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Polarization and exchange effects in elastic scattering of electron with atoms and ions*

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Laser-induced electron diffraction (LIED), in which elastic scattering of the returning electron with the parent ion takes place, has been used to extract atomic potential and image molecular structures with sub-Å precision and exposure time of a few femtoseconds. So far, the polarization and exchange effects have not been taken into account in the theoretical calculation of differential cross section (DCS) for the laser-induced rescattering processes. However, the validity of this theoretical treatment has never been verified. In this work, we investigate the polarization and exchange effects on electron impact elastic scattering with rare gas atoms and ions. It is found that, while the exchange effect generally plays a more important role than the polarization effect in the elastic scattering process, the exchange effect is less important on electron–ion collisions than on electron–atom collisions, especially for scattering in backward direction. In addition, our calculations show that, for electron–atom collisions at incident energies above 50 eV, both the polarization and exchange effects can be safely neglected, while for electron–ion collisions, both the polarization and exchange potentials do not make substantial contributions to the DCS at incident energies above 20 eV and scattering angles larger than 90°. Our investigation confirms the validity of the current LIED method.

Keywords: polarization, exchange, elastic scattering, differential cross sections

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1. Introduction

Collisions of electrons with atoms and ions are the basic physical processes that provide a unique diagnostic probe of the fundamental interactions in many-electron systems. While elastic scattering of electrons from neutral atoms has been extensively studied both experimentally and theoretically, experimental difficulties have limited the investigations on elastic scattering of electrons from ions. So far, measurements of cross sections for electron elastic scattering in free-electron ion collisions have been scarce. However, in recent years, there has been a large amount of experimental data available for differential cross section (DCS) of elastic scattering of electrons with singly charged atomic ions[1–5] as well as molecular ions.[6] These experimental DCSs were extracted from the measured two-dimensional (2D) momentum distributions for high energy photoelectrons in high-order above threshold ionization (HATI) based on the quantitative rescattering (QRS) model (see Ref. [7] and references therein).

The main philosophy of the QRS model is that the yields of laser-induced rescattering processes, which comprise elastic scattering, excitation, ionization, and recombination of the returning electron with the parent ion, can be expressed as a product of the returning electron wave packet (RWP) with various field-free electron–ion scattering cross sections. Among all the laser-induced rescattering processes, HATI is the simplest one in which the electron–ion elastic collision takes place. According to the QRS model, the 2D momentum distributions for high energy photoelectrons in HATI can be factorized as the RWP and the laser-free electron–ion elastic scattering DCS. It has been well documented that the RWP which can be evaluated from the second-order strong field approximation[8] depends only on the laser parameters. Owing to this property of the RWP, one is able to remove the laser's influence and thus obtains the electron–ion elastic collision DCSs at large scattering angles from 100° to 180° and in a wide range of incident energy from the experimentally measured laser-induced electron diffraction (LIED) momentum distributions.

LIED has attracted wide interests in strong laser physics since it was first proposed to serve as a new tool to probe ultrafast molecular dynamics by Zuo *et al.*[9] two decades ago. It has been demonstrated that LIED can be used to extract the atomic potential[10] and to probe the detailed information about the electronic orbital and the position of the nuclei in molecules.[11] Furthermore, LIED has also been applied to molecular imaging with sub Å precision and exposure time of a few femtoseconds.[6] To our knowledge, in the theoretical treatment of LIED, the polarization and exchange effects have never been taken into account in the DCS calculations for electron–ion elastic scattering. However, since the incident electron influences the charge distribution of the target, an electric dipole is induced in the target during the collision,

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and the magnitude of the induced dipole depends on the polarizability. In the meantime, the scattering electron can potentially exchange with any of the bound electrons in the target. It has been well recognized that the effects of the charge cloud polarization in the target and exchange of the scattering electrons with the bound electrons are important in electron scattering from atoms, ions, and molecules, especially for low collision energies.

According to the semiclassical rescattering model,[12,13] in the LIED, one of the bound electrons that is first tunnel ionized near the peak of the laser's oscillating electric field is subsequently driven by the laser field and has the chance to return back to the parent ion when the field changes direction, and then serves as an incident electron colliding with the parent ion. The maximum kinetic energy that a returning electron can gain from the field is $3.17U_{\rm p}$, where $U_{\rm p}$ is the electron ponderomotive energy, which is proportional to the laser intensity. For a typical laser pulse with a wavelength of 800 nm and a peak intensity of 1.0×10^{14} W/cm^2, $U_{\rm p}=6$ eV, and hence the incident energy of the returning electron is less than 20 eV.

In this paper, we examine the energy dependence of the polarization and exchange effects in elastic scattering of electron with atoms and ions. The goal of the present work is to verify the validity of the current theoretical treatment of electron–ion elastic scattering in LIED.

Atomic units $m_{\rm e}=\hbar=e=1$ are used throughout the paper unless otherwise indicated.

2. Scattering potential

We consider elastic scattering of electrons with Ne and Ar atoms as well as Ar^+ ion, and employ the standard potential scattering theory to evaluate the elastic scattering DCSs. The details of the standard potential scattering theory have been presented in our previous paper.[14] Here only the scattering potentials used in the numerical calculations are given.

The static potential $V_{\rm s}(r)$ of the target atom (ion), obtained by averaging over the motion of the target electrons, is given by

$$V_{\rm s}(r) = -\frac{Z}{r}+\sum_{i=1}^{N}\int|\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)|^2 \times\frac{1}{|\boldsymbol{r}-\boldsymbol{r}_i|}\,{\rm d}\boldsymbol{r}_1\,{\rm d}\boldsymbol{r}_2\cdots{\rm d}\boldsymbol{r}_N, \tag{1}$$

where Z is the nuclear charge of the target, $\boldsymbol{r}$ and $\boldsymbol{r}_i$ $(i=1,2,\ldots,N)$ are the position vectors of the projectile and the bound state electrons with respect to the nucleus, and N is the total number of bound electrons in the target. For the cases considered in the present work, $N=Z$ for neutral atoms and $N=Z-1$ for singly charged ions. $\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)$ is the antisymmetrized Hartree–Fock wave function of the target, which is expressed in terms of the Slater-type orbitals

$$\Phi_{nl}(\boldsymbol{r})=R_{nl}(r)Y_{lm}(\hat{\boldsymbol{r}}), \tag{2}$$

where $Y_{lm}(\hat{\boldsymbol{r}})$ are the spherical harmonics and R_{nl} is the radial wave function given by

$$R_{nl}(r)=\sum_{i=1}^{M_{nl}}c_i\frac{1}{\sqrt{(2n_i)!}}(2\xi_i)^{n_i+1/2}r^{n_i-1}\,{\rm e}^{-\xi_i r}. \tag{3}$$

The parameters c_i, n_i, ξ_i, and M_{nl} for each of the orbitals are given by Clementi and Roetti.[15]

The effect of polarization on the projectile can be modeled by adding a polarization potential to the static potential. Here we take the polarization potential to be of the Buckingham type[16]

$$V_{\rm p}(r)=-\frac{\alpha r^2}{2(r^2+d^2)^3}, \tag{4}$$

where α is the static dipole polarizability which is taken to be 2.68 for Ne,[17] 11.10 for Ar,[18] and 6.85 for Ar^+.[19] The parameter d is energy dependent which is determined by fitting the calculated cross sections for elastic scattering of electrons with the corresponding experimental measurements. For elastic scattering of electrons by Ar, the values of the parameter d for various incident energies are given in Ref. [16].

The polarization potential given in Eq. (4) is a local approximation to represent the non-local effect of polarization. Similarly, to take into account the exchange of the projectile with the bound electron, the non-local exchange potential is often replaced by a local approximation, too. This is mainly due to the difficulties involved in obtaining solutions to the integro-differential equation for the continuum electron wavefunction in the Hartree–Fock approximation.[20] Based on the semiclassical exchange approximation, Riley and Truhlar[21,22] proposed a local exchange (LE) potential, which takes the form

$$V_{\rm ex}(r)=\frac{1}{2}\left[(E-V_{\rm d})-\sqrt{(E-V_{\rm d})^2-(-)^S2\beta\rho(r)}\right], \tag{5}$$

where E is the incident energy of the projectile, $V_{\rm d}$ is the direct interaction potential, namely, $V_{\rm d}=V_{\rm s}+V_{\rm p}$, S is the total spin of the projectile electron and one of the bound electrons in the target with which the projectile electron exchanges, and ρ is the radial charge density of the N-electrons, which is given by

$$\rho(r)=\sum_{n=1}^{N_0}\sum_{l=0}^{n-1}N_{nl}|R_{nl}(r)|^2. \tag{6}$$

Here N_0 is the number of occupied shells in the target and N_{nl} is the number of electrons in the orbital (n,l).

In Eq. (5), the parameter β depends on the target, and so does the total spin S of the two exchanging electrons. For rare gas atoms, the total spin of the ground state is zero. When exchange between the projectile electron and one of the atomic electrons takes place, the spin of the rare gas atoms remains

singlet. Therefore, the projectile electron can only exchange with an identical spin atomic electron. As a result, the total spin of the two exchanging electrons would be triplet, i.e., $S = 1$. Furthermore, it should be noted that only half the atomic electrons will have spins identical to the projectile, indicating that the atomic density which is used should correspond to half the density for the full atom. Therefore, β is set equal to 1/2.

While the exchange potential for rare gas atoms can be determined with no ambiguity, the choice of the exchange potential for ions is somehow arbitrary. Firstly, there exists an ambiguity in the total spin of the two exchanging electrons. Although the total spin for the exchange of the projectile electron with one of the closed shell electrons in the target ion remains triplet, it is not clear if the projectile electron exchanges with an open shell electron, since in this case the total spin could be either triplet or singlet. Secondly, there are many different ways to construct the exchange potential. In this paper, we employ three different models for the local exchange potential which have been proposed originally for the exchange of the ejected electron with a bound electron in the residual ion in the process of electron impact ionization of Ar,[20] equivalent to the exchange of the projectile electron in elastic scattering by Ar^+. The first model for the exchange potential for elastic scattering from an open shell ion is taken to be the same as that for elastic scattering from a closed shell atom, as given by Eq. (5). Since only triplet spin is involved in this local exchange potential, we label the first model as LET. However, it is intuitively more reasonable to treat the exchange of the projectile electron with one of the bound electrons in the closed shell and the open shell separately. Therefore, a combination of triplet and singlet potentials should be used. In the second model, the local exchange potential is expressed as a sum of a triplet potential accounting for the exchange between the projectile electron and the bound electron in a closed shell, which comprises the inert core and four of the 3p electrons, plus a singlet potential for the exchange of the projectile electron with the remaining 3p electron. This model is referred to as LE1 since only one of the five 3p electrons is regarded as the open shell. The LE1 model can be expressed as

$$V_{\rm ex}(r) = \frac{1}{2}\left[(E-V_{\rm d}) - \sqrt{(E-V_{\rm d})^2 - (-)^{S_1} 2\beta_1\rho_1(r)}\right] + \frac{1}{2}\left[(E-V_{\rm d}) - \sqrt{(E-V_{\rm d})^2 - (-)^{S_2} 2\beta_2\rho_2(r)}\right], \tag{7}$$

where $S_1 = 1$, $\beta_1 = 1/2$, $S_2 = 0$, and $\beta_2 = 1$. ρ_1 and ρ_2 represent the radial charge densities of $N-1$ electrons in the closed shell and one 3p electron in the open shell, respectively. Nevertheless, there is no guarantee that any arbitrary four p-electrons will necessarily form a singlet state. This implies that there exists an ambiguity in classifying the closed shell and the open shell in Ar^+. In the third model, only the inert core is treated as closed and all five 3p electrons are regarded as open. This model is referred to as LE5 and it takes the same form as LE1 except that ρ_1 and ρ_2 in Eq. (7) are the radial charge densities of the inert core and five 3p electrons, respectively.

3. Results and discussion

We have performed theoretical calculations of the DCSs for elastic scattering of electrons by Ne and Ar atoms as well as Ar^+ ion. We aim to investigate the energy dependence of the polarization and exchange effects on elastic scattering of electron with atoms and ions. Although the theoretical model employed in this paper is the same as that used by Nahar and Wadehra,[16] the separate quantitative contributions to the DCSs from the polarization and exchange potentials were not presented in Ref. [16]. Here, to demonstrate the effects of the charge cloud polarization in the target and exchange of the projectile electron with the bound electron, the DCSs by using the static potential only ("s"), the static potential plus local polarization potential ("sp"), the static potential plus local exchange potential ("se"), and the static potential with both local polarization and exchange potentials ("spe") are calculated separately. It should be noted that in the "se" calculations, $V_{\rm d}$ in Eq. (5) is replaced by $V_{\rm s}$ to exclude the effect of polarization.

In Fig. 1, we present the calculated DCSs for elastic scattering of electrons by Ne at incident energies of 5 eV, 10 eV, 20 eV, 50 eV, 70 eV, and 100 eV respectively, which are compared with the corresponding experimental measurements.[23–26] The values of the parameter d used in the local polarization potential, Eq. (4), for the incident energies considered here are given in Table 1. First of all, it is surprising to see from Figs. 1(a)–1(c) that while the calculated DCSs for scattering from the static potential only deviate substantially from experiment for incident energies of 5 eV, 10 eV, and 20 eV, very good agreement between the theoretical results and the experimental data is achieved when both the polarization and exchange potentials are included. It can also be seen that by taking into account the exchange effect, both the absolute magnitude and the angular distribution of the DCSs observed in experiment at large scattering angles are well reproduced. On the other hand, both the magnitude and the minimum in the DCSs predicted by the "sp" calculations are quite different from the experiment. This clearly indicates that the exchange potential plays a more significant role in the elastic scattering than the polarization potential.

The polarization and exchange effects are expected to decrease with the increase of energy, as demonstrated in Figs. 1(d)–1(f) for incident energies above 50 eV. Again, the "spe" results and the experimental data are on top of each

other. Nevertheless, compared with the experiment, the calculations of "sp", "se", and even "s" can be regarded as satisfactory at least for scattering angles larger than 60° with the experimental error taken into account.

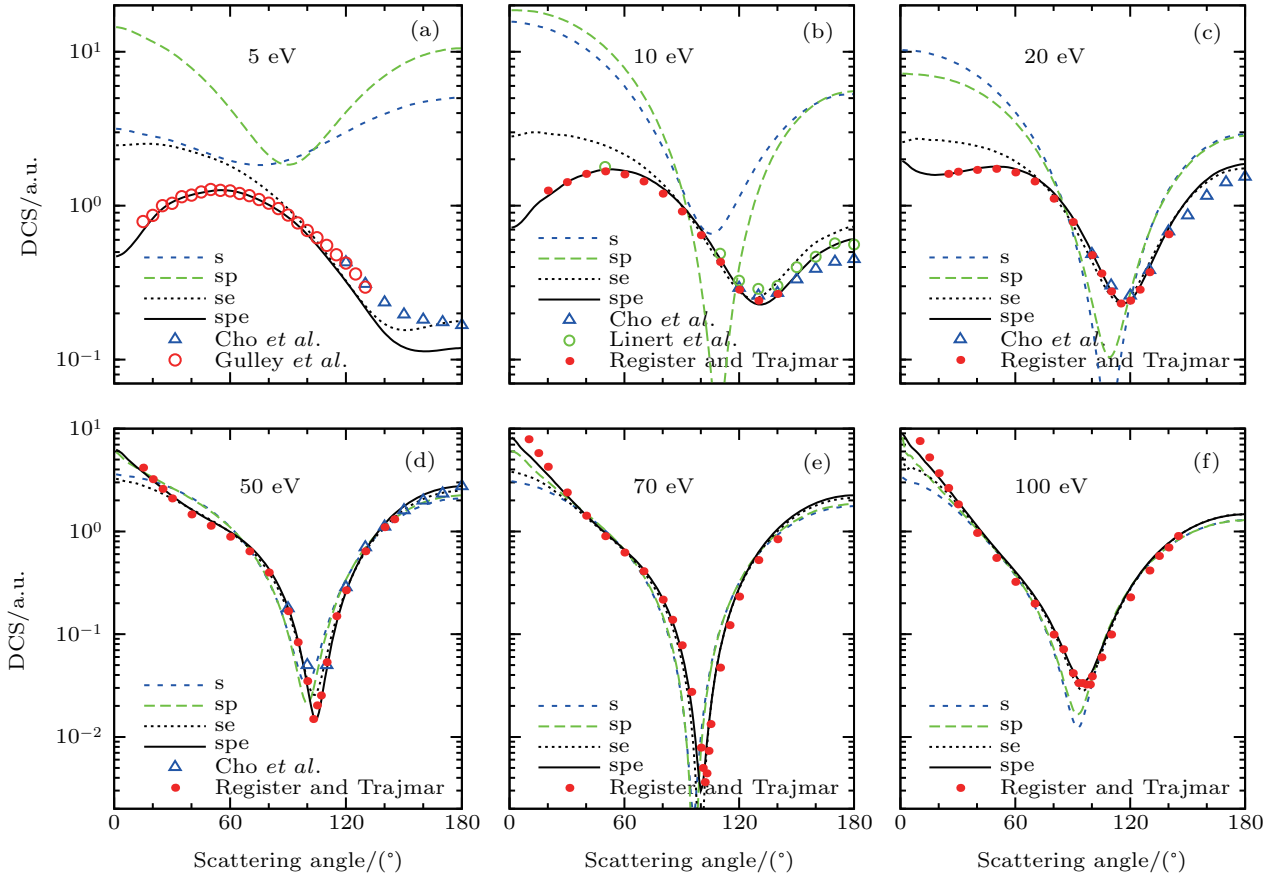


Fig. 1. (color online) Differential cross sections for elastic scattering of electrons by Ne at incident energies of (a) 5 eV, (b) 10 eV, (c) 20 eV, (d) 50 eV, (e) 70 eV, and (f) 100 eV. The experimental data are taken from Chao *et al.*,[23] Gulley *et al.*,[24] Linert *et al.*,[25] and Regester and Trajmar.[26]

Table 1. The values used for parameter d for elastic scattering of Ne at various impact energies.

E/eV	5	10	20	50	70	100
d/a.u.	1.10	1.00	0.95	1.00	1.00	1.20

Figure 2 displays the comparison of the calculated DCSs with the experimental measurements[16,27–30] for elastic scattering of electrons by Ar. Similar to the situation for Ne shown in Fig. 1, the "spe" DCSs are also in excellent agreement with the experimental data for all the incident energies considered here. Compared to the potential scattering of Ne, the DCSs of Ar have more structure, exhibiting two minima in both the forward and the backward directions. It has already been shown that, in general, the heavier the atom is, the more abundant structure the elastic collision DCSs exhibit (for example, see Fig. 10 in Ref. [8] and Fig. 9 in Ref. [31]). The reason is that heavier atoms have more bound electrons, resulting in more complex distributions of the charge density. This is also true for electron impact excitation.[32]

In Fig. 2, the experimentally measured DCSs show that, for incident energies below 10 eV, the position of the minimum in the forward direction moves to larger scattering angles with decreasing depth as the incident energy increases, while the position and the depth of the dip in the backward direction change reversely. It is interesting to see that, as the incident energy increases from 10 eV to 20 eV, a deep minimum in the forward direction appears again, and becomes even deeper at 50 eV. On the other hand, the depth of the dip in the backward direction keeps increasing from 20 eV to 100 eV with the position moving back and forth. Both of the depths and positions of the minima are critical in the DCSs in which the structure information of the target is imprinted.

In the theoretical calculations for the elastic scattering of electrons by Ar, the static potential completely fails to predict the double-dip structure in the DCSs observed in experiment for incident energies below 20 eV, and so does the static plus polarization potential, although obvious differences exist between the "s" and "sp" results. The agreement between theory and experiment is greatly improved if the exchange potential is included since, at least, the dip in the backward direction is well reproduced by the "se" calculations. As a matter of fact, the minima in both the forward and the backward directions can be reproduced by the static plus exchange potential for incident energies above 10 eV. Again, this indicates that the exchange potential is more important than the polarization potential.

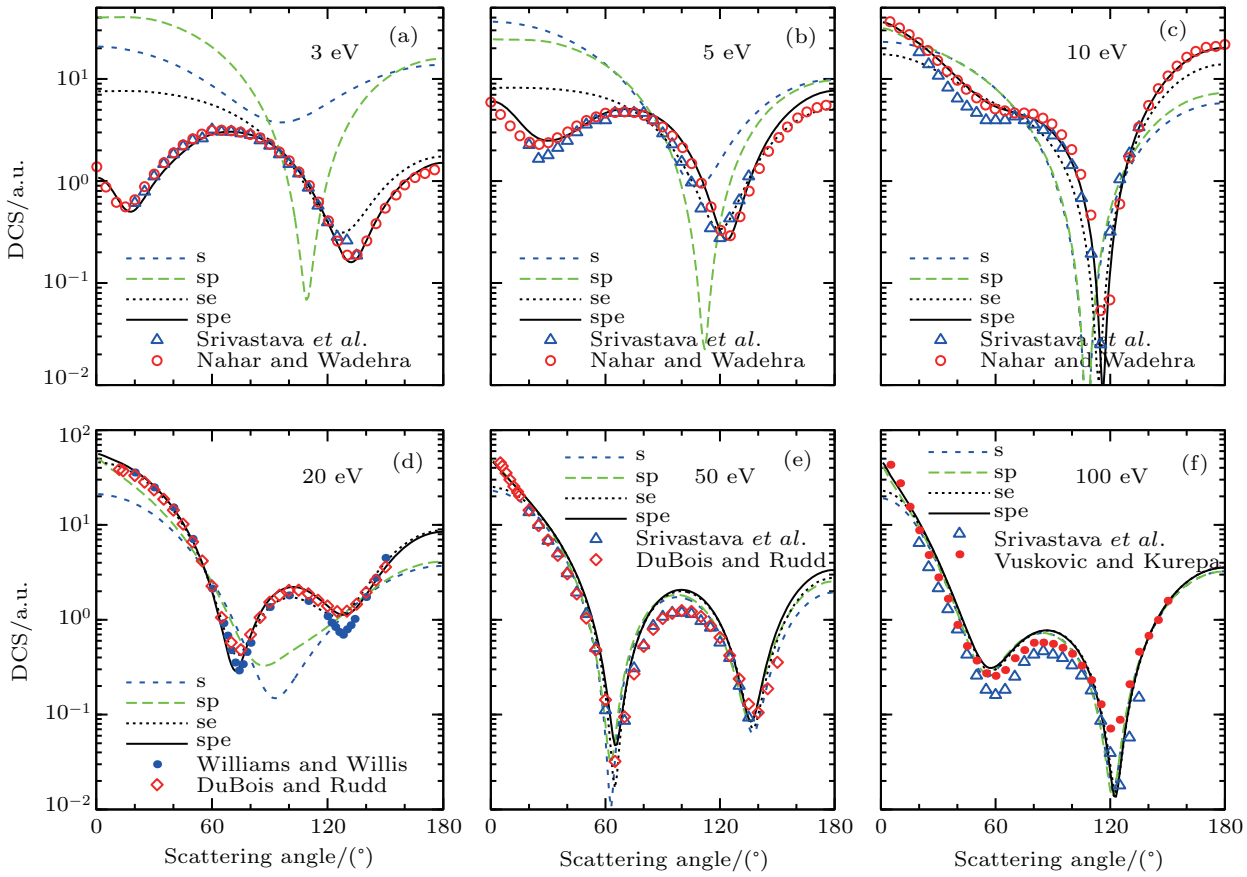


Fig. 2. (color online) Differential cross sections for elastic scattering of electrons by Ar at incident energies of (a) 3 eV, (b) 5 eV, (c) 10 eV, (d) 20 eV, (e) 50 eV, and (f) 100 eV. The experimental data are taken from Srivastava *et al.*,[27] Nahar and Wadehra,[16] Williams and Willis,[28] DuBois and Rudd,[29] and Vušković and Kurepa.[30]

For both Ne and Ar, as demonstrated in Figs. 1 and 2, the polarization and exchange effects can be safely neglected for incident energies higher than 50 eV, provided that slight discrepancies between theory and experiment at scattering angles close to 0° and 180° are acceptable.

It should be noted that the "spe" DCSs depend on the parameter d in Eq. (4). To see the effect of variation of d on the DCSs, in Fig. 3, we show the calculated "spe" DCSs with different values of d for elastic scattering of electrons with Ne and Ar. Here, only the calculated DCSs for incident energies below 20 eV are plotted together with the corresponding experimental data, since the polarization effect is less significant at higher incident energies. It can be seen from Fig. 3 that variation of d has an important effect on both the structure and the magnitude of the calculated DCSs, especially at low collision energies and forward scattering angles. For Ne, as shown in Figs. 3(a)–3(c), by increasing the value of d, the curve of DCSs in the forward direction could be moved up and the location of the maximum shifts to smaller angles. Variation of d also affects the DCSs in the forward scattering angles significantly for Ar, as shown in Figs. 3(d)–3(f), whereas the shape of the DCSs in the backward scattering remains almost the same.

Recall that the ultimate goal of the present work is to test the significance of the polarization and exchange effects in LIED in which the laser-induced electron scattering with the parent ions is treated as laser–free electron scattering with the target ions. For traditional scattering processes, experimental measurements of cross sections at backward angles up to 180° are typically formidable due to the mechanical constraints of the electron spectrometer. In LIED, on the contrary, only the backward scattering cross sections can be extracted from the HATI photoelectron momentum distributions, in which the elastic scattering cross sections in the forward directions are imbedded in the signal of direct ionization and hence are inaccessible. The backward scattering cross sections generally carry more structure information of the targets due to the fact that large angle scattering results from collisions with small impact parameters such that the electron probes the effective potential distribution inside the electron cloud of the target. Consequently, a more sophisticated theoretical description is required.

For elastic scattering of electrons with ions, the difficulty is associated with how to deal with the exchange between the projectile electron and an open shell electron. As discussed in the above section, there exists an ambiguity in the description of the exchange potential in local approximation. Following the prescriptions of Biava *et al.*,[20] here, we also try three different models for the LE potential, namely, LET, LE1, and

LE5, for elastic scattering of electrons by Ar^+. The success or failure of a LE potential should be decided by whether or not, and to what extent, using such a potential improves the agreement between the experimental data and the calculated results based on a no-exchange model. Biava *et al.*[20] have examined the accuracy of the LE potential for electron impact ionization of the p-shell electron of Ar and found that the LE approximation is reliable for ionization leading to s-state vacancies but not p-state vacancies.

In Fig. 4, the calculated DCSs are compared with the experimental data and the existing theoretical results for elastic scattering of electrons by Ar^+ at 16 eV. The experimental data for scattering angles in the forward direction are taken from the measurement of Brotton *et al.*[33] for traditional electron–Ar^+ collision, and those for large scattering angles in the backward direction are extracted from HATI spectra by Micheau *et al.*[34]

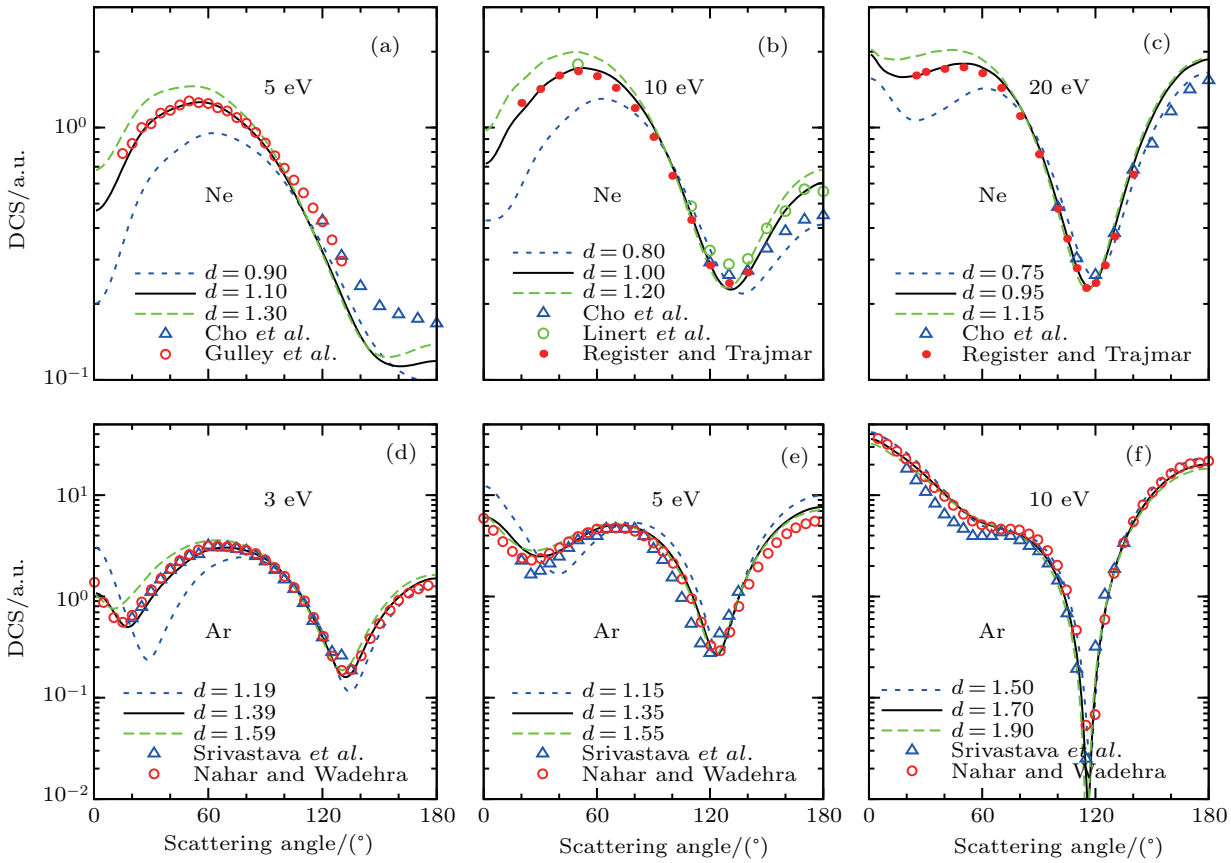


Fig. 3. (color online) Comparison of the calculated differential cross sections using "spe" potential with different values of the parameter d in Eq. (4) with the experimental measurements for elastic scattering of electrons by Ne at incident energies of (a) 5 eV, (b) 10 eV, (c) 20 eV, and Ar at incident energies of (d) 3 eV, (e) 5 eV, (f) 10 eV, respectively. The experimental data are taken from Chao *et al.*,[23] Gulley *et al.*,[24] Linert *et al.*,[25] and Regester and Trajmar[26] for Ne, and Srivastava *et al.*,[27] and Nahar and Wadehra[16] for Ar.

To examine the accuracy of the three LE models, in Fig. 4(a), we present the calculated "spe" results based on LET, LE1, and LE5 respectively. The parameter d in Eq. (4) is taken to be 2.0. It should be noted that for elastic scattering of electrons with ions, variation of d has less significant effect on the calculated DCSs compared to the situation for atoms, since the polarizabilities for ions are much smaller than those for neutral atoms. One can see that although both the LET and LE1 reproduce the overall shape of the measured DCSs, the LE1 model describes the depth of the minimum observed in experiment more accurately, and is in better agreement with the coupled HF calculations performed by Brotton *et al.*[33] It should be noted that the LET model has some defects when it is used for electron–ion collisions. The most likely problem with the LET model is that half the charge density of the inert ion used in Eq. (5) represents a fractional number of electrons, which is somewhat unphysical. It should also be noted that, for traditional electron–Ar^+ collision, the choice of S_2 in Eq. (7) for the LE1 model is somewhat ambiguous. However, for laser-induced electron scattering with the parent ion Ar^+, it is guaranteed that $S_2 = 0$ (note that the other four 3p-electrons in Ar^+ are assumed to have a net spin of zero) since the projectile electron is initially in the ground state, a singlet spin state, and the total spin is preserved during ionization in the laser field.[35] In contrast, the LE5 generates the DCSs which are substantially different from the experimental measurements.

The comparison shown in Fig. 4(a) demonstrates that the LE1 is the best among the three local exchange potential mod-

els for elastic scattering of electrons by Ar^+. Therefore, in the "se" and "spe" calculations shown in Fig. 4(b), only the LE1 model is used. One can see from Fig. 4(b) that the "sp" and "spe" DCSs are very close to the "s" and "se" calculations, respectively, indicating that the polarization effects are less important compared to the situation of elastic scattering of electrons by neutral atoms. While the minimum in the forward direction is shallower in both the "s" and "sp" calculations, by including the exchange potential LE1, the agreement between the experimental data and the calculated results is improved at the forward scattering angles around 35° and 75°. For DCSs in the backward direction, the experimental data exhibit a minimum which is above all of the theoretical predictions. This might be due to the fact that the background in the experimental measurements has not been removed cleanly.

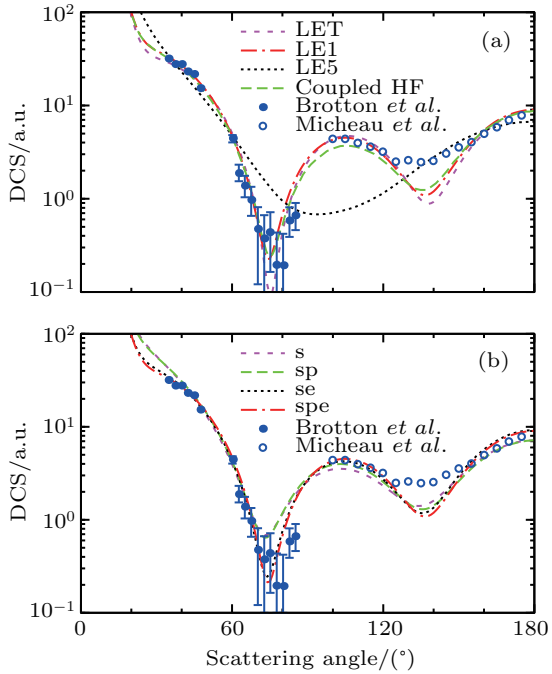


Fig. 4. (color online) Differential cross sections for elastic scattering of electrons by Ar^+ at incident energy of 16 eV. The experimental data are taken from Brotton *et al.*[33] and Micheau *et al.*[34] The coupled HF calculations are taken from Brotton *et al.*[33]

In Fig. 5, we show the similar comparison between the calculated DCSs and the experimental measurements of Greenwood *et al.*[36] as well as the *R*-matrix calculations of Griffin and Pindzola[37] for elastic scattering of electrons by Ar^+ at 3.3 eV. In the experimental measurements, the instrumental angular profile has an effective angular spread decreasing almost linearly from 15° at the scattering angle of 120° to 5° at 170°. In order to facilitate a direct comparison of the theoretical results with the experiment data, for all the calculated DCSs plotted in Fig. 5, including the *R*-matrix results, a convolution has been performed with Gaussian functions representing the instrumental profile. First of all, it is surprising to see in Fig. 5(a) that, except for LE5, all the present theoretical models reproduce the DCSs similar to the *R*-matrix results at scattering angles larger than 150°, which deviate tremendously from the experimental observations. Only in a small range of scattering angles between 120° and 140° can the experimental measurements be well predicted by the *R*-matrix calculations, where both the LET and LE1 predict lower minimum than that observed in experiment. Similar to the case shown in Fig. 4, again, the LE1 is the best while the LE5 is the worst model of exchange potential. Here, the parameter d in Eq. (4) is taken to be 1.5 which is adjusted in the way such that the calculated "spe" DCSs based on LE1 are in best agreement with the *R*-matrix results.

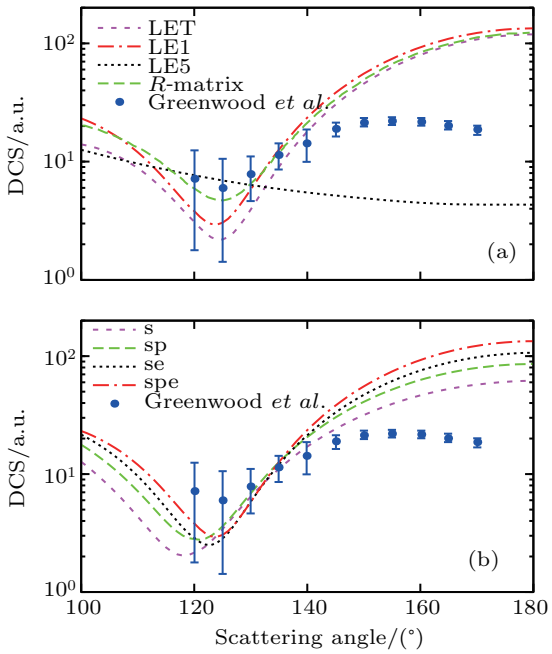


Fig. 5. (color online) Differential cross sections for elastic scattering of electrons by Ar^+ at incident energy of 3.3 eV. The experimental data are taken from Greenwood *et al.*[36] The *R*-matrix results are taken from Griffin and Pindzola.[37]

The effects of the polarization and exchange potentials are demonstrated in Fig. 5(b). By taking into account the polarization effect, the "sp" calculations shift the minimum position to larger angles with respect to the "s" calculations, and so does the "se" calculations in which the exchange potential is included. Finally, the "spe" calculations predict the minimum position at the largest scattering angle which is in good agreement with experiment. It should be noted that, in both the "se" and "spe" calculations, the exchange potential LE1 is used. Although the agreement with experiment cannot be regarded as satisfactory, both the polarization and exchange effects, as expected, become more important at the incident energy of 3.3 eV compared to the case in which the incident energy is 16 eV, as shown in Fig. 4.

4. Conclusions

We have investigated the polarization and exchange effects on elastic scattering of electrons with atoms and ions.

Numerical calculations of differential cross sections based on the standard potential scattering theory have been performed for elastic scattering of electrons by Ne and Ar at incident energies from 5 eV to 100 eV, and by Ar^+ at 3.3 eV and 16 eV. By including both the polarization and exchange potentials, the present theoretical results are in very good agreement with experiment for all the cases considered in the present paper, except for electron–Ar^+ collision at 3.3 eV. Even for electron–Ar^+ collision at 3.3 eV, the present "spe" DCSs are also very close to the *R*-matrix calculations.

The present numerical calculations agree with the well-known general trend that the polarization and exchange effects are very significant at low energies but become weaker as the energy increases. It has been found that, for elastic scattering of electrons with neutral atoms, both the polarization and exchange effects can be safely neglected for incident energies higher than 50 eV. Comparison of the theoretical results with the experimental data also reveals that the exchange potential plays a more important role than the polarization potential. Whereas, although it is more difficult to deal with the exchange between the projectile electron and the bound electron in an open shell, it has been found that the exchange effect is less important on electron–ion collisions than on electron–atom collisions, especially for scattering in the backward direction, provided that a proper local exchange potential is used. In the meanwhile, the polarization of ions is also depressed since the charge distribution of the core is more tightened compared to that of atoms.

In conclusion, for elastic scattering, both the polarization and exchange effects on electron–ion collisions are not as important as those on electron–atom collisions. Since only slight differences exist between the "s" and "spe" calculated DCSs for elastic scattering of electrons by Ar^+ at 16 eV, it is reasonable to deduce that both the polarization and exchange effects can be ignorable for elastic electron–ion collisions at energies above 20 eV. This indicates that the current theoretical treatment of LIED is valid.

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