Simple local potentials for elastic scattering of electrons by noble-gas atoms

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We study the performance of a simple l-dependent but otherwise local electron–noble-gas potential consisting of the direct electrostatic terms plus a $1/r^4$ polarization potential, which merges into a constant for $r \leq r_0$, r_0 depending on the target atom and the partial wave. This simple one-parameter potential reproduces low-energy elastic-scattering data by helium, neon, and argon, as well as the most advanced and sophisticated *ab initio* calculations. In a partial wave containing at least one occupied single-particle state in the target atom, the condition that the highest-lying bound state in the local potential has maximum overlap with the corresponding Hartree-Fock single-particle state of the atom, may serve as criterion for determining r_0.

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The theoretical description of low-energy electron scattering by inert-gas atoms has received considerable attention for several years [1–7]. Recent studies have been performed with potentials derived approximately on the basis of *ab initio* methods [4–7] or without explicit reference to a potential by solving a multiconfiguration Hartree-Fock (MCHF) problem for the electron-plus-atom system [8]. Earlier calculations based on simple phenomenological potentials [9] had few accurate experimental data for guidance. Accurate experimental phase shifts for electron scattering by inert gases became available relatively late [10], when theoretical work had already reached a high degree of sophistication, and the agreement obtained between theory and experiment is indeed quite satisfactory [5,8]. Probably due to this success there are relatively few detailed studies on how well simple phenomenological potentials are able to reproduce the accurate phase-shift data available today.

In this paper we study the performance of extremely simple potentials for the interaction of electrons with noble-gas atoms. The electron-atom potential contains the electrostatic attraction by the atomic nucleus (charge number Z) and the electrostatic repulsion by the N atomic electrons characterized by a charge density $-e\rho(\mathbf{r})$ [11]:

$$V_{es}(\mathbf{r}) = -Z\frac{e^2}{r} + \int \frac{e^2 \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 r' . \tag{1}$$

All remaining contributions due to correlation, polarization, etc. are summarized in a simple one-parameter term

$$V_{ec} = \begin{cases} -\alpha_d/2r^4, & r > r_0 \\ -\alpha_d/2r_0^4, & r \leq r_0, \end{cases} \tag{2}$$

where α_d is the (experimentally known) dipole polarizability of the target atom, and r_0 is an energy-independent distance at which the potential (2) merges into a constant.

At first sight, the potential (1)+(2) appears to lack consideration of exchange effects. One dominant consequence of exchange effects is that the wave function of the projectile electron is orthogonal to the single-particle wave functions of the electrons in the target atom [12]. The electrostatic potential (1) is dominantly attractive at

small separations and may, together with the correlation and polarization potential (2), support bound states quite similar to the electronic states in the target atom. This is in fact the case for the potentials used in this paper, so the automatic orthogonality of scattering wave functions to the bound states in the potential largely accounts for exchange effects and the requirements of the Pauli principle. Exchange effects which go beyond this (automatically fulfilled) orthogonality requirement are neglected.

The potential (2) has in fact been used on top of a local approximation to the exchange potential in a study of the s- and p-wave phase shifts in electron-helium scattering by Câmpeanu [13]. Nahar and Wadehra [14] used a similar ansatz with a smooth cutoff and an energy-dependent cutoff parameter to describe electron-argon scattering. Our present ansatz is one level simpler than Refs. [13] and [14] in that it contains no explicit consideration of exchange effects beyond the automatically fulfilled orthogonality condition.

Using potentials consisting of the electrostatic potential (1) and the regularized polarization potential (2) we calculated the scattering phase shifts for elastic scattering of electrons on He, Ne, and Ar. The polarizabilities α_d were taken from Ref. [15] and are (in atomic units): 1.38 for helium, 2.66 for neon, and 11.08 for argon. In each partial wave the (energy-independent) radius parameter r_0 was adjusted to give best agreement with the experimental phase shifts of Williams [10] in the energy region up to 20 eV where accurate data are available. The resulting values of the radius parameter r_0 and the rms deviation σ between calculated and experimental phase shifts are listed in Table I. Table I also contains the overlaps $\langle \phi_{nl} | \phi_{HF} \rangle$ between the bound states ϕ_{nl} (if any) in our local potential and the corresponding single-particle Hartree-Fock wave function(s) illustrated, e.g., for neon in Fig. 1. The overlaps in Table I are indeed all very close to unity, and solving the radial Schrödinger equation subject to the condition that the scattering wave be orthogonal to the single-particle (Hartree-Fock) bound states (if any) occupied by target-atom electrons in the respective partial wave leads only to marginal adjustments in r_0 and marginal improvements in σ.

TABLE I. Values of the parameter r_0 and performance of the simple local potential consisting of (1) and (2) for elastic electron scattering on helium, neon, and argon. σ is the rms deviation of the calculated phase shifts from the experimental values (Ref. [10]) (in units of π) in the energy range from zero to 20 eV. The last column shows the overlaps $\langle \phi_{nl} | \phi_{HF} \rangle$ of the occupied single-particle Hartree-Fock states (if any) in the target atom with the corresponding bound states ϕ_{nl} in the local model potential. The numbers in parentheses are the results obtained when the cutoff parameter r_0 is not fitted, but derived via the maximum-overlap criterion described in the text.

Element	Phase	r_0	σ	At. Orb.	Overlap
He	s	1.01	4.7×10^{-3}	$1s$	0.9975
		(0.95)	(2.3×10^{-2})		(0.9998)
	p	1.25	3.8×10^{-3}		
	d	1.88	5.3×10^{-4}		
Ne	s	0.974	3.6×10^{-3}	$1s$	0.9994
				$2s$	0.9993
		(1.00)	(9.2×10^{-3})		(0.9994)
	p	1.03	2.9×10^{-3}	$2p$	0.9994
		(1.02)	(5.6×10^{-3})		(0.9997)
	d	1.11	1.1×10^{-3}		
Ar	s	1.53	1.0×10^{-2}	$1s$	0.9998
				$2s$	0.9966
				$3s$	0.9973
		(1.57)	(1.7×10^{-2})		(0.9976)
	p	1.63	5.1×10^{-3}	$2p$	0.9961
				$3p$	0.9975
		(1.60)	(1.2×10^{-2})		(0.9977)
	d	1.83	2.1×10^{-2}		
	f	2.25	1.5×10^{-3}		

In the energy range up to about 20 eV, the short-ranged behavior of the potential is only important in the low partial waves listed in Table I. Higher partial waves are adequately described by the effective range formula [16,17]

$$\tan\delta = \frac{\pi\alpha_d}{(2l+3)(2l+1)(2l-1)} k^2 , \tag{3}$$

which only contains the dipole polarizability α_d as input. As an example Fig. 2 shows the differential cross section for scattering by neon at an electron-impact energy of 20 eV. The experimental points are from Ref. [18], the curve is from a calculation based on the potential (1)+(2) for partial waves up to $l = 2$ and complemented by the phase shifts from the effective range formula (3) for higher partial waves up to $l = 400$, where the differential cross sections have converged sufficiently.

The results obtained with the one parameter potential (1)+(2) are compared with the results obtained with more sophisticated methods in Table II. The columns list the rms deviations between calculated and experimental phase shifts for each partial wave in He, Ne, and Ar. AE stands for the adiabatic exchange approximation of McEachran and Stauffer [4] and PO stands for the polarized orbital calculation of Duxler, Poe, and La Bahn [19] in the helium case and of Dasgupta and Bhatia [6] for

neon and argon, respectively. In both the AE and PO calculations the electron-atom potential contains a complicated nonlocal contribution in order to account for exchange and polarization effects. The most advanced calculations are the MCHF calculations of Saha [8] which do not explicitly refer to an electron-atom potential. The phase shifts calculated by the AE, PO, and MCHF methods were not always given at the same energies as the experimental data of Williams. In order to have a sufficiently large and uniform set of numbers for compar-
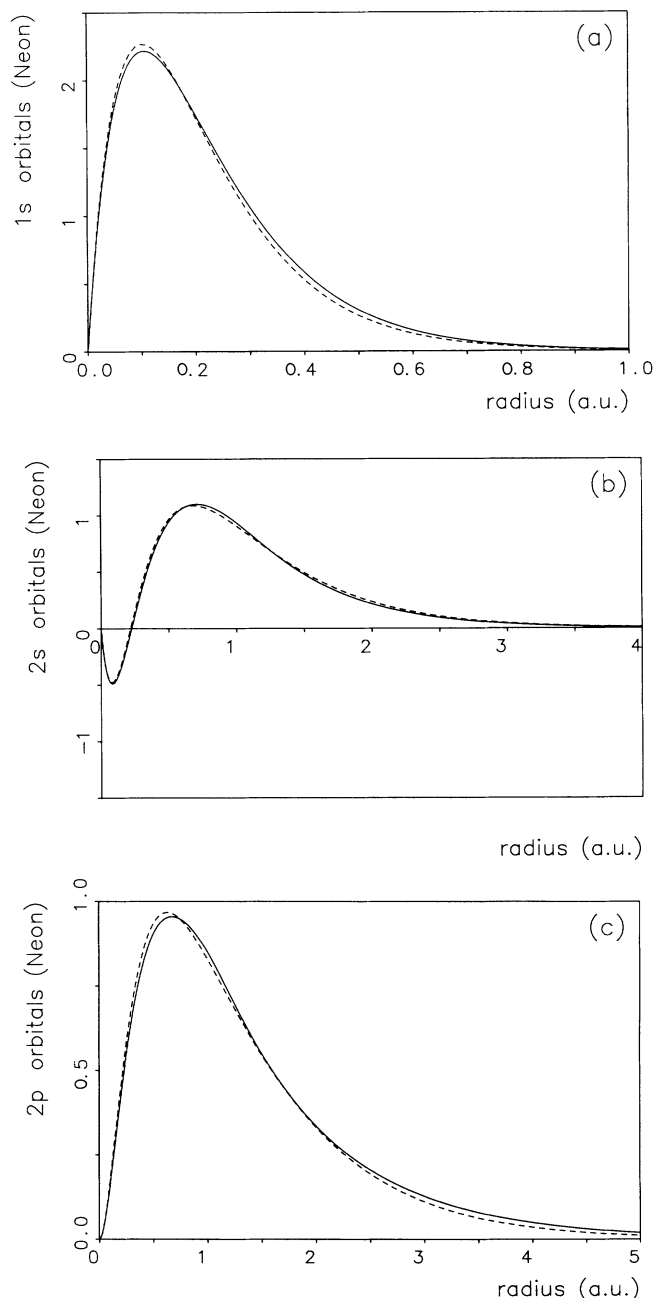

FIG. 1. The solid lines show the radial wave functions of the bound s states (a and b) and of the bound p state (c) in the local potential (1)+(2) for electron scattering on neon. The dashed lines show the corresponding Hartree-Fock single-particle wave functions.
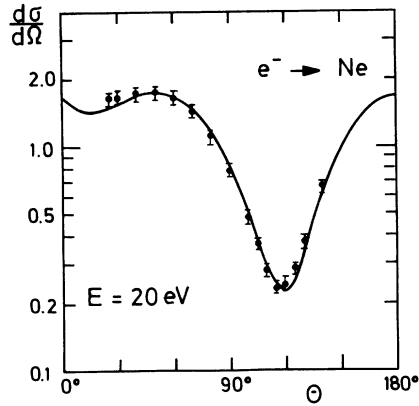
FIG. 2. Differential cross section for elastic scattering of electrons by neon at 20 eV. The experimental points are from Register and Trajmar [18], the curve was calculated using the (1)+(2) potential in partial waves up to $l=2$. Higher partial waves up to $l=400$ were included by the effective range formula (3).

TABLE II. rms deviations between calculated and experimental (Ref. [10]) phase shifts (in units of $10^{-3}\pi$) for elastic scattering of electrons by noble-gas atoms at energies up to 20 eV. The performance of the present simple local potential (1)+(2) is compared with the adiabatic exchange potential (AE) of McEachran and Stauffer (Ref. [4]), the polarized orbital potential (PO) of Duxler (Ref. [19]) for helium, and of Dasgupta and Bhatia (Ref. [6]) for neon and argon, respectively, and with the MCHF calculations of Saha (Ref. [8]).

Element	Phase	AE	PO	MCHF	This work
He	s	12	13	6.5	4.7
	p	7.4	2.9	1.6	3.8
	d	0.97	1.1	0.42	0.53
Ne	s	7.1	6.6	1.6	3.6
	p	2.7	2.7	2.9	2.9
	d	2.0	2.6	1.2	1.1
Ar	s	7.3	15	5.8	10
	p	4.4	5.4	4.6	5.1
	d	37	61	9.2	21
	f	1.9	2.2	4.3	1.5

ison we interpolated the calculated values via a spline routine and evaluated the rms deviation using the 27 (helium) or 22 (neon, argon) data points given by Williams. The phase shifts calculated with the present potential (1)+(2) are shown together with the experimental data in Fig. 3. In each case the phase is drawn to start at $n_b\pi$, where n_b is the number of bound states in the respective partial wave. In this way all phase shifts would converge to zero in the high-energy limit according to Levinson's theorem, if the simple potential model were valid for all energies.

The simple one-parameter local potential consisting of

(1) and (2) describes the available experimental phase shifts in the energy range up to 20 eV with a rms deviation σ of less than $1°$ in all cases except for the s wave $(1.8°)$ and the d wave $(3.8°)$ in the electron-argon scattering. In the latter case, where there is a pronounced resonance at about 14 eV, our results are nevertheless closer to the data than the AE and PO results.

For helium and argon the present results are also better than the fits of Refs. [13] and [14], respectively, where the deviation between calculated and experimental phase shifts is 1.5 to six times larger than in our calcula-
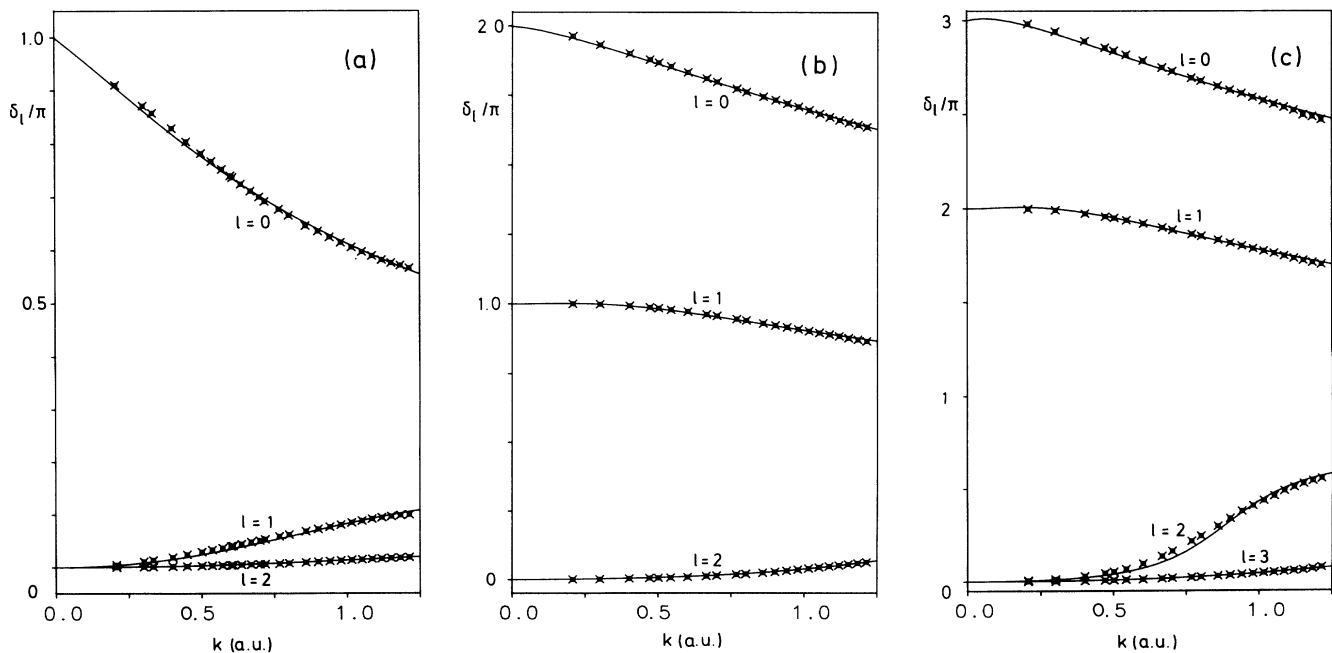

FIG. 3. Experimental (crosses [10]) and calculated (solid lines) phase shifts for elastic electron scattering on helium (a), neon (b), and argon (c).

tion. The fact that the fit in Ref. [13] used the same cutoff parameter r_0 in the s and p waves is compensated by the freedom of choosing one of five different local approximations to the exchange potential. The calculation in Ref. [14] also uses an l-independent cutoff parameter, but it is adjusted independently at each energy and shows considerable nonsystematic variations at low and intermediate energies.

All in all the simple (1)+(2) potential containing one phenomenological parameter in each partial wave performs better than most of the available potentials and even compares favorably with the most advanced *ab initio* calculations, namely the MCHF calculations of Saha. For the d wave in argon the MCHF calculation of Saha, which does not explicitly refer to an electron-atom potential, is the only one yielding a rms deviation of roughly the same magnitude as can be achieved in the other cases. The rms deviations obtained with the various potentials under investigation are larger by a factor 2 (our calculation), three (Ref. [14]), four (AE) and seven (PO).

The theoretical foundation for the (1)+(2) potential becomes sounder if there is an independent criterion for determining the parameter r_0 without having to refer to data. The fact that the fitted potentials support bound states of more than 99% overlap with the bound Hartree-Fock single-particle states points towards the following possible criterion for determining r_0: in a given partial wave l choose r_0 such that the overlap between the highest bound state and the Hartree-Fock single-particle wave function with the same number of radial nodes is a maximum. Reference to the highest bound state follows from the observation that the overlap of the lower-lying bound states with the corresponding Hartree-Fock single-particle states is always close to unity and rather insensitive to the value of r_0.

The above criterion of maximum overlap makes a lot of sense in the more general context of justifying local potentials for electron-atom scattering. As long as the target atom is well described by a Hartree-Fock wave function the orthogonality of the scattering wave function to the occupied Hartree-Fock single particle states is a strict consequence of the requirements of the Pauli principle, and it is brought about in the static exchange model by complicated nonlocal contributions in the potential. A local potential without bound states resembling the occupied Hartree-Fock single-particle states would violate this orthogonality requirement. Maximizing the overlap between the bound states in the potential and the occupied single-particle states in the target atom means optimizing the fulfillment of the orthogonality requirement.

We have redone the calculations with parameters r_0 determined by the maximum-overlap criterion described above. The results are listed in parentheses in Table I. The values r_0 obtained by applying the maximum-overlap criterion agree to within a few percent with the best-fit values. The rms deviation of the calculated phase shifts from the experimental values is of course larger when using the potentials based on the maximum-overlap criterion (which now contain no fitting parameter), but they are still of the same order of magnitude as the results of the AE and PO calculation (see Table II).

Summary. As far as elastic scattering at comparatively low energies goes, the complicated effects of exchange and correlation in the interaction of an electron with a helium, neon, or argon atom appear to be adequately described by a single (energy-independent) parameter in each partial wave. In the ansatz used in the present paper this parameter is the distance r_0 at which the asymptotic polarization potential merges into a constant. The requirements of the Pauli principle are largely accounted for by the automatic orthogonality of the scattering waves to the bound states of the local potential, which simulate the occupied single-particle states in the target atom. In a given partial wave containing at least one occupied single-particle state in the target atom, the condition that the highest-lying bound state in the local potential has maximum overlap with the corresponding Hartree-Fock single-particle state of the target atom may serve as a criterion for determining the parameter r_0. The values of r_0 determined in this way agree to within a few percent with the values obtained by fitting phase shifts to experimental data. Apparently the correct value of the dipole polarizability and good fulfillment of the orthogonality condition required by the Pauli principle are the key ingredients needed to reproduce experimental phase shift data in the low-energy region.

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