Relativistic effect in low-energy elastic scattering of electrons by inert-gas atoms

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Relativistic corrections must be made in a description of the elastic scattering of low-energy electrons by neon, argon, krypton, and xenon atoms. The interaction of an electron with an atom has been modeled by several spherically symmetric potentials. Numerical calculations have been carried out by the phase-function method and also through direct integration of the radial relativistic Dirac equation and the nonrelativistic Schrödinger equation. At energies below 1 eV, the difference between the values of the total cross section for the relativistic and nonrelativistic cases increases with increasing atomic number Z.

The cross section for elastic low-energy scattering of an electron by an argon atom was first calculated by Holtsmark[1] through a solution of the radial Schrödinger equation in a Hartree potential along with polarization forces. Nonrelativistic calculations of the total cross section for the elastic scattering of an electron by inert-gas atoms with various polarization and exchange potentials were carried out in Refs. 2–5. In 1991, Saha reported[6] the results of calculations in which the scattered electron was incorporated at the outset in a multiconfiguration nonrelativistic Hartree–Fock method. Experimental values were found for the total and partial cross sections for the elastic scattering of an electron by argon in Refs. 7–12.

In the present letter we use the phase-function method[13,14] to solve the radial relativistic Dirac equation and the nonrelativistic Schrödinger equation for elastic scattering by a spherically symmetric potential $V(r)$ which falls off more rapidly than r^{-1} at infinity. In an effort to test the results found by the phase-function method, we also carried out a direct integration of the radial Dirac and Schrödinger equations and then joined the results with the asymptotic solutions.

The normalized solutions of the radial Dirac equation[15] for the large component $g(r)$ and the small one $f(r)$ are

$$g(r)=\sqrt{\frac{E+mc^2}{2E}}A_{jl}(r)[\cos\delta_{jl}(r)j_l(pr)-\sin\delta_{jl}(r)\,\eta_l(pr)], \tag{1}$$

$$f(r)=l^{l-l'+1}\sqrt{\frac{E-mc^2}{2E}}A_{jl}(r)[\cos\delta_{jl}(r)j_{l'}(pr)-\sin\delta_{jl}(r)\,\eta_{l'}(pr)]. \tag{2}$$

Here j is the total angular momentum, l is the orbital angular momentum, $l'=2j-l$, E is the total energy of the electron, m is its mass, $\hbar$ is Planck's constant, c is the velocity

of light in vacuum, $p=\sqrt{E^2/c^2-m^2c^2/\hbar}$ is the wave vector, and $j_l(pr)$ and $\eta_l(pr)$ are spherical Bessel and Neumann functions, which were found in Ref. 16. The phase function[1)] $\delta_{jl}(r)$ and the amplitude function $A_{jl}(r)$ (Ref. 14) satisfy the system of equations[2)] of Ref. 13 with the boundary conditions $\delta_{jl}(0)=0, A_{jl}(\infty)=1$:

$$\frac{d}{dr}\delta_{jl}(r)=\frac{V(r)(pr)^2}{\hbar c}\left\{\sqrt{\frac{E+mc^2}{E-mc^2}}[\cos\delta_{jl}(r)j_l(pr)-\sin\delta_{jl}(r)\eta_l(pr)]^2\right.$$
$$\left.+\sqrt{\frac{E-mc^2}{E+mc^2}}[\cos\delta_{jl}(r)j_{l'}(pr)-\sin\delta_{jl}(r)\eta_{l'}(pr)]^2\right\}, \tag{3}$$

$$\frac{d}{dr}A_{jl}(r)=-\frac{A_{jl}(r)V(r)(pr)^2}{\hbar c}$$
$$\times\left\{\sqrt{\frac{E+mc^2}{E-mc^2}}[\cos\delta_{jl}(r)j_l(pr)-\sin\delta_{jl}(r)\eta_l(pr)]\right.$$
$$\times[\cos\delta_{jl}(r)\eta_l(pr)-\sin\delta_{jl}(r)j_l(pr)]$$
$$+\sqrt{\frac{E-mc^2}{E+mc^2}}[\cos\delta_{jl}(r)j_{l'}(pr)-\sin\delta_{jl}(r)\eta_{l'}(pr)]$$
$$\left.\times[\cos\delta_{jl}(r)\eta_{l'}(pr)+\sin\delta_{jl}(r)j_{l'}(pr)]\right\}. \tag{4}$$

We now take the nonrelativistic limit in Eqs. (3) and (4). In this case we have

$$\sqrt{(E+mc^2)/(E-mc^2)}\to 2mc/\hbar k, \quad \sqrt{(E-mc^2/(E+mc^2)}\to 0, \quad p\to k$$

[the nonrelativistic expression for the kinetic energy is $E_k=(\hbar k)^2/2m$]. We find equations for the phase function and the amplitude function[3)] (Ref. 14) under the boundary conditions $\delta_l(0)=0, A_l(\infty)=1$:

$$\frac{d}{dr}\delta_l(r)=\frac{2m}{h^2}V(r)kr^2\{[\cos\delta_{jl}(r)j_l(kr)-\sin\delta_{jl}(r)\eta_l(kr)]^2\}, \tag{5}$$

$$\frac{d}{dr}A_l(r)=\frac{2m}{h^2}A_l(r)V(r)kr^2\{[\cos\delta_l(r)j_l(kr)-\sin\delta_l(r)\eta_l(kr)]$$
$$\times[\cos\delta_l(r)\eta_l(kr)-\sin\delta_l(r)j_l(kr)]\}. \tag{6}$$

For scattering of a nonrelativistic particle by a potential with a characteristic depth on the order of mc^2, it is necessary to incorporate relativistic corrections. Accordingly, we cannot ignore the second term in Eq. (3) and simply go over to Eq. (5).

Let us apply these equations to the problem of the scattering of a low-energy electron by an inert-gas atom. We adopt a scattering potential

$$V(r)=V_a(r)+V_p(r)+V_{ex}(r), \tag{7}$$

where $V_a(r)$ is the potential of the unperturbed atom, which is the sum of the Coulomb potential of the interaction of the nucleus with a uniform charge distribution and the

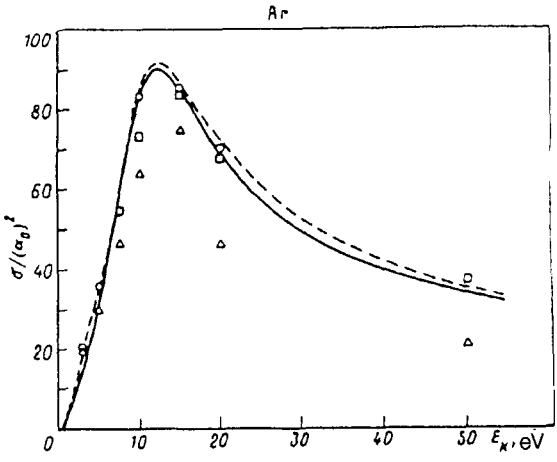

FIG. 1. Total scattering cross section σ, in atomic units, versus the kinetic energy of the electron, E_k in eV, for Ar. Solid curve—Results of a relativistic calculation; dashed curve—results of Ref. 6; points—experimental. ○) Ref. 7; △) Ref. 8; □) Ref. 9.

potential of an interaction with the electron density $\rho(r)$, found in the Hartree–Fock–Slater model of a unified atomic field in the relativistic approximation, $V_p(r)$ is the polarization potential, and $V_{ex}(r)$ is the exchange potential.

To determine the effect of the models used for the polarization and exchange potentials on the value found for the total cross section for elastic scattering of an electron by an argon atom, we carried out three series of numerical calculations with the following polarization potentials $V_p(r)$ and exchange potentials[4] $V_{ex}(r)$:

(1) with the polarization potential of Ref. 2 and the exchange potential of Ref. 18;
(2) with the polarization potential of Ref. 19 and the exchange potential of Ref. 18;
(3) with the polarization potential of Ref. 2 and the exchange potential of Ref. 20.

Figure 1 shows relativistic results[5] for the first model potentials, in comparison with calculations by Saha[6] and experimental data of Refs. 7–9. The cross section for the elastic scattering of an electron with a kinetic energy $E_k = 10^{-8}$ eV is $\sigma_{rel} = 51$ when relativistic corrections are taken into account (these are atomic units), while it is $\sigma_{nrel} = 44$ when these corrections are ignored. This difference is determined by the fairly deep potential of the unperturbed atom, $V_a(r)$, in which the characteristic momentum of the electron is relativistic, as was verified by an additional series of calculations in which the polarization potential $V_p(r)$ and the exchange potential $V_{ex}(r)$ were ignored.

In a second series of calculations, in which we changed the polarization potential $V_p(r)$, we found that the total elastic cross section changed only negligibly (by an amount on the order of 2%) in the entire energy range. In a third series of calculations, in which we changed the exchange potential $V_{ex}(r)$, we found a substantial difference from the previous results at kinetic energies $E_k \sim 1$ eV. At $E_k = 10^{-8}$ eV we found $\sigma_{rel} = 1630$, in atomic units. For kinetic energies E_k above 3 eV, all three calculations of the total cross section yield results in agreement with experimental data. In all three versions, the cross sections for the elastic scattering of an electron at a kinetic energy $E_k = 10^{-8}$ eV, according to the relativistic and nonrelativistic calculations, differ by about 15%. At low energies, the cross section depends strongly on the shape of the exchange

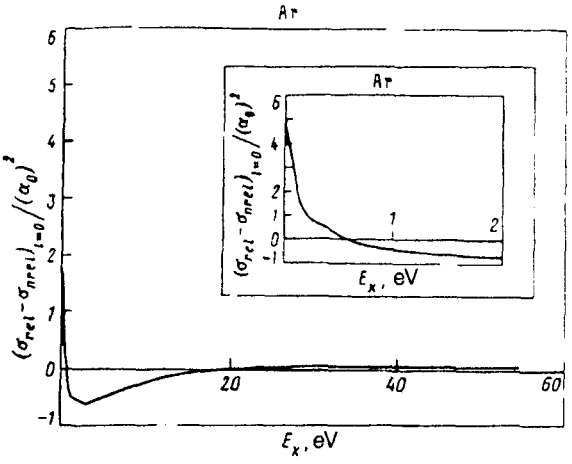

FIG. 2. Difference between the partial elastic cross sections for electron scattering for the s wave in the relativistic and nonrelativistic cases, in atomic units, for the Ar atom. The independent variable is the kinetic energy of the electron, E_k, in eV.

potential. An additional series of calculations, similar to the third except that we varied the contribution of the Riley exchange potential[20] [$V_{ex}(r)=nV_{ex}(r)$ (Ref. 20), where $0\leq n\leq 1$], confirmed this behavior.

Relativistic effects are significant in the cross section for the elastic scattering of an electron by an argon atom at low kinetic energies ($E_k < 5$ eV) for the s and p waves. With increasing E_k, the number of partial waves increases, and the relativistic effect in the total cross section σ falls off. Figure 2 shows the difference between the relativistic and nonrelativistic partial cross sections for the s wave. Figure 3 shows the difference between the sum of the relativistic partial cross sections $p_{1/2}$ and $p_{3/2}$ and the nonrelativistic partial cross section for the p wave for the case of the polarization potential $V_p(r)$ from Ref. 2 and the exchange potential $V_{ex}(r)$ from Ref. 18.

The difference between the results for the s-wave scattering phase shifts in the

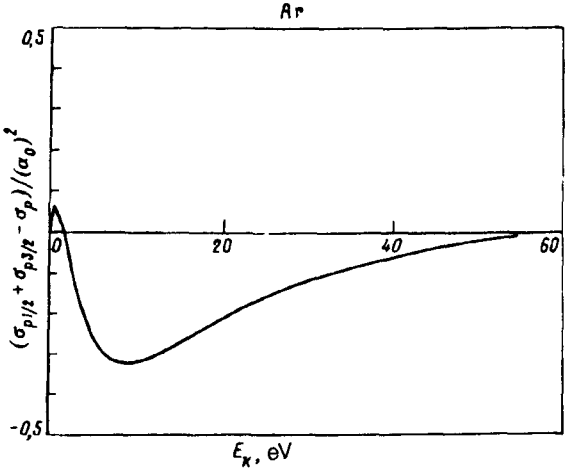

FIG. 3. Difference between the sum of the relativistic partial cross sections $p_{1/2}$ and $p_{3/2}$ for the elastic scattering of an electron and the nonrelativistic partial cross section for the p wave, in atomic units, for the Ar atom. The independent variable is the electron energy E_k, in eV.

relativistic and nonrelativistic methods, ignoring spin–orbit forces, shows that the difference between the total elastic cross sections found by these methods apparently cannot be explained by the spin–orbit coupling.

The use of the relativistic and nonrelativistic phase-function methods makes it possible to determine the particular distances at which relativistic effects come into play. For a fairly deep potential $V(r)$ we are no longer justified in discarding the second term from Eq. (3) in taking the nonrelativistic limit, since this term contributes to the value of the phase function $\delta_{jl}(r)$ when the equation is integrated. This conclusion is supported by a direct numerical integration of Eq. (3) with and without the second term.[6)] By studying the s-wave ($l=0$) phase function as a function of the distance from the center of the nucleus of the argon atom for an electron kinetic energy $E_k=10^{-8}$ eV, we found that the relativistic corrections begin to increase at distances r on the order of 2 a.u.

The difference between the relativistic and nonrelativistic results of calculations of the cross section for the elastic scattering of an electron by an atom stems from the depth of the unperturbed atomic potential $V_a(r)$, which in turn depends on the atomic number Z. We carried out calculations of the total cross section for the elastic scattering of an electron by atoms of the inert gases neon ($Z=10$), argon ($Z=18$), krypton ($Z=36$), and xenon ($Z=54$)[with the polarization potential $V_p(r)$ from Ref. 2 and the exchange potential $V_{ex}(r)$ from Ref. 18].

The results[17] show that, at low electron kinetic energies, the difference between the relativistic and nonrelativistic calculations increases substantially with increasing atomic number Z: At the energy $E_k=10^{-8}$ eV for the Ar atom, the relativistic cross section differs from the nonrelativistic one by 15%, and it differs from that of the heaviest atom, Xe, by 192%.

The accuracy of the experimental data currently available is such that even simple model potentials seem to be in good agreement with experiment. The most systematic theoretical nonrelativistic calculations[6] by the multiconfiguration Hartree–Fock method, incorporating an electron in the continuum, require immensely powerful computer systems such as the CRAYs. Our study has shown that relativistic corrections influence the values of the phase shifts and cross sections for elastic scattering. The method which we have used to solve the radial Dirac equation by the phase-function method can also be applied to other problems in which one needs to find only the scattering phase shift, not the wave function.

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[1)]Here $\delta_{jl}(\infty)=\delta_{jl}$ is the phase shift of the elastic scattering.

[2)]See Ref. 17 for a detailed derivation.

[3)]The phase function $\delta_l(r)$ and the amplitude function $A_l(r)$ of the Schrödinger equation depend on only the orbital angular momentum l; at nonrelativistic energies we have $\delta_l \approx \delta_{l+1/2,l} \approx \delta_{l-1/2,l}$, $p \approx k$.

[4)]The parameters of the potentials and their exact shapes can be found in Ref. 17.

[5)]The nonrelativistic results are not shown here, because of the small scale of this figure.

[6)]This approach is equivalent to a numerical integration of Eq. (5) for the nonrelativistic polarization method.

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