Elastic scattering of low-energy electrons by Ne, Ar, Kr, and Xe

R. Haberland, L. Fritsche, and J. Noffke
Institut für Theoretische Physik der Technischen Universität Clausthal, D-3392 Clausthal-Zellerfeld, Federal Republic of Germany
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We treat low-energy electron scattering by atoms within a Kohn-Sham-type one-particle theory. In applying this theory, all many-body effects involved in the projectile-target interaction are absorbed into a one-particle potential. Hence, one merely has to solve an elementary potential-scattering problem. However, there are two crucial points to be observed in the construction of the scattering potential. (1) The Kohn-Sham-type exchange-correlation potential must be formed by using correlation factors which are required to have certain asymptotic and integral properties. (2) Since the scattering process is viewed as being quasistationary, the unbound projectile state must be modified by a bell-jar-type envelope function to account for the effect of a finite residence time in the target where the projectile causes a finite perturbation. During this time the entire system has to be treated as consisting of $N+1$ indistinguishable electrons which in a Kohn-Sham-type theory are described by only $N+1$ self-consistent one-particle states. Once the analytical forms of the correlation factors and the envelope function have been chosen, the calculational procedure is completely parameter-free. Although it is considerably simpler than well-established methods in this field, it provides comparably good results on differential cross sections and scattering-induced polarizations in a wide range of impact energies (5—100 eV).

I. INTRODUCTION

In a recent paper (hereafter referred to as I), Fritsche *et al.*[1] have shown that electron scattering by atoms can consistently be treated by employing a Kohn-Sham-type one-particle scheme. Within that approach exchange and correlation is accounted for by introducing model pair correlation functions which are subject to certain N-representability conditions obeyed by the exact pair correlation functions. The $(N+1)$-electron system consisting of the projectile and the N-electron target is described then by a set of $N+1$ one-particle equations where exchange and correlation is absorbed into a potential which contains these model functions. The one-particle potential thus constructed differs favorably from commonly used local-density approximations in that it shares the virtues of the latter but does not suffer from the obvious failure in describing the proper asymptotic behavior for large electron-nucleus separations. This property becomes particularly evident when one is dealing with limiting cases such as hydrogen or negative ions. In the case of hydrogen, the effective one-particle potential reduces exactly to that of the nuclear Coulomb potential as it should. On the other hand, negative ions prove to be generally stable when treated within that scheme. Moreover, as has been shown by Fritsche and Gollisch,[2,3] affinity energies turn out to be in relatively good agreement with the experiment. It is particularly the latter result that has encouraged studies on the applicability of the new approach to the $(N+1)$-electron problem of electron scattering by atoms. An important point of this scheme resides in the assumption that the projectile can, during its passage through the atom, be viewed as being localized within the target and that it is nondistinguishable from the N target electrons in that state. The entire system can be treated then by self-consistently solving $N+1$ one-particle equations as in atomic structure calculations. All many-body effects involved in the action of the projectile on the target are thus adequately accounted for. The advantage gained over other $(N+1)$-electron theories of scattering consists in the fact that the perturbed target states are iteratively recalculated within the self-consistency procedure so that one is definitely dealing with only $N+1$ states all the time. This is distinctly different from conventional methods which are based on (in principle infinite) expansions in terms of fixed bound and unbound target states describing the perturbed occupied states in the presence of the projectile. (For a review of these methods see, e.g., Burke and Williams[4] and Callaway.[5]) Since the actual perturbation is small and the convergence of these expansions accordingly slow, the calculational procedure is a relatively delicate one. In a straightforward approach, one would need a large number of unbound states in the expansions to mimic the perturbed states. To make the calculation manageable one has to put up with certain inconsistencies or auxiliary constructs, e.g., pseudostates whose selection is not at all a trivial matter.

At first sight, our approach appears to be open to discussion as well, as the Kohn-Sham one-particle scheme has only been proven to apply to ground states. We deliberately omit here discussing the problem as to what extent one is justified in applying this theory to the scattering problem which deals with excited $(N+1)$-electron states. An extensive study on this subject will be published elsewhere.

The most intriguing question to be dealt with is how one is to treat the scattering process in a quasistationary fashion although the actually occurring perturbation of

the target clearly reflects the fact that there is only a finite residence time of the projectile during which it can mediate a finite effect on the target. It becomes particularly obvious from our one-particle description of the scattering process that this perturbational effect would be vanishingly small if we were to assume the projectile in a stationary one-particle state whose contribution to the effective potential within the target would be of the order $(4\pi/3)r_{\rm eff}^3/V$ where $r_{\rm eff}$ is the effective target radius and V the volume of the scattering chamber. Curiously, this basic problem of scattering theory, i.e., the question of how to choose the normalization of the projectile state, is rarely addressed. In the present paper we adopt the plausible view that the projectile is during some residence time localized within a sphere of radius $r_{\rm eff}$ defined by the uppermost occupied target state obtained within the self-consistent calculation. Since the latter implies indistinguishability of the $N+1$ electrons involved, our assumption just accounts for the fact that the incoming electron loses its identity as it trespasses that sphere. Consequently, the electron emerging from the atom after the scattering will very likely be some other electron irrespective of whether or not the energy is conserved in the process.

The method of determining the localization volume put forward in I was much more involved than the one which will be used here. Moreover, the former method led to differential cross sections for collision energies below 20 eV which were in poor agreement with the experiments. Hence, the progress achieved by the present paper in providing significantly better results is primarily connected with a simpler and physically more adequate description of the projectile localization. We have, in addition, introduced a slightly different projectile envelope function which allows a favorable modification of the long-range behavior of the effective one-particle potential. Details on this subject will be presented in Sec. II. Section III is entirely devoted to results obtained for the scattering by Ne, Ar, Kr, and Xe in the energy regime of 5–100 eV. In Sec. IV we shall draw some conclusions from the improvements achieved and discuss possible further development along the lines of the present paper.

II. THEORY

As indicated in the foregoing section, we shall not dwell here at any length on how to justify applying the Kohn-Sham theory[6] to the excited $(N+1)$-electron system under study. We rather refer to the observation that a simpleminded extension of this theory to, for example, x-ray absorption of atoms (see Gollisch[7]) or to photoemission (see, e.g., Noffke and Fritsche[8] and Leschik *et al.*[9]) yields in many cases surprisingly good agreement with the experiments.

Applying the Kohn-Sham scheme to the problem at hand amounts to self-consistently solving $N+1$ one-electron equations which read

$$H_s\psi_{is}(\mathbf{r})=\varepsilon_{is}\psi_{is}(\mathbf{r}) , \tag{1a}$$

where

$$H_s=-\tfrac{1}{2}\nabla^2+U_s(\mathbf{r}) \tag{1b}$$

and $s=\pm 1$ denotes the two spin orientations of an electron. (If not differently stated, all quantities are given in Hartree units.)

The potential $U_s(\mathbf{r})$ is a functional of the charge density $\rho_s(\mathbf{r})$ and of the correlation factors $f_{s's}(\mathbf{r}',\mathbf{r})$. The latter are connected with the pair correlation functions $g_{s's}(\mathbf{r}',\mathbf{r})$ through

$$g_{s's}(\mathbf{r}',\mathbf{r})=1-f_{s's}(\mathbf{r}',\mathbf{r})$$

and have the general properties

$$f_{s's}(\mathbf{r}',\mathbf{r})=f_{s's}(\mathbf{r},\mathbf{r}') , \tag{2a}$$

$$f_{s's}(\mathbf{r}',\mathbf{r})\leqq 1 , \tag{2b}$$

$$f_{ss}(\mathbf{r},\mathbf{r})=1 , \tag{2c}$$

$$\int \rho_{s'}(\mathbf{r}')f_{s's}(\mathbf{r}',\mathbf{r})d^3r'=\delta_{s's} , \tag{2d}$$

$$f_{s's}(\mathbf{r}',\mathbf{r})\to\delta_{s's}1/N_s \quad \text{as} \quad |\mathbf{r}-\mathbf{r}'|\to\infty , \tag{2e}$$

where

$$N_s=\int \rho_s(\mathbf{r})d^3r .$$

The equations (2d) are commonly referred to as "sum rules." (For more details see, e.g., I.) The potential $U_s(\mathbf{r})$ consists of three parts: the nuclear Coulomb potential of the atomic scatterer

$$U_n(\mathbf{r})=-\frac{Z}{r} , \tag{3a}$$

where Z is the atomic number, and the nucleus is assumed to be centered at $r=0$; the classical Coulomb potential

$$U_c(\mathbf{r})=\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3r' ; \tag{3b}$$

and the exchange-correlation potential

$$U_{\rm xc}^{(s)}(\mathbf{r})=-\sum_{s'}\int \frac{\rho_{s'}(\mathbf{r}')f_{s's}(\mathbf{r}',\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}d^3r' - \tfrac{1}{2}\sum_{s',s''}\rho_{s''}(\mathbf{r})\int \frac{\rho_{s'}(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|}\frac{\delta f_{s's''}(\mathbf{r}',\mathbf{r})}{\delta\rho_s(\mathbf{r})}d^3r' , \tag{3c}$$

where $\delta f_{s's''}(\mathbf{r}',\mathbf{r})/\delta\rho_s(\mathbf{r})$ is the functional derivative of $f_{s's''}(\mathbf{r}',\mathbf{r})$ with respect to ρ_s. For a detailed derivation of (3c) see, e.g., Fritsche and Gollisch.[2] The functional derivatives of the correlation factors can only be reduced to simple analytical expressions if the factors for $s'\neq s$ are assumed to be negligibly small for all r' and r and if the true $\mathbf{r}',\mathbf{r}$ dependence of $f_{ss}(\mathbf{r}',\mathbf{r})$ is approximated by

$$f_{ss}(|\mathbf{r}'-\mathbf{r}|/A_s(\mathbf{r})) ,$$

where $A_s(\mathbf{r})$ is determined by the sum rule (2d). For details on the derivation of

$$\delta f_{ss}(|\mathbf{r}'-\mathbf{r}|/A_s(\mathbf{r}))/\delta\rho_s(\mathbf{r})$$

the reader is referred to the paper by Gunnarsson *et al.*[10]

In cases where relativistic effects are non-negligible (as for scattering by Kr and Xe), the Schrödinger-type equations (1) have to be replaced by the corresponding Dirac

equations. The form of the potential is not affected by this. (See I for details.)

Following the arguments of I, we assume the correlation factors to have the following approximate form:

$$f_{s's}(\mathbf{r}',\mathbf{r})=\delta_{s's}\left[1+\left[\frac{|\mathbf{r}'-\mathbf{r}|}{A_s(\mathbf{r})}\right]^2\right]^{-5/2}, \tag{4}$$

where $A_s(\mathbf{r})$ is determined by requiring (4) to satisfy (2d). The ansatz (4) represents a particular case of the form $f_{ss}(|\mathbf{r}'-\mathbf{r}|/A_s(\mathbf{r}))$ discussed above. Obviously, this expression conforms to the fundamental requirements [2(b)–2(d)] to be satisfied by $f_{s's}(\mathbf{r}',\mathbf{r})$. The choice of a Lorentzian to the $\frac{5}{2}$ power appears to be rather arbitrary. We could just as well have chosen a Gaussian, for example. Atomic structure calculations based on different choices of this kind have shown, however, that key quantities like $\rho_s(\mathbf{r})$ and the total energy are only slightly affected by a change of the analytical form of $f_{ss}(|\mathbf{r}'-\mathbf{r}|/A_s(\mathbf{r}))$. This is a consequence of the fact that the requirements 2(b)–2(d) represent relatively severe constraints, in particular the sum rule (2d) which has to be satisfied for any $\mathbf{r}$. Compared to other possible choices, the expression (4) offers some practical advantages in determining $A_s(\mathbf{r})$ from (2d) and in evaluating $U_{\rm xc}^{(s)}(\mathbf{r})$. Moreover, this form of $f_{ss}(|\mathbf{r}'-\mathbf{r}|/A_s(\mathbf{r}))$ has proved to be particularly suited in atomic structure calculations with emphasis on negative ions. (See Fritsche and Gollisch.[2,3])

Further, we set

$$\rho_s(\mathbf{r})=\rho_{s'}(\mathbf{r})=\tfrac{1}{2}\rho(\mathbf{r}) \tag{5}$$

which applies to the case of an unpolarized projectile electron incident on a closed-shell atom.

In order to retain the separability of the Schrödinger equation (1a) we assume $\rho(\mathbf{r})$ to be spherically symmetric

$$\rho(\mathbf{r})=\rho(r) . \tag{6}$$

This represents, of course, an approximation only, since the charge density

$$\rho(\mathbf{r})=\sum_{\substack{s,i\\(\text{occupied})}}|\psi_{is}(\mathbf{r})|^2 \tag{7}$$

is made up from contributions of slightly perturbed occupied target states and from that of the unbound one-particle state $\psi_u(\mathbf{r})$ describing the incident and scattered electron

$$\psi_u(\mathbf{r})=\psi_{\rm in}(\mathbf{r})+\psi_{\rm out}(\mathbf{r}) . \tag{8}$$

The charge contribution associated with the latter is inevitably nonspherical as a result of which the self-consistent target charge density can no longer be spherically symmetry. The property (6) of $\rho(\mathbf{r})$ is ensured by forming the spherical average of the actual charge density after each iteration step. As in I, we allow for localization of the projectile by choosing a plausible form of an envelope function whose half-width is given by some effective radius $r_{\rm eff}$. We then multiply (8) by this envelope function and use the resulting new unbound one-particle state $\psi_u'(\mathbf{r})$ to calculate its contribution to the total charge density. In I the envelope function was assumed to be a Gaussian so that $\psi_u'(\mathbf{r})$ attained the form

$$\psi_u'(\mathbf{r})=A\exp[-\tfrac{1}{2}(r/r_{\rm eff})^2]\psi_u(\mathbf{r}) , \tag{9}$$

where the constant A ensured proper normalization

$$\int|\psi_u'(\mathbf{r})|^2 d^3r=1 .$$

The method used in determining $r_{\rm eff}$ was a relatively clumsy and in some cases unreliable one. Moreover, the envelope function ought to preserve the original form of $\psi_u'(\mathbf{r})$ inside the target as best as possible which in retrospect makes a Gaussian a relatively unfavorable choice. The localization described by (9) was thought to automatically ensure a correct asymptotic behavior of $U_s(\mathbf{r})$ for large r. A closer study preceding the present work revealed, however, that the long-tail behavior of $U_s(\mathbf{r})$ was $\propto 1/r^3$ rather than $\propto 1/r^4$. Finally, it had been overlooked that $\psi_u'(\mathbf{r})$ is no longer orthogonal to the target states as a result of which $\rho(\mathbf{r})$ is not given exactly by (7) any more. The shortcomings of the previous method in describing the projectile localization can be entirely removed by proceeding along the following lines.

(1) The Gaussian is replaced by a Fermi distribution function. Hence, $\psi_u'(\mathbf{r})$ attains the form

$$\psi_u'(\mathbf{r})=A\{\exp[(r-r_{\rm eff})/t_D]+1\}^{-1}\psi_u(\mathbf{r}) , \tag{10}$$

where A is again a normalization constant, and t_D is determined by the requirement that the radial derivatives of $\psi_u'(\mathbf{r})$ and that of the uppermost occupied target state $\psi_b(\mathbf{r})$ agree at $r=r_{\rm eff}$. The latter radius is chosen to be the classical turning point associated with the radial part of $\psi_b(\mathbf{r})$.

(2) The localized projectile state (10) is subsequently orthogonalized with respect to all target states so that the total charge density can be formed according to (7).

(3) The exact functional derivatives of the correlation factors in (3c) are calculated in complete analogy to the method suggested by Gunnarsson *et al.*[10]

(4) Because the correlation factor for unlike spins is according to (4) assumed to vanish identically, $U_s(\mathbf{r})$ cannot be expected to vary $\propto 1/r^4$ for very large r. (See Williams and von Barth.[11]) Nevertheless, $U_s(\mathbf{r})$ constructed with the use of (4) displays for not too large distances an approximate $1/r^4$ behavior as shown in Fig. 1. [The dashed straight line refers to the long-range behavior of $U_s(\mathbf{r})$ associated with a Gaussian-like localization as used in I.] We have forced $U_s(\mathbf{r})$ to obey an exact $1/r^4$ dependence for large distances beyond the minimum in Fig. 1 by setting $r^4U_s(\mathbf{r})$ equal to a constant as indicated by the dotted line. This procedure has proved to be possible and unambiguous in all cases.

The modifications (2) and (3) do not give rise to sizable changes of the differential cross sections within the energy regime of 5–100 eV, whereas modification (4) slightly affects the results below 10 eV.

Except for the above four amendments, the calculational scheme remains the same as that used in I. Once the self-consistent scattering potential $U_s(\mathbf{r})$ has been determined, the direct scattering amplitude f and the spin-flip amplitude g can be obtained by employing the partial-

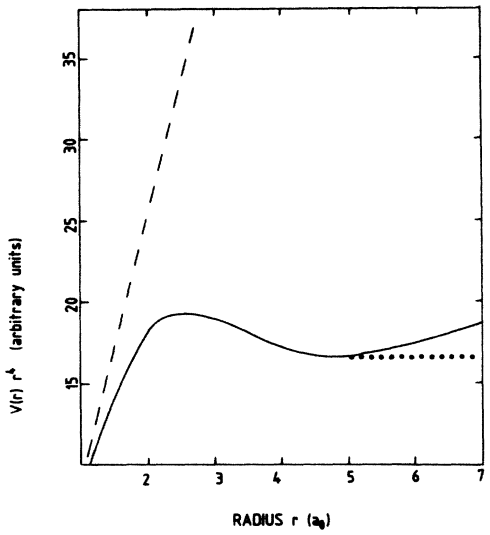

FIG. 1. Long-range behavior of the scattering potential $V(r)$. Since the r dependence of the true potential is $\propto 1/r^4$ we have plotted $-r^4V(r)$: — — —, Fritsche *et al.* (Ref. 1); —— this work. For distances beyond the minimum of the solid curve the potential used in calculating the scattering amplitudes f and g has been continued according to the dotted line.

wave method as described in I. From these two complex functions one can readily derive the following quantities of particular interest.

The differential cross section

$$\frac{d\sigma}{d\Omega} = |f|^2 + |g|^2 ,$$

the total cross section

$$\sigma = \int (|f|^2 + |g|^2) d\Omega ,$$

and the Sherman function

$$S = i\frac{fg^* - f^*g}{|f|^2 + |g|^2}$$

which describes the scattering-induced polarization of an initially unpolarized electron beam. There are two further quantities which have been of interest in connection with recent triple-scattering experiments:

$$T = \frac{|f|^2 - |g|^2}{|f|^2 + |g^2|}$$

and

$$U = i\frac{fg^* + f^*g}{|f|^2 + |g|^2} .$$

The quantities S, T, U describe the change of the polarization components of a polarized electron beam by the scattering process (for details see, e.g., Kessler[12]).

III. RESULTS

The method described in the preceding section has been applied to electron scattering by Ne, Ar, Kr, and Xe atoms for impact energies ranging from 5 to 100 eV. To ensure sufficient accuracy all calculations were carried out by using partial waves up to a maximum angular momentum of $l=14$. The overall agreement with the experiments is very satisfactory considering the fact that the calculations do not contain adjustable parameters. We want to emphasize again that these calculations are based on a fixed number of self-consistent one-particle states, viz., N target states plus one projectile state. Nevertheless, they cover a range of impact energies from well below excitations of the target to way above the ionization threshold. Toward lower impact energies the differential cross section becomes, of course, increasingly sensitive to possible peripheral departure of the scattering potential from its true r dependence. Hence, the relatively good agreement obtained lends some credit to the adequacy of our method.

Although the contribution of the projectile state to the total charge density varies it spatial dependence as the impact energy goes up, the effect on r_{eff} is zero on the scale of interest. Naturally, the radial derivative of $\psi_b(\mathbf{r})$ at $r = r_{\text{eff}}$ picks up that variation much more sensitively. This is reflected in the energy dependence of t_D shown in Table I, where we have also compiled data on r_{eff} and the total elastic cross section for the atoms studied.

In presenting our results on differential cross sections, we have limited ourselves to including only one respective example from other theoretical sources. We have chosen two recent papers by McEachran and Stauffer[13] who use a carefully crafted polarized orbital approximation which is conceptually quite different from our approach and covers essentially the same material on the same target atoms. Our results are generally drawn with solid lines, those referring to McEachran and Stauffer are dashed unless differently stated.

TABLE I. Calculated values r_{eff}, t_D, and total elastic cross sections σ (in atomic units) for impact energies ε_i of 5—100 eV.

	ε_i (eV)	r_{eff}	t_D	σ
Ne	5	0.7	0.8	11.8
	10	0.7	0.7	14.4
	20	0.7	0.6	14.5
	50	0.7	0.5	12.0
	100	0.7	0.3	9.7
Ar	5	1.3	1.0	36.2
	10	1.3	1.0	64.5
	20	1.3	1.6	70.5
	50	1.3	1.1	33.3
	100	1.3	0.4	23.2
Kr	5	1.6	0.7	54.7
	10	1.6	0.8	85.6
	20	1.6	1.0	79.4
	50	1.6	1.1	51.3
	100	1.6	0.8	32.5
Xe	5	2.1	0.6	104.3
	10	2.1	0.8	129.0
	30	2.1	1.2	65.8
	60	2.1	0.5	31.8
	100	2.1	1.1	30.1

A. Neon

Fig. 2 shows differential cross sections for Ne compared with experimental results of Register and Trajmar,[14] Brewer *et al.*,[15] and Williams and Crowe.[16] For impact energies above 20 eV these results are obviously very well represented by our theory except for the deep minimum at 50 eV around a scattering angle of 105°. For lower energies our calculation tends to overestimate the experimental values around the maximum at ~55°. Nevertheless, there is a striking improvement over the earlier calculations in I which are shown with dash-dotted lines. Hence, the departure of those curves from the experimental results does not primarily originate from asphericity affects as suggested in I but is mainly caused by an inadequate description of the projectile localization.

B. Argon

Experimental results on scattering by Ar are available from the works of Srivastava *et al.*[17] and Williams and Crowe.[16] The differential cross sections are shown together with the respective theoretical curves in Fig. 3. The results for 5 eV impact energy around the minimum at 30° appear to favor neither of the two theories. However, unpublished results of Andrick and Bitch quoted by Bell *et al.*[18] as well as the R-matrix calculations of the latter authors confirm our results within that range of scattering angles. Also, the results for 10 eV [Fig. 3(b)] are clearly in favor of our calculation. At higher energies, the experimental values are mostly overestimated by the theory within the entire range of scattering angles. This may be due to the fact that the elastic differential cross section is influenced by the presence of inelastic channels which has not been accounted for in our calculation.

C. Krypton

Figure 4 presents the experimental results by Srivastava,[17] Jost,[19] and Williams and Crowe,[16] together with those of the two theories. Again, around the first minimum of the differential cross section at 5 eV the theoretical curves depart from the experimental data in

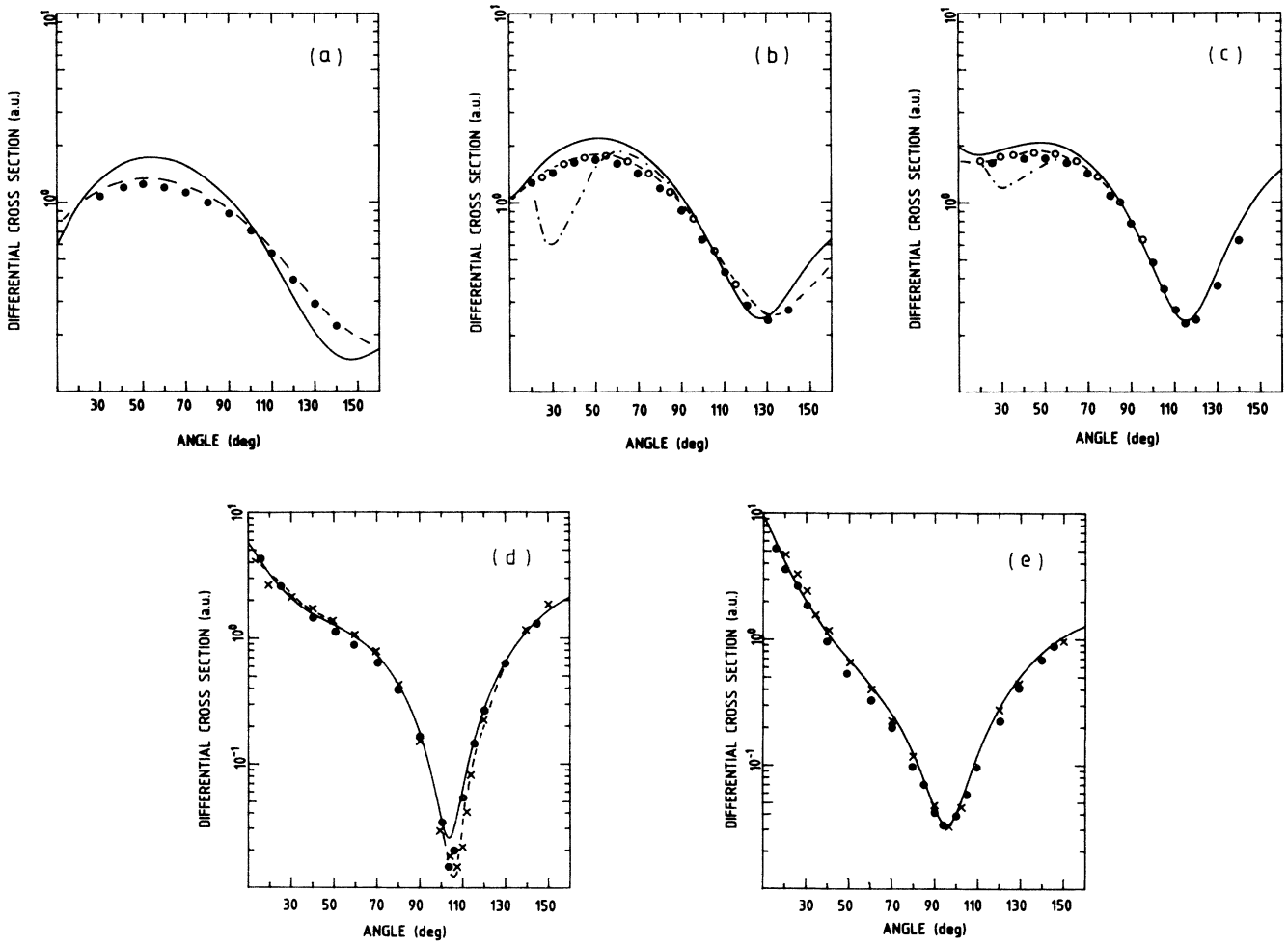

FIG. 2. Differential cross sections for elastic scattering of electrons by Ne atoms (in atomic units): (a) 5 eV, (b) 10 eV, (c) 20 eV, (d) 50 eV, (e) 100 eV. Experiment: ●, Ref. 14; ○, Ref. 15; ×, Ref. 16. Theory: ——, present work; — — —, McEachran and Stauffer (Ref. 13); —·—·—·, Fritsche *et al.* (Ref. 1).

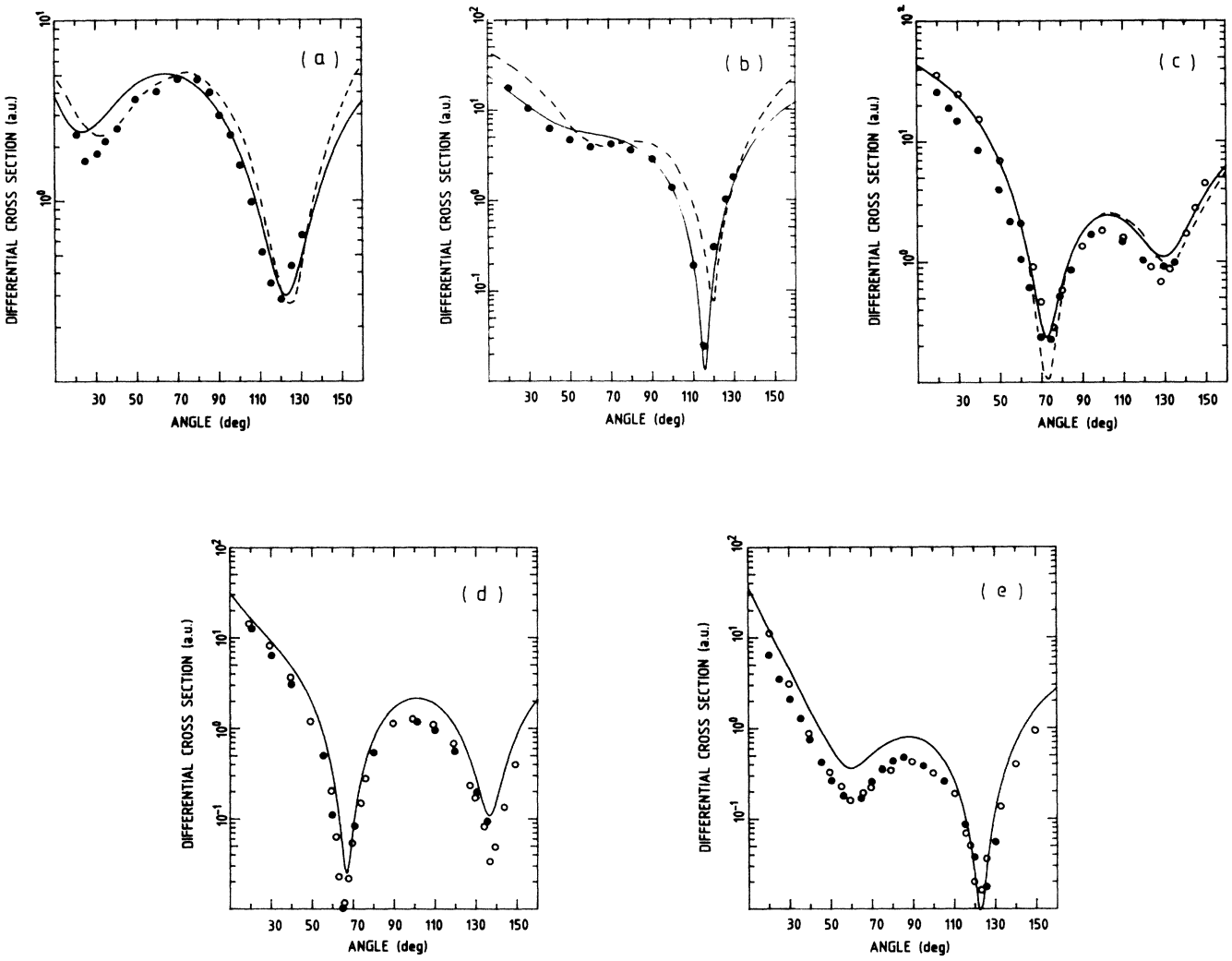

FIG. 3. Differential cross sections for elastic scattering of electrons by Ar atoms (in atomic units): (a) 5 eV, (b) 10 eV, (c) 20 eV, (d) 50 eV, (e) 100 eV. Experiment: ●, Ref 17; ○, Ref. 16. Theory: ——, present work; — — —, McEachran and Stauffer (Ref. 13). The theoretical results of McEachran and Stauffer at 50 eV are not included because they coincide with the present results.

different ways. Surprisingly, the minimum around 75° seen in the experimental data at 10 eV is clearly missing in our theory which otherwise neatly follows the trend of the observed angle dependence. At 20 and 50 eV our results agree slightly better with the measurements than those of McEachran and Stauffer[13] yet generally confirm our conjecture on the effect of overshooting the experimental results.

As the atomic number of the scatterer becomes larger, spin-orbit coupling gives rise to an ever increasing polarization of the scattered (initially unpolarized) electron beam. We have calculated the angle dependence of this polarization for three impact energies. The results are shown in Fig. 5 and compared with experimental data of Beerlage *et al.*[20] and Schackert.[21] At 10 and 20 eV the calculations compare very satisfactorily with the observed data. At higher energies discrepancies develop. Our theory does not predict the large polarization effect around 65° seen at 50 eV. Also, the large positive polarization around 45° found by Schackert[21] is not confirmed.

D. Xenon

In this case we may again refer to measurements by Jost[19] and by Williams and Crowe.[16] The experimental and theoretical material is compiled in Fig. 6. Considerably worse than in the case of Ar and Kr, our calculations deviate markedly from the data measured at 5 eV. A comparison with the results of McEachran and Stauffer[13] appears to suggest that there might be a slight advantage of their theory in the regime of low impact energies. This is not the case as follows from Fig. 6(b) showing the differential cross section at 10 eV. Experiments by Jost[19] clearly indicate that there is only one minimum around 115° close to that predicted by our theory. At 30 eV and even more so at 50 eV (not shown in the figures) both cal-

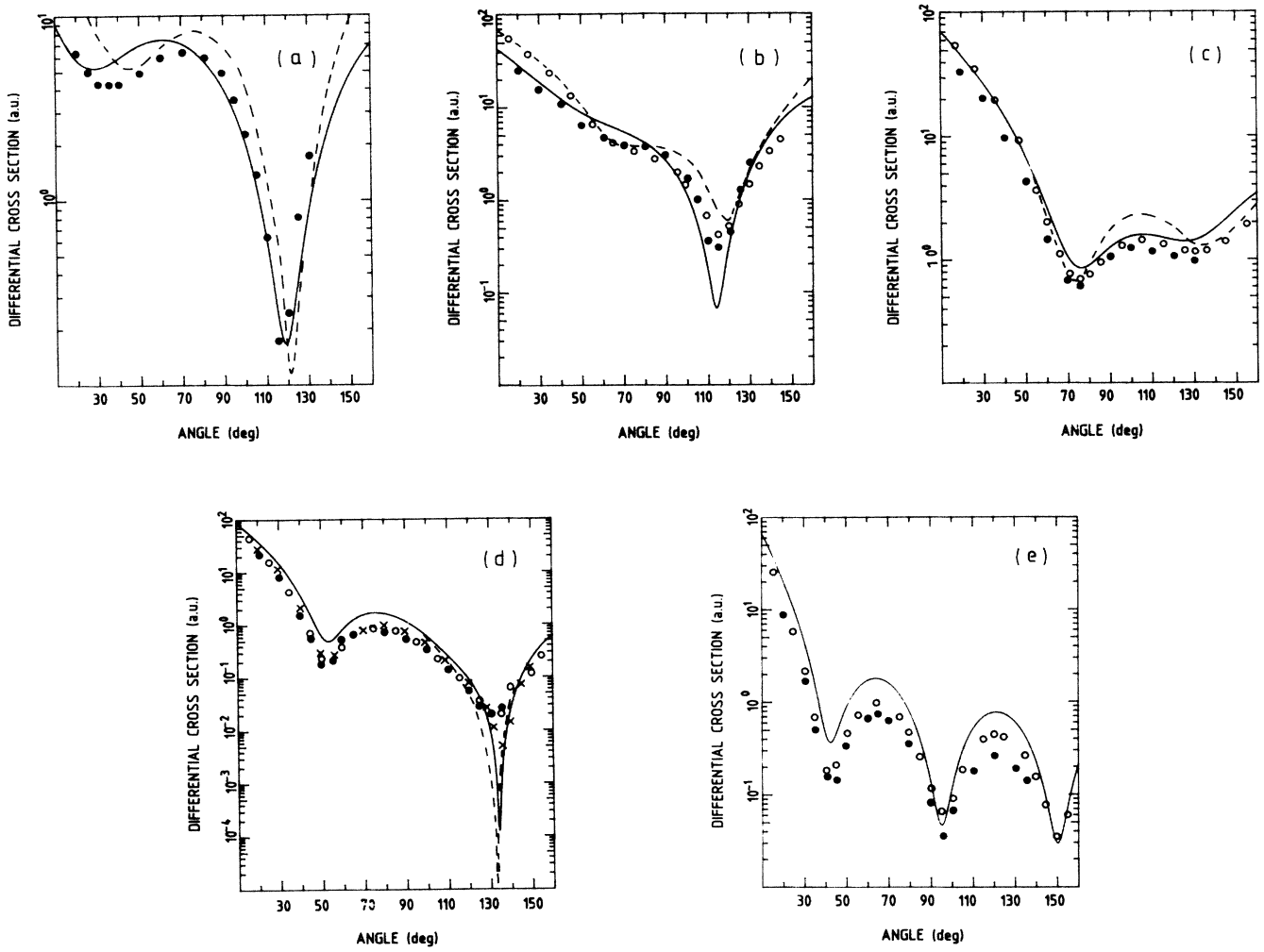

FIG. 4. Differential cross sections for elastic scattering of electrons by Kr atoms (in atomic units): (a) 5 eV, (b) 10 eV, (c) 20 eV, (d) 50 eV, (e) 100 eV. Experiment: ●, Ref. 17; ○, Ref. 19; ×, Ref. 16. Theory: ——, present work; — — —, McEachran and Stauffer (Ref. 13).

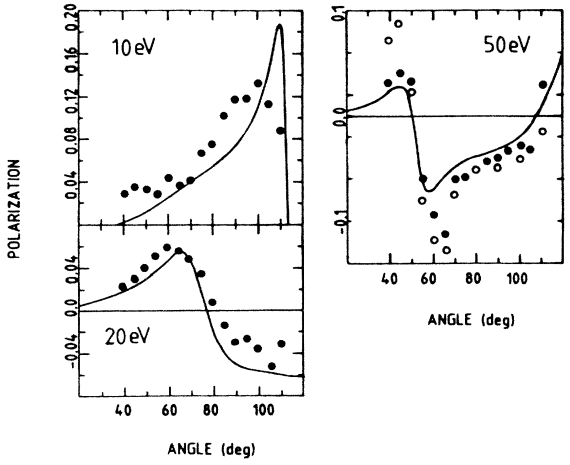

FIG. 5. Polarization of electrons elastically scattered by Kr atoms at 10, 20, and 50 eV. Experiment: ●, Ref. 20; ○, Ref. 21. Theory: ——, this work.

culations yield practically identical results. At higher energies (30 eV and above) the angle dependence of the differential cross section develops complicated structures which makes an assessment of the theoretical results difficult if not impossible. The experimental situation is affected by this as well. At 60 eV, for example, the measurements by Jost[19] and those by Williams and Crowe[16] arrive in the range of 25°—100° at appreciably different results as can be seen from Fig. 6(d). When the impact energy is raised to 100 eV we find again good agreement with the data of Jost[19] as regards the principal features of the angular dependence. As in the case of Ar and Kr, the absolute values obtained from theory are generally too large.

Our results on the Sherman function at 50, 60, and 100 eV are shown in Fig. 7. Essential features of the experiments by Berger *et al.*,[22] Klewer *et al.*,[23] and Schackert[24] are obviously well described by these curves. This applies in particular to the sign and to the zeros of the measured

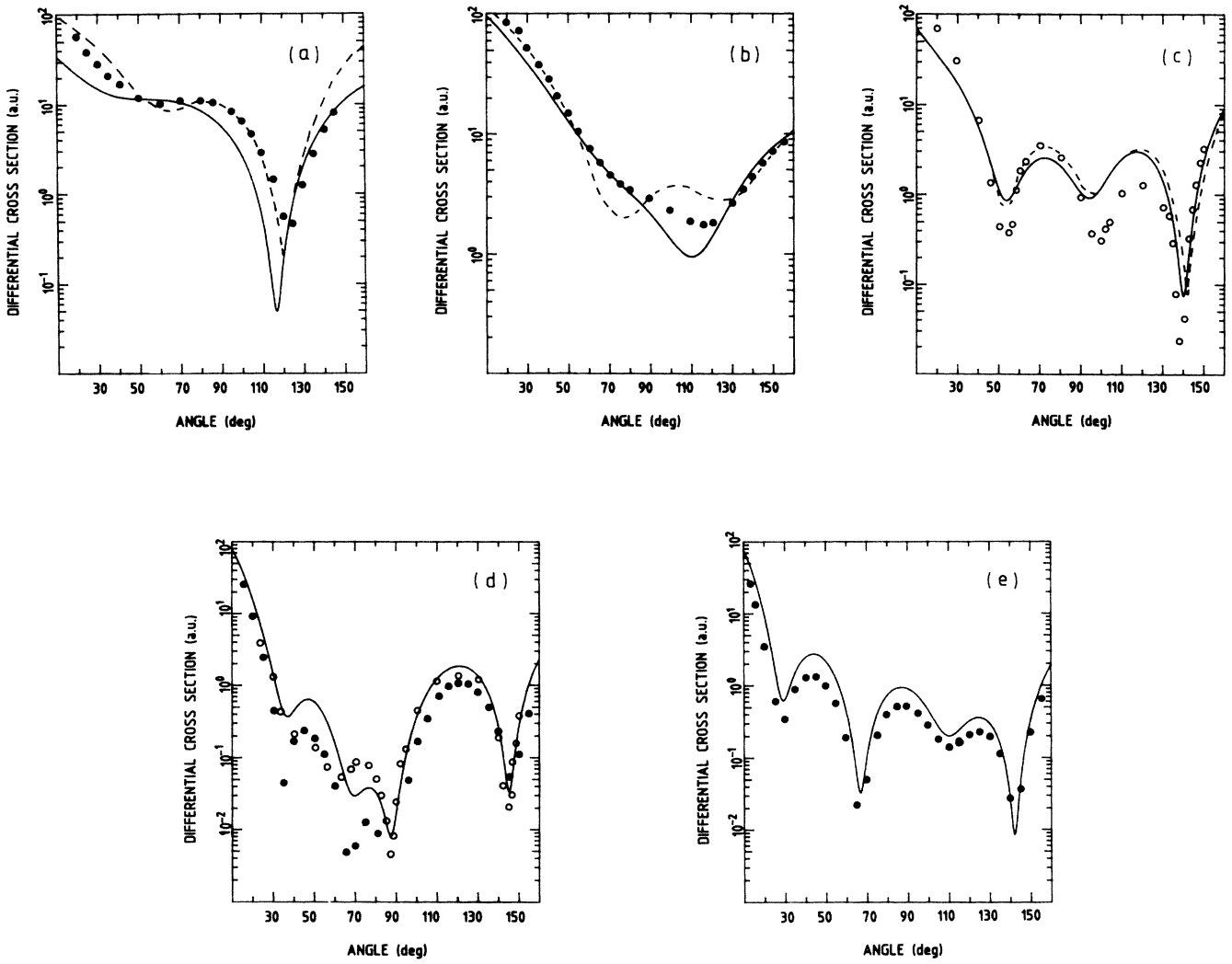

FIG. 6. Differential cross sections for elastic scattering of electrons by Xe atoms (in atomic units): (a) 5 eV, (b) 10 eV, (c) 30 eV, (d) 60 eV, (e) 100 eV. Experiment: ●, Ref. 19; ○, Ref. 16. Theory: ——, this work; — — —, McEachran and Stauffer (Ref. 13).

angle dependence of S. Figures 8 and 9 present analogous results on the T and U parameter. The calculated curves show only moderate agreement with the respective measurements of Berger.[25] Still, there is an obvious one-to-one correspondence between distinct structures seen in the experiment and those predicted by theory.

IV. CONCLUSIONS

We have shown that a simple Kohn-Sham-type theory of electron scattering by noble-gas atoms is capable of satisfactorily describing the wealth of data provided by various experimental groups. It appears to be particularly rewarding that the Kohn-Sham theory retains its considerable predicting power in a field of application where it has been expected to fail. In addition, our results on the scattering-induced polarization lends strong support to our method of accounting for relativistic effects by substituting Dirac-type equations for the one-particle Schrödinger equations and by adequately including exchange in the presence of spin-orbit coupling. (Although Strange *et al.*[26] have independently arrived at a similar scheme, there is no exact one-to-one correspondence between their potential and ours. Whether the expression given by these authors works similarly well in the case considered here has not yet been shown.) There is a number of obvious improvements the present method suggests making. First of all, the correlation factors for electrons of unlike spins have so far been assumed to vanish identically. It appears to be not too difficult, however, to go beyond that present level by incorporating approximate forms of these factors which conform to the sum rule (2d) and ensure proper asymptotic behavior according to (2e). In finding appropriate forms of these correlation factors it

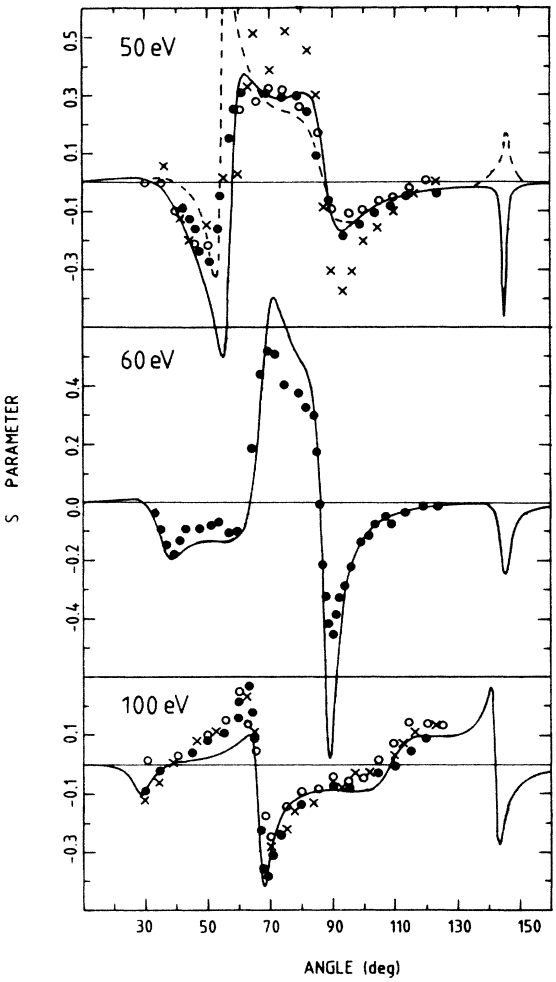

FIG. 7. S parameter for elastically scattered electrons by Xe atoms at impact energies of 50, 60, and 100 eV. Experiment: ●, Ref. 22; ○, Ref. 21; ×, Ref. 23. Theory: — — —, Fritsche (Ref. 1); ——, this work.

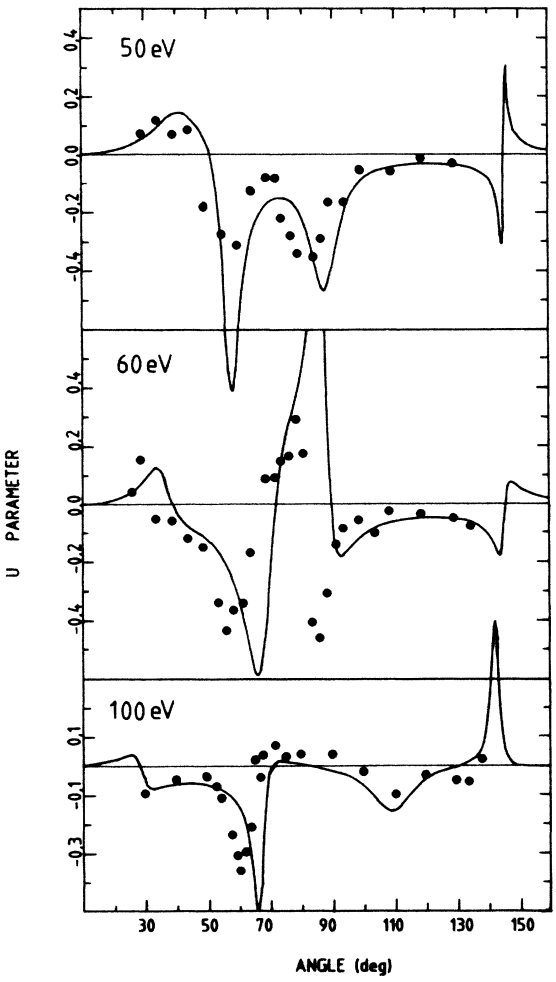

FIG. 9. U parameter for elastically scattered electrons by Xe atoms at impact energies of 50, 60, and 100 eV. Experiment: ●, Ref. 25. Theory: ——, this work.

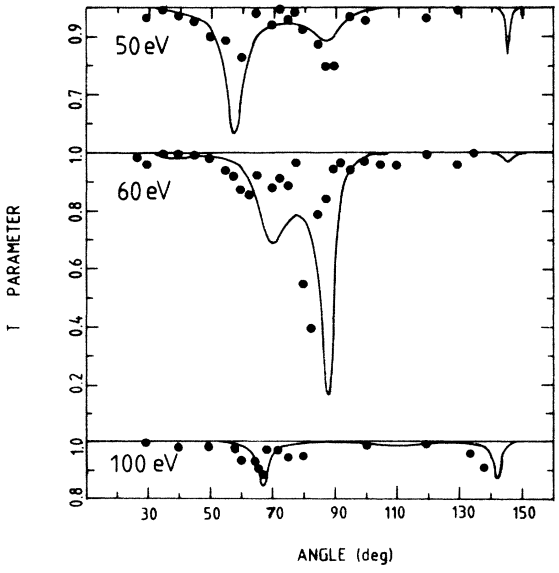

FIG. 8. T parameter for elastically scattered electrons by Xe atoms at impact energies of 50, 60, and 100 eV. Experiment: ●, Ref. 25. Theory: ——, this work.

is certainly advisable to consult configuration-interaction (CI) calculations for the systems in question. Work in this direction is in progress. Furthermore, asphericity effects brought about by nonspherical contributions of the projectile state to the total charge density should be accounted for. Finally, since the presence of inelastic channels gives rise to modifications in the elastic channels, the present theory should be extended accordingly.

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