Intra-atomic relativistic effects on the spin polarization in low-energy electron scattering from Ca, Sr, Ba, and Yb atoms

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(Received 6 February 1995)

The influence of intratarget relativistic effects on electron spin polarization is studied for low-energy electron scattering from Ca, Sr, Ba, and Yb atoms, for which a low-lying d-wave shape resonance is predicted. The motion of the scattering electron is described by solving the continuous-state Dirac-Fock equations plus a parameter-free correlation-polarization potential. The targets are represented using Dirac-Fock, Cowan's quasirelativistic Hartree-Fock, and nonrelativistic Hartree-Fock wave functions, in which the intra-atomic (also called the indirect) relativistic effects are incorporated in varying degrees. It is shown that the intra-atomic relativistic effects, in particular the spin dependence of the Dirac-Fock one-electron orbitals, create apparent quantitative changes in the spin polarization parameters around the d-wave shape resonances.

PACS number(s): 34.80.Bm, 34.80.Nz

I. INTRODUCTION

In the past few years, there has been growing interest in electron scattering from alkaline-earth-metal atoms [1–8], as evidence of the stable negative ions Ca^-, Sr^-, Ba^-, and Ra^- has been provided by both theories [9] and experiments [10]. Studies of the spin-dependent electron scattering by atoms make it possible to obtain more detailed information about the spin-dependent interactions between the electron and target, and provide more sensitive examination of theoretical approaches. Spin polarization of electrons elastically scattered from alkaline-earth-metal atoms was given by Dzuba *et al.* [3,6], Yuan and Zhang [5], and Kumar *et al.* [8]. The detailed variations of electron spin polarization with collision energies and scattering angles were provided in our previous study [5], and the results show that the spin-orbit interaction is increased considerably around the low-lying shape resonance.

According to Sin Fai Lam and Baylis [11], the relativistic effects in electron scattering by atoms can be described in terms of direct and indirect effects. The direct relativistic effect arises from substituting the Dirac equation for the Schrödinger equation to describe the motion of the projectile electrons in an atomic field, and the indirect relativistic effect from the changes of the target electron density due to relativity and the spin-dependent character of the one-electron orbitals of a full relativistic atomic wave function for bound electrons. The indirect effect is actually the consequence of the intra-atomic relativistic effects in the collisions. Most recently, the R-matrix method for the Breit-Pauli Hamiltonian [12] and the relativistic R-matrix method for one-electron alkali-metal atoms of Thumm and Norcross [13] were applied to the very-low-energy electron collision with the Cs atom, where the author [12] found somewhat surprising discrepancies of the spin polarization parameters between their results [12,13] and suspected that it was due to the Breit-Pauli approach to treat the relativistic effects. In the scheme of Thumm and Norcross [13], the closed core of the target was approximated with a model potential and the spin dependence of the core electron orbitals was not taken into account either. Electron scattering by neutral Hg atoms was studied by Wijesundera, Grant, and Norrington [14] using the Dirac R-matrix method based on the same relativistic Hamiltonian for both bound and continuous electrons, and the authors attributed the changes of their results mainly to the differences in account of the relativistic effects, compared to the earlier calculations of Scott, Burke, and Bartschat [15] and of Bartschat and Burke [16] based on the Breit-Pauli Hamiltonian. In our previous calculation of the spin-dependent collisions with alkaline-earth-metal atoms [5], the direct relativistic effect was treated adequately by using Dirac equation for free electrons, while the method of Cowan and Griffin [17] was used to treat the redistribution of electron density due to relativity by including relativistic correction terms in the nonrelativistic equations and the spin split of the bound electron orbitals was averaged out to give the target wave function in nonrelativistic form. Most recent results show that the intra-atomic relativistic effects, in particular the explicit spin dependence of the bound electron orbitals, can create apparently quantitative changes in spin polarizations of low-energy electron scattering by rare-gas atoms [18]. Therefore, the considerations to the intra-atomic relativistic effects in our previous calculation [5] should be improved to incorporate all the important physics in the calculation of such very sensitive quantities as the electron spin polarizations. The purpose of the present calculation is to study the importance of the intra-atomic relativistic effects, mainly the explicit spin dependence of the full relativistic bound electron orbitals, in the calculations of spin polarizations of low-energy electron scattering from Ca, Sr, Ba, and Yb atoms around the low-lying d-wave shape resonance. The only published result of the Yb atom is due to Dzuba and Gribakin [6]. It is also interesting to compare the results of the Yb atom obtained using different methods. Unless otherwise specified, atomic units are used throughout the paper.

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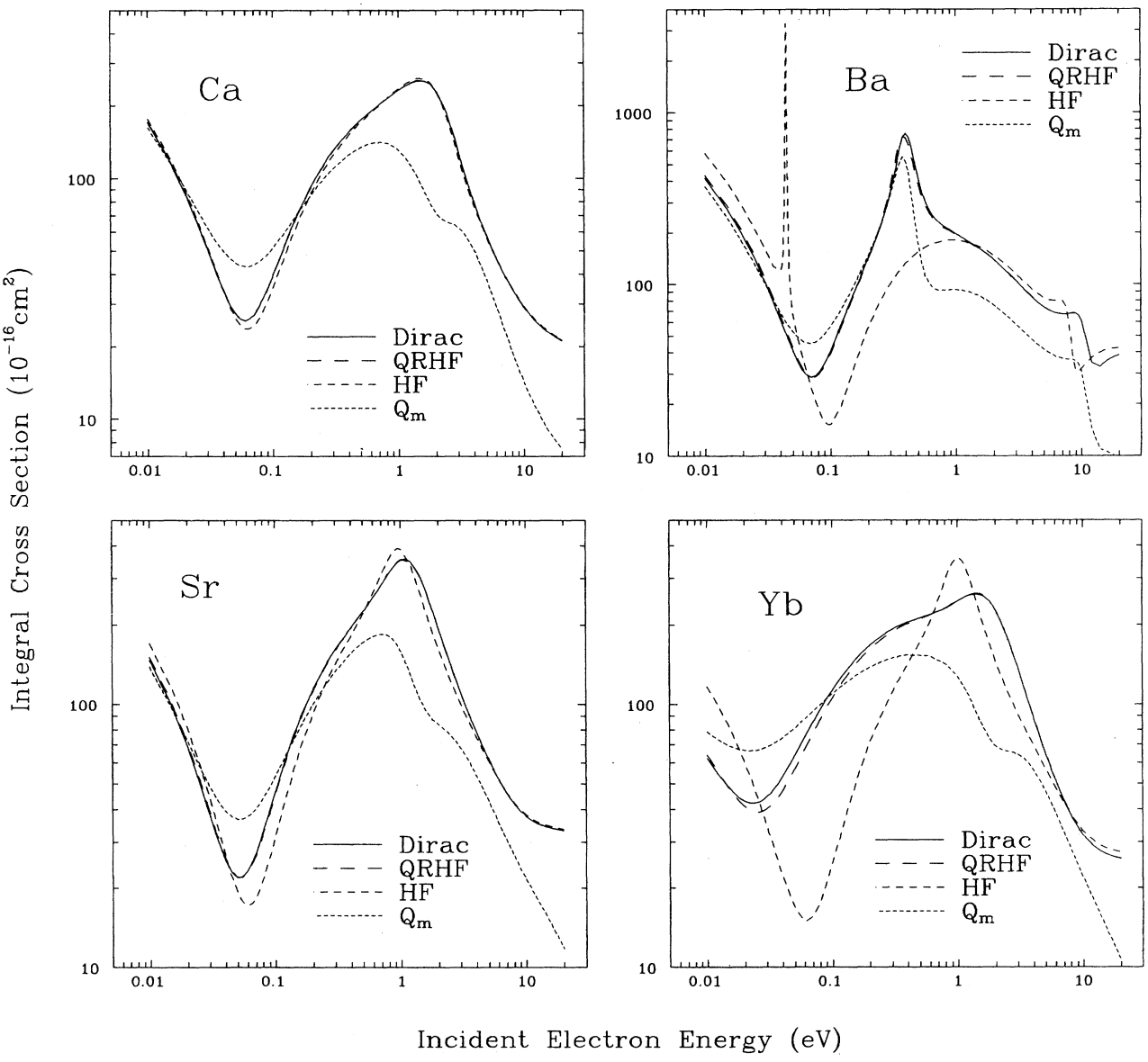

FIG. 1. Integral cross sections of Ca, Sr, Ba, and Yb atoms. Solid lines labeled Dirac are the results of the first set obtained with Dirac-Fock atomic wave functions; the longest dashed lines labeled QRHF are the results of the second set obtained with Cowan's QRHF atomic wave functions (please note that the longest dashed QRHF lines coincide or nearly coincide with the corresponding solid Dirac lines); the middle dashed lines represent the results of set three obtained with Hartree-Fock atomic wave functions; the shortest dashed lines labeled Q_m are the momentum transfer cross sections of the first set. Explanations for the three different sets are given in the text.

II. THEORY

A. Scattering equation

The continuous wave functions of the projectile electrons are described by using the Dirac-Fock equations [19,20]:

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right)P_\kappa(r)=\left\{\frac{2}{\alpha}+\alpha[E-V(r)]\right\}Q_\kappa(r)+X_Q(r) \tag{1}$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right)Q_\kappa(r)=-\alpha[E-V(r)]P_\kappa(r)+X_P(r),$$

where $X_Q(r)$ and $X_P(r)$ are the exchange terms and the detailed forms can be found in Ref. [19] for continuous wave functions and in Ref. [20] for the bound state case. The potential $V(r)$ consists of the static potential and a parameter-free correlation-polarization potential [21] to approximate the distortion and polarization of the target induced by the projectile electron. The equation set (1) is solved by the iterative technique with the asymptotic forms of $P_\kappa(r)$ and $Q_\kappa(r)$ at large r:

$$P_\kappa(r)/r\sim j_l(kr)\cos\delta_l^{\pm}-n_l(kr)\sin\delta_l^{\pm}, \tag{2}$$

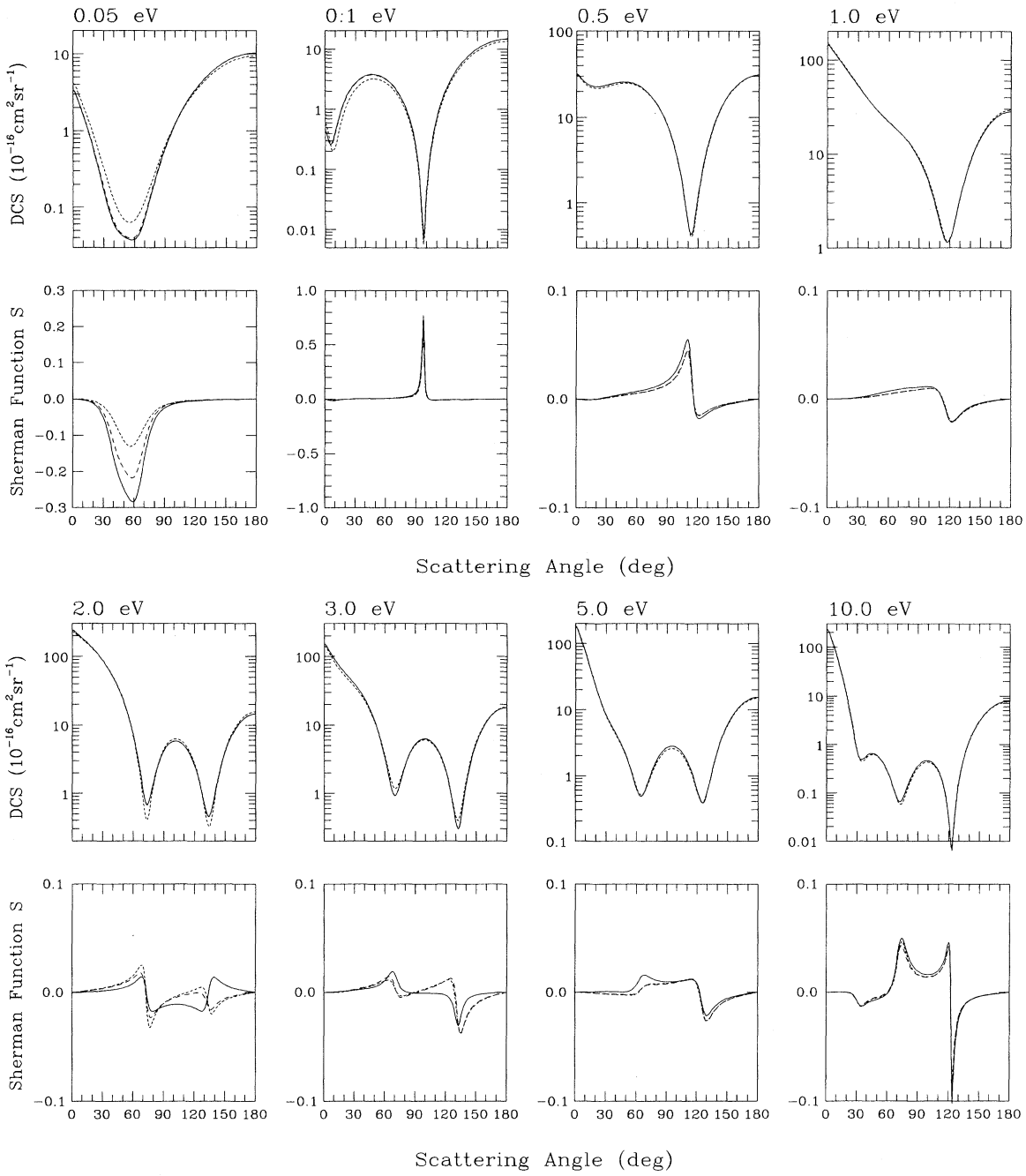

FIG. 2. The DCS and the Sherman function of e-Ca scattering. Solid lines represent the results of the first set; long dashed lines are the results of the second set (please note that in this set DCS lines coincide or nearly coincide with the corresponding first set DCS lines); short dashed lines are results of the last set.

$$Q_\kappa(r)/r \sim \alpha\left(\frac{E}{E\alpha^2+2}\right)^{1/2}[j_{l\pm1}(kr)\cos\delta_l^{\pm}-n_{l\pm1}(kr)\sin\delta_l^{\pm}], \tag{3}$$

where $k=(2E+\alpha^2E^2)^{1/2}$ is the momentum of the incident electron. The phase shifts δ_l^+ and δ_l^- are, respectively, corresponding to the quantum numbers $\kappa=-l-1\,(j=l+1/2)$ and $\kappa=l\,(j=l-1/2)$. In terms of the spin-up and spin-down phase shifts, the expressions of the direct and spin-flip scattering amplitudes are

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

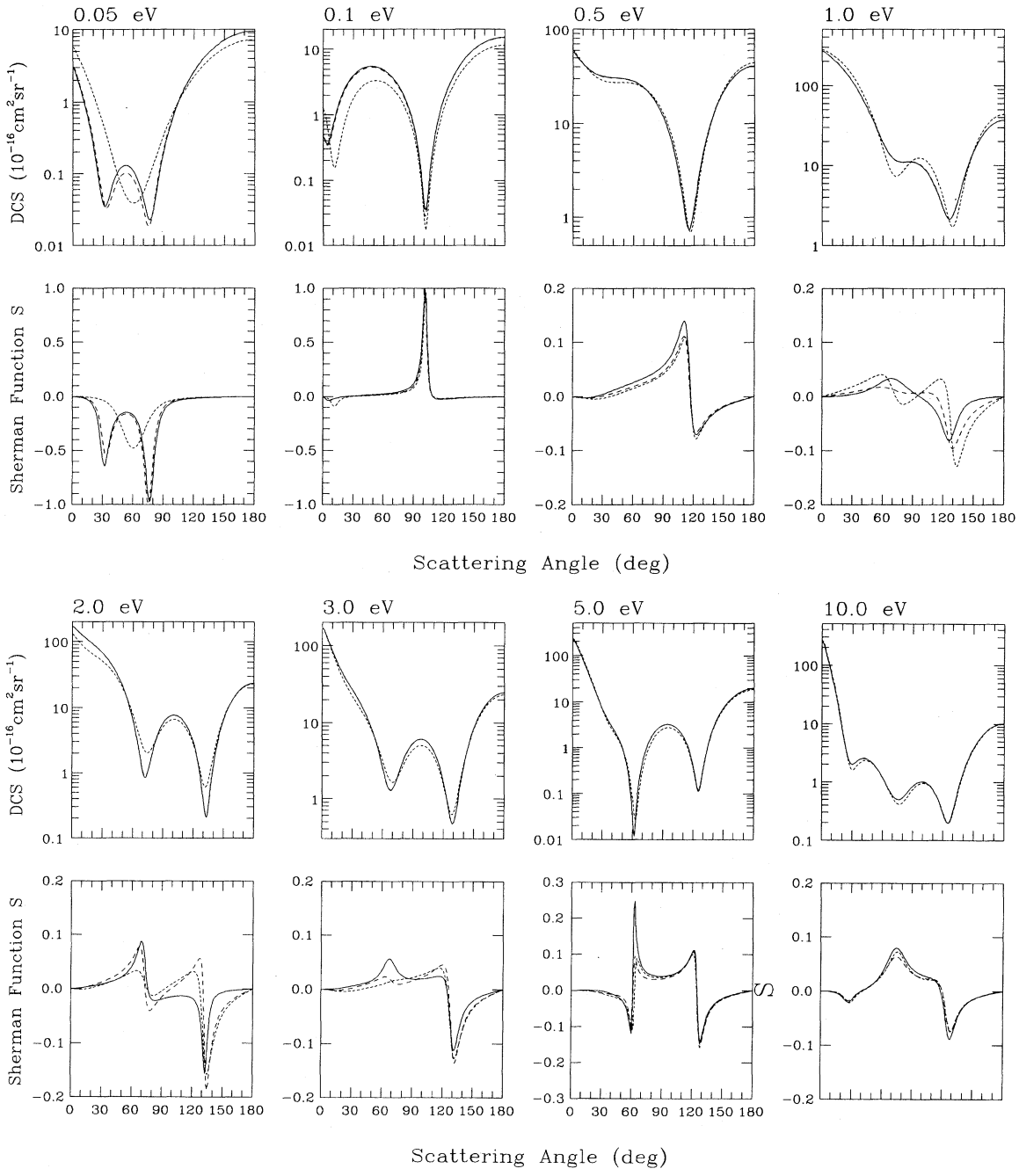

FIG. 3. As in Fig. 2 but for e-Sr scattering (please note that the DCS lines of the first two sets coincide or nearly coincide with each other).

$$g(\theta)=\frac{1}{2ik}\sum_l [\exp(2i\delta_l^-)-\exp(2i\delta_l^+)]P_l^1(\cos\theta), \quad (5)$$

where $P_l(\cos\theta)$ and $P_l^1(\cos\theta)$ are the Legendre polynomial and the Legendre associated functions, respectively. The differential cross section of the unpolarized electron scattering $\sigma_u(\theta)$ and the spin polarization parameter S have the forms [22]

$$\sigma_u(\theta)=|f|^2+|g|^2, \qquad S(\theta)=i\frac{fg^*-f^*g}{|f|^2+|g|^2}. \quad (6)$$

The Sherman function S describes the spin polarization of the scattered electrons if the incident electron beam is unpolarized.

B. Atomic wave function

In order to study the importance of the intra-atomic relativistic effects, three different kinds of atomic wave functions are used in Eq. (1) to generate three corresponding sets of results: in the first set, Dirac-Fock atomic wave functions

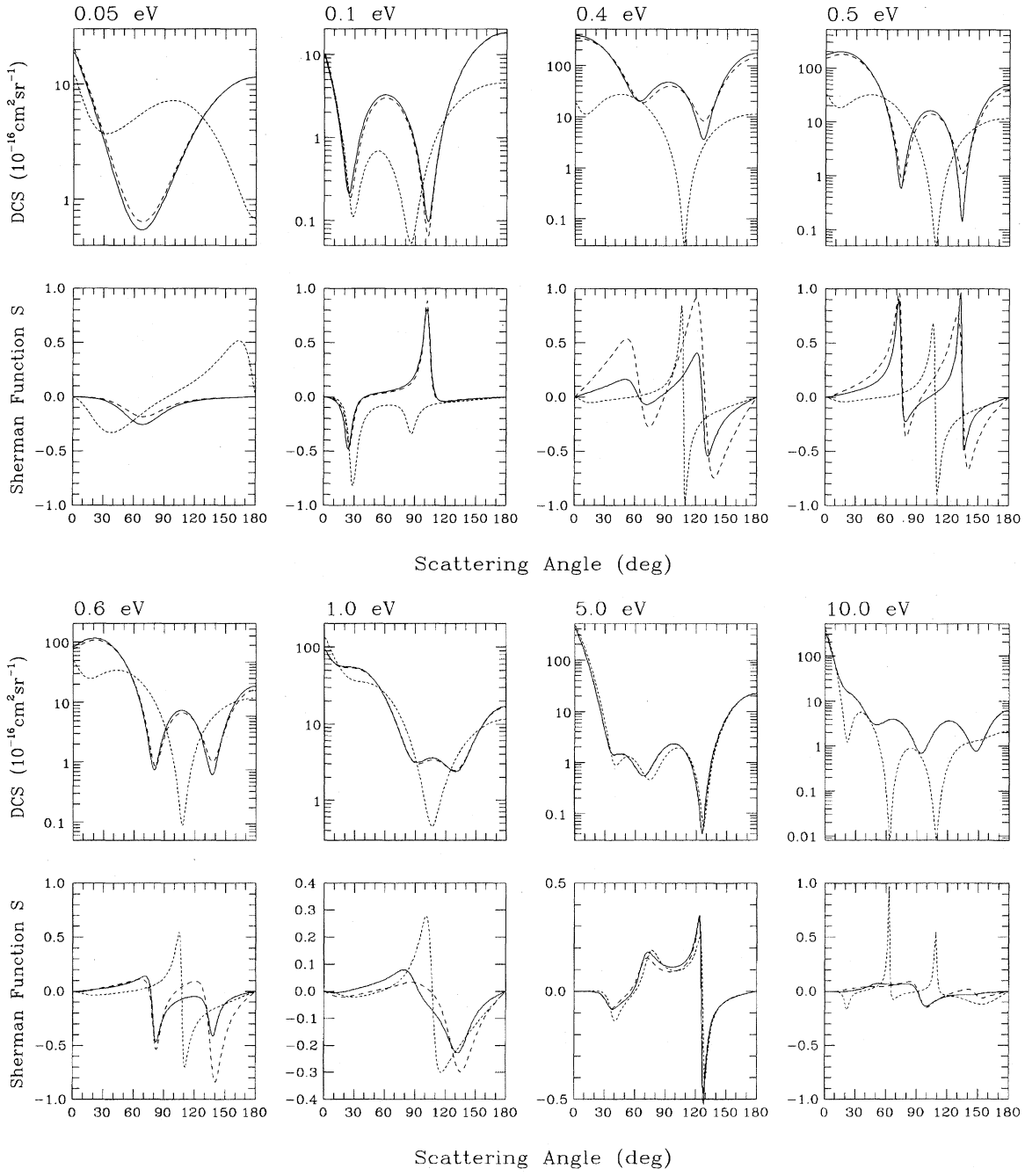

FIG. 4. As in Fig. 2 but for e-Ba scattering.

obtained by using the MCDF computer program of Grant *et al.* [20] are applied to the description of the bound electrons; in the second set, Cowan's quasirelativistic Hartree-Fock (QRHF) atomic wave functions [17] are used for bound electrons; and the Hartree-Fock atomic wave functions are employed for bound electrons in the last set.

The direct relativistic effect is considered equally by using Eq. (1) for the continuous electron in all three sets of results, but the intra-atomic relativistic effects are considered in varying degrees. In the first set, the changes of the electronic charge distribution of the target due to relativity as well as the spin-dependent character of the one-electron orbitals are taken into account by using the Dirac-Fock atomic wave function. In the second set, the QRHF atomic wave functions are applied to the calculations of the potential $V(r)$ and the exchange terms. So the intra-atomic relativistic effects are considered partly for the electronic density changes and the spin split of the bound one-electron orbitals was neglected. In the last set, the intra-atomic relativistic effect is completely neglected by using a nonrelativistic Hartree-Fock wave function in the calculations of the potential $V(r)$ and the exchange terms.

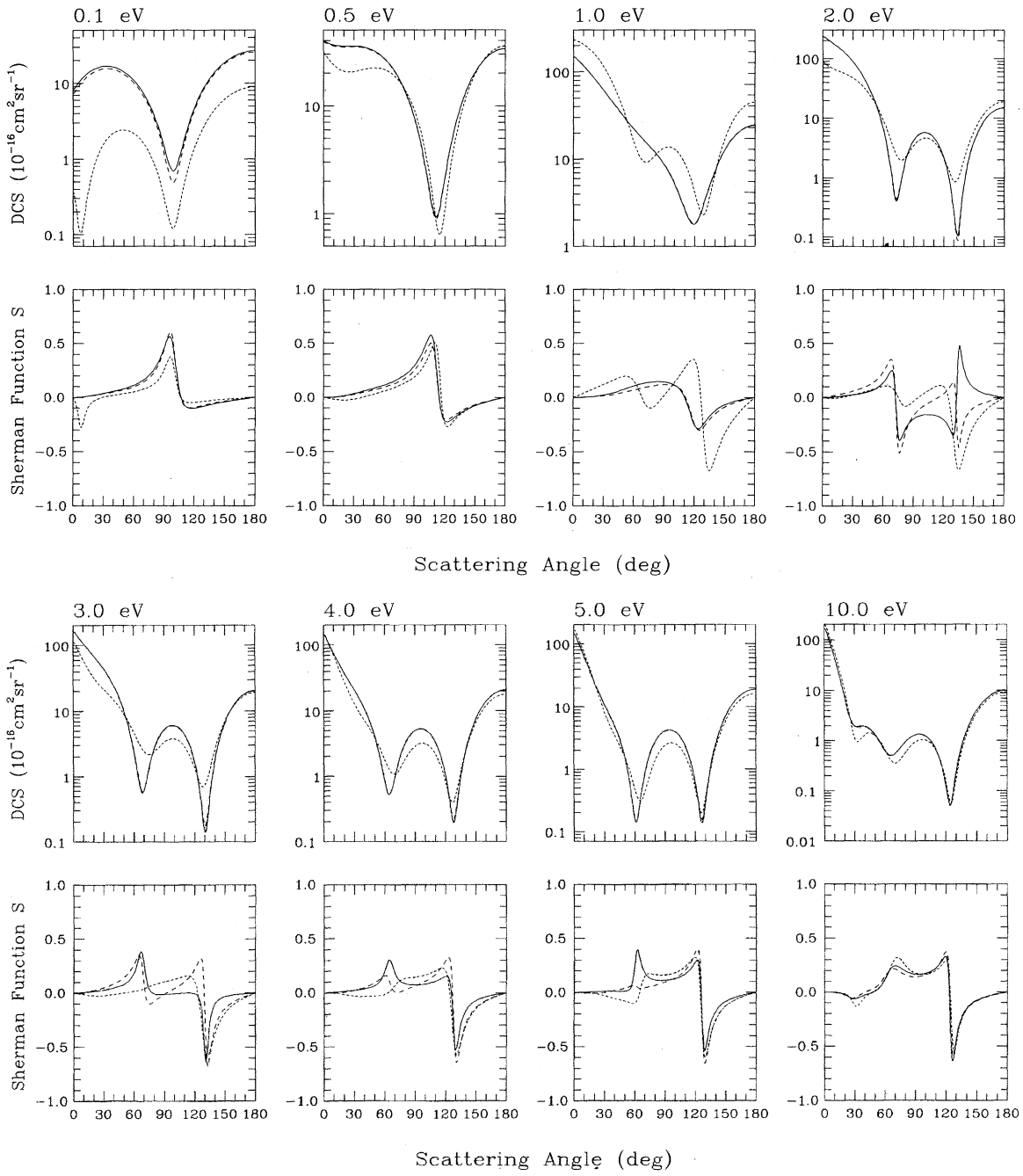

FIG. 5. As in Fig. 2 but for e-Yb scattering.

It is worthwhile to mention that the same exact nonlocal exchange formula in relativistic form is employed in all three sets of calculations. When QRHF and nonrelativistic Hartree-Fock bound electron orbitals are employed in the calculations of the exchange terms, the small component of the bound electron orbitals contained in the exchange formula is set to be zero and the spin split of the bound electron orbitals is also neglected. Calculations using the Dirac-Fock atomic wave functions with and without the small component in the exchange terms are also compared, but the difference is negligible. Therefore, the same Eq. (1) and the same expressions of the static potential, correlation-polarization potential, and exchange terms are used in all the present calculations. The differences between the different models are originally from the bound electron orbitals, which are different only in the inclusion of the relativistic effects.

III. RESULTS AND DISCUSSION

A. Integral elastic cross sections

In recent years, there have been a few calculations about the low-energy electron collisions with Ca, Sr, Ba, and Yb

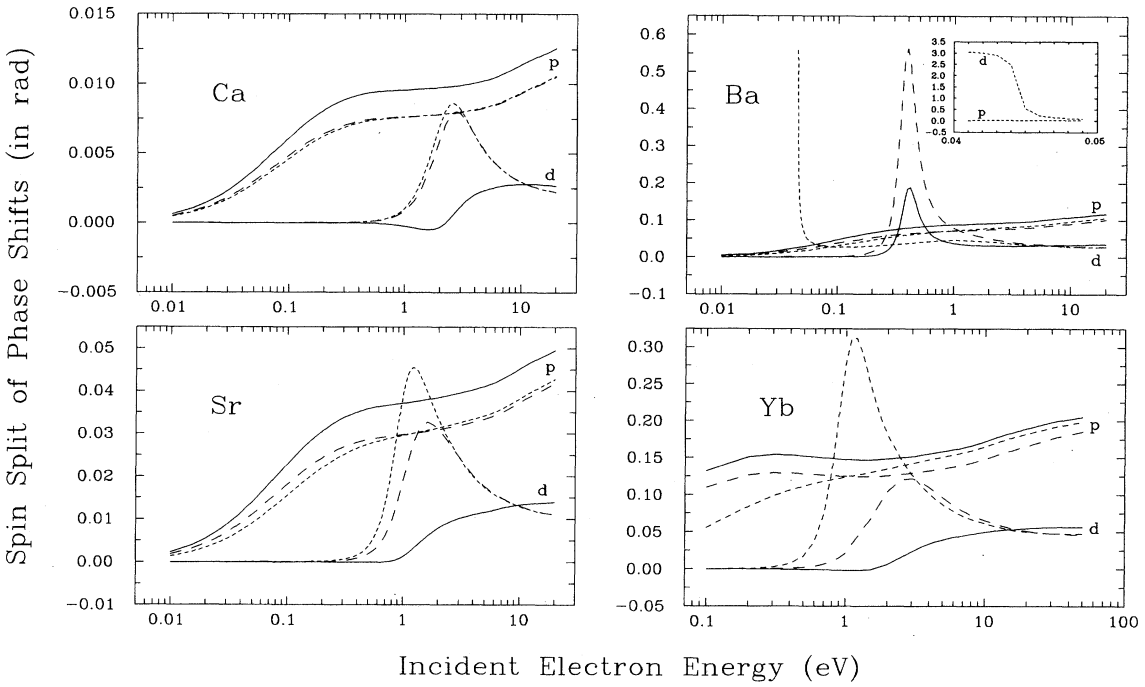

FIG. 6. The spin splits of the phase shifts of p and d waves. The meaning of the lines is the same as in Fig. 2.

atoms using varieties of methods [1–7]. The calculation for the Yb atom was given in the most recent article of Dzuba and Gribakin [6]. The general features of the reported results are a low-lying d-wave shape resonance and a bound p-wave negative ion orbital. In the results of Dzuba and Gribakin [6], a bound d-wave negative ion orbital of Ba and a p-wave shape resonance near zero energy of Yb were predicted, but other evidence for their predictions is absent.

In Fig. 1, three sets of the present integral cross sections, as defined in Sec. II B, are plotted and labeled Dirac, QRHF, and HF, respectively. In the results of Gribakin *et al.* [4], momentum transfer cross sections were reported. In order to make a comparison, the momentum transfer cross sections of the present first set results labeled Q_m are also shown in this figure. The qualitative shapes of the curves of Ca, Sr, and Ba atoms are the same as other theories [4,7], but serious quantitative differences among all the reported results exist in both the values of the cross sections and positions of the low-lying shape resonances. The present predication for the position of the d-wave shape resonance of the Yb atom is congruent with the result of Dzuba and Gribakin [6], but the $p_{3/2}$ shape resonance peak predicted by them near zero energy is moved into the bound state by the present calculation. The general behavior of the present cross section of the Yb atom towards zero energy is different from theirs. The importance of the intra-atomic relativistic effects with the increase of the nuclear charge can be seen by identifying the discrepancies between the corresponding curves of the first and third sets. The discrepancies of the HF curves from the corresponding Dirac and QRHF curves increase rapidly from Ca to Yb atoms. On the whole, the influence of the intra-atomic relativistic effects is to reduce the strength of the interaction between the projectile and the target. In particular, when the HF wave function is applied to bound electrons, the $d_{3/2}$ state of Ba is moved into the negative energy and the $d_{5/2}$ state displays a very sharp resonance between 0.04 eV and 0.05 eV. Note here that the plotted Dirac and QRHF curves coincide with each other for Ca, Sr, and Ba atoms, and show only slight discrepancies below 0.5 eV for the Yb atom. So the QRHF atomic wave function is efficient to treat the influence of the intra-atomic relativistic effects on integral cross sections from intermediate to heavy atoms.

B. Differential cross section and electron spin polarizations

The spin polarizations of electron collisions with alkaline-earth-metal atoms were studied by Yuan and Zhang [5,23] and by Dzuba *et al.* [3,6]. We focus our discussion on electron spin polarizations, as the intra-atomic relativistic effects will produce pronounced changes in the spin polarizations around the d-wave shape resonant energies. From the results of the integral cross sections, it could be concluded that the electronic charge redistribution of the targets due to relativity can be treated effectively by Cowan's quasirelativistic scheme. The major difference between the QRHF and Dirac-Fock atomic wave functions is the explicit spin dependence of the one-electron orbitals of Dirac-Fock theory, and one will see that this diversity will create considerably quantitative or even qualitative changes in the electron spin polarizations. Parallel to the above discussions of the integral cross sections, three sets of data are presented in this subsection for differential cross section (DCS) and electron spin polarization parameter S.

In Fig. 2 absolute DCS and the spin polarization parameter S of e-Ca scattering are presented at a few selected energies. The DCS curves of the first and second sets cannot be distinguished from each other except near the minimum value at 0.05 eV, and have a very small difference from the

curve of the third set. The relativistic effects are generally small for the Ca atom because of the small nuclear charge. Except in the Ramsauer-Townsend (RT) region (below 0.1 eV) the degree of spin polarization is very low. The increase of the degree of spin polarization around the RT minimum point has been already pointed out in our previous paper [5], but Cowan's QRHF wave functions were used there for atomic electrons. From 0.5 eV to 5 eV the magnitude of the Sherman function is very small, but the changes due to the spin split of the Dirac-Fock one-electon orbitals appear apparently. It is interesting to note that the S parameter curves of the second and third sets come close to each other and show apparent distinctions from the corresponding one of the first set, although the DCS curves show the contrary agreement. The effect of the Dirac-Fock orbitals on the S parameter can also be seen at 0.05 eV, where the first curve shows a considerably quantitative difference from the second one. At 10 eV, the intra-atomic relativistic effects have relatively small influences on the spin polarization, and the general shape of the S curves is determined by the direct relativistic effect.

In Fig. 3 the DCS and the S parameter are plotted for the Sr atom. High degree spin polarizations are also produced in the RT region. The relativistic effects for the Sr atom are much stronger than those for the Ca atom as the larger nuclear charge. Except at 0.05 and 0.1 eV, DCS curves of the first and second sets cannot be distinguished either, but the corresponding third DCS curve shows more apparent quantitative or even qualitative differences. It is clearer that the changes of the DCS are mainly due to the charge redistribution and treated adequately in Cowan's quasirelativistic scheme. At 1.0, 2.0, and 3.0 eV, the S parameter curves of all three sets show substantial disparity from each other. The neglect of intra-atomic relativistic effects in the Hartree-Fock bound electron wave functions causes larger changes in the DCS's, and in turn larger changes in the S parameters. The Dirac-Fock orbitals cause the changes of the S parameters between the first and second sets of data, which are considerable from 1.0 eV to 3.0 eV. At 5.0 and 10.0 eV the general shape of the curves is determined by the direct relativistic effect.

In Fig. 4 the DCS and the S parameter of electron collision with Ba atoms are presented. It has been shown in the integral cross sections that the neglect of the intra-atomic relativistic effects causes drastic changes in the low-lying shape resonance structures with the $d_{3/2}$ state being moved into the bound states. Therefore, the general features of the angular dependences of DCS and S parameter of the third set data are completely different from those of the first and second ones at the plotted energies except 5.0 eV. Around the d-wave shape resonance peak, the differences between the DCS curves of the first and second sets are apparent only near the minimum points, but the corresponding changes in the S parameter are very large over quite wide scattering angles from 0.4 eV to 1.0 eV. The degree of spin polarization at 0.4 eV is reduced significantly in the first set of data. This reduction can be understood from the spin split of the phase shift (see below). The increase of the d-wave phase shift spin split around the d-wave shape resonances is weakened substantially when Dirac-Fock orbitals are used. In Fig. 1, the integral cross section curves of Ba have a shoulder and a minimum point between 5 eV and 20 eV, but the positions of these structures of the HF curves are quite different from those of the Dirac and QRHF curves. It could be understood that the DCS and S parameter of the third set have quite large discrepancies from the corresponding curves of the first and second sets in this energy region. As an example, the energies and angles, where a very deep DCS minimum structure occurs with a high degree of spin polarizations, would be quite different for these different sets of results. These structures are produced at 10 eV in the third set of results.

In Fig. 5 the DCS and S parameter of electron scattering from Yb atoms are plotted at a few selected energies. The general shapes of the DCS and S parameter of Yb atom below 0.5 eV are similar for the three curves. Large discrepancies among the S parameters of all the three sets begin from 1.0 eV up to 5 eV. It is worthwhile to point out again that the pronounced differences between the S parameters of the first and second sets of data are mainly due to the spin split of the Dirac-Fock bound electron orbitals, and that only small corresponding changes in DCS around minimum points are produced by this factor. The spin polarization of the electron collision with the Yb atom was provided by Dzuba and Gribakin [6] only at 0.19 eV. The present data at 0.1 and 0.5 eV are in qualitative agreement with the results of Dzuba and Gribakin.

The results presented in this section indicate that the spin dependence of the Dirac-Fock one-electron orbitals is much more essential for the electron spin polarization during collision processes than for the integral as well as differential cross sections, and that only consideration to the charge density changes in Cowan's QRHF wave functions and other similar quasirelativistic theories is not enough to take the influences of the intra-atomic relativistic effect on these quantities into account. This is also applied to the model potentials in which the explicit spin-dependent character of the bound electron orbitals is not incorporated adequately. Studies of electron spin polarizations could provide not only the stringent examination about the treatment of the direct relativistic effect but also a close test about the consideration of the intra-atomic relativistic effects.

C. The spin split of the phase shifts

The energy dependences of the spin splits of the phase shifts $\Delta\delta_l = \delta_l^- - \delta_l^+$ of p and d waves are plotted in Fig. 6. Three set results mentioned above are included in this figure to display the importance of the spin dependence of the relativistic one-electron orbitals from a different point of view. The general energy dependence of the p-wave $\Delta\delta_l$ is determined by the direct effect and the three curves have similar behavior, but considerably quantitative differences are caused at the energies above 0.1 eV by the intra-atomic effect, particularly by the spin-dependent character of the Dirac-Fock one-electron orbitals. It is obvious that the divergence of the curves of the first set from the corresponding curves of the second and the third sets of Ca and Sr atoms is almost completely induced by the spin dependence of the Dirac-Fock orbitals, as it is the common factor of the second and third sets of data different from the first one. The d-wave $\Delta\delta_l$ around the d-wave shape resonance energies is enhanced in the second and third sets of results for all the

plotted atoms resulting from the increase of the spin-orbit interactions of the d-wave electrons around the d-wave shape resonances, but the action of the Dirac-Fock bound electron orbitals is to cancel the increase of the d-wave spin split of the phase shift induced by the spin-orbit interaction almost completely except for Ba atoms, for which the width of the shape resonance is the smallest one and the increased spin-orbit interaction is much stronger than any other atoms.

In conclusion, the Dirac-Fock, Cowan's QRHF, and the nonrelativistic Hartree-Fock atomic wave functions are chosen to make comparison calculations to study the importance of the intra-atomic relativistic effects including both the charge distribution changes due to relativity and the explicit spin dependence of the relativistic bound electron orbitals in the calculations of low-energy spin-dependent electron collisions with atoms. The results show that considerations of the explict spin-dependent character of the bound electron orbitals in a formalism are essential to the calculation of electron spin polarization. The conclusion can also be applied to the various model potentials, but one would be reminded that it is derived from the calculations of low-lying d-wave shape resonance scattering from closed shell atoms, and that studies for other type collisions are also needed. The trend of the cross section of Yb atoms towards zero energy is predicted differently from the previous result, and further studies on very-low-energy collisions are expected with more accurate methods.

ACKNOWLEDGMENTS

The author would like to thank Professor Qiren Zhou of Jilin University for valuable help in using the MCDF computer program. This work was supported by the National Natural Science Foundation of China under Grant No. 19374019 and by the Chinese Research Association of Atomic and Molecular Data.

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