant at small angles, whereas the direct scattering is most significant at large angles in the spin-flip scattering amplitude.

In summary, by comparing our results for the Stokes parameters, it can be inferred that at an incident electron energy of 50 eV the direct relativistic effect is more important than the indirect relativistic effect for cesium atoms, whereas the opposite is true for gold atoms. By comparing our results for the STU parameters of electron-cesium scattering with those from the RDW method, it can be deduced that it is the direct relativistic effect that leads to the invalidity of the fine-structure approximation for cesium atoms.

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