PHYSICAL REVIEW
LETTERS

VOLUME 16 | 20 JUNE 1966 | NUMBER 25

RELATIVISTIC VERSUS NONRELATIVISTIC SCATTERING OF SLOW ELECTRONS*

Larry Spruch
Physics Department, New York University, New York, New York
(Received 20 May 1966)

Relativistic effects can be important in the elastic scattering of particles incident with arbitrarily small velocities, provided the potential is sufficiently attractive to accelerate the particles to high velocities during the collision. One example is the scattering of slow electrons by a heavy atom stripped of most of its electrons. Numerical results presented in a recent Letter[1] indicated that relativistic (R) effects were significant in the more interesting case of the scattering of slow electrons (2 to 200 eV) by neutral heavy atoms; the phase shifts, δ, determined from the Schrödinger (S) and Dirac (D) equations were found to differ appreciably. Serious doubt has been cast[2] on the foundation of the calculation; arguments presented here should compound the doubt.

An equivalent one-body potential, obtained in the Hartree-Fock or some other such approximation, was used.[1] The same potential was used in the S and D equations in the scattering analysis. Rotenberg pointed out the inconsistency of this approach. (If the S equation describes scattering inadequately, it should also describe bound states inadequately and should not be used to determine the potential to be inserted into the D equation.) Proceeding phenomenologically, he chose two potentials, one for the S and one for the D equation, to match the binding energies of the valence electron of the low-lying levels of Na (and Cs). (The almost hydrogen-like higher levels demand only that the potential approach $-e^2/r$ for large r.) He found the nonrelativistic (NR) and R phase shifts (relative to Coulomb phase shifts) both for $l=0$ and for $l=1$ for the scattering of electrons by singly ionized Na (and Cs) to be rather close to one another. (The relativistic splitting of the $l=1$ phase shifts for $j=\frac{1}{2}$ and $j=\frac{3}{2}$ was small.)

[We will not concern ourselves with the question of why, for Hg, for example, the δ's obtained[1] from the S equation with a potential obtained with a NR approach were so different from the δ's obtained from the D equation with a potential obtained from (very approximate) R approach, nor of why different NR potentials lead to δ's that differ so greatly one from the other.]

We argue on somewhat broader grounds that R effects are probably not very important. The approach has both the advantages and the disadvantages of a formal treatment as opposed to a numerical calculation, namely, it is much more general—the details of the potential play almost no role—and it provides more insight but no explicit estimate of R effects. We make no pretense at rigor or complete generality.

Consider electron scattering by a spherically symetric neutral atom. Proceeding phenomenologically, we introduce in the NR approach a one-body potential V_λ containing spin-orbit coupling; the S partial-wave scattering equations that determine the phase shifts are

$$[T_l + V_\lambda - E]\Psi_\lambda(r) = 0, \tag{1}$$

where $V_\lambda(r) = U(r) + \lambda W(r)$, E is the incident kinetic energy, T_l is the kinetic-energy operator appropriate to angular momentum l, and $\lambda = l$ for $j = l + \frac{1}{2}$ and, for $l \neq 0$, $\lambda = -l-1$ for $j = l - \frac{1}{2}$. U and W are not yet specified in detail, but we take them to be spin and energy independent, and, for the moment, short-ranged. For the R approach, we choose a potential $v_D(r)$ satisfying these same properties. Manipulating the D equation with v_D into an equation of S form, the new potential is energy dependent and contains spin-orbit coupling. [See, for example, Eq. (2) of Ref. 1.] The energy dependence disappears upon neglecting E relative to mc^2, which one can do lightheartedly at the energies under consideration. The S form of the D equation is then

$$[T_l + v_\lambda - E]\psi_\lambda(r) = 0, \tag{2}$$

where $v_\lambda(r) = u(r) + \lambda w(r)$. u and w are short-ranged, and spin and energy independent. The S and D equations will lead to the same scattering if we choose v_D such that $v_\lambda(r) = V_\lambda(r)$, but we shall now see that such a stringent requirement is not necessary to achieve a near equality of the low-energy R and NR phases.

Let us assume that the electron and the atom can form one and only one $l = 0$ ionic bound state of very small binding energy, E_B, where $E_B = \frac{1}{2}\gamma^2\hbar^2/m$. (States with binding energies greater than $2E_B$ could be permitted.) For sufficiently small incident energies, it follows from NR effective range theory that $k\cot\delta(\mathrm{NR}, l = 0) \simeq -\gamma$. (See any nuclear theory text.) This remarkable result shows, excluding pathologies, that all short-ranged potentials that give the correct binding give practically the same low-energy $l = 0$ phase shift. v_λ (which here reduces to $v_0 = u_0$) will be short-ranged since v_D is, and we therefore have $k\cot\delta(\mathrm{R}, l = 0) \simeq -\gamma$. Thus, for γ and k exceedingly small, relativistic effects will be exceedingly small even though v_0 may contain highly singular terms. The argument is almost identical in form for a bound state characterized by $l \neq 0$ and $j = \pm\frac{1}{2}$.

In the NR case, the applicability of effective-range theory does not demand that V_λ be energy independent. This restriction can be dropped to allow a more realistic optical-model potential. The restriction can very likely be dropped in the R case as well.

In the significant regions of space we expect the spin-dependent part of the interaction to be small compared to the spin-independent part, and we expect $V_\lambda(r)$ to be roughly equal to $v_\lambda(r)$, but the argument presented is independent of the validity of these expectations.

As was pointed out to me by M. Ruderman, it is interesting, because of the simplicity of the Klein-Gordon (KG) equation, to compare the results obtained from the KG and S equations. Consider the problem of determining the low-energy scattering of a spinless particle by a center of force, when all that is known is that the interaction is spherically symmetric and short-ranged, and that a bound state of angular momentum l of the particle exists with a binding energy $E_B \ll mc^2$. We allow the possibility of there being regions of space within which the strength of the interaction is not negligible compared to mc^2. Choosing the vector potential to be zero, we can write the KG equation as

$$[(E_T - V_{KG})^2 - p^2c^2 - m^2c^4]\bar{\psi} = 0,$$

where E_T is the total energy and $V_{KG}(r)$ is energy independent. We have, equivalently,

$$[T_l + (E_T/mc^2)V_{KG} + (V_{KG}^2/2mc^2) - (p_0^2/2m)]\bar{\psi} = 0,$$

where p_0 is the incident momentum. For $p_0 \ll mc$, this reduces to an ordinary S equation with a potential $\bar{v}(r) = V_{KG} + (V_{KG}^2/2mc^2)$, with no restrictions on the strength of V_{KG}. If we choose V_{KG} such that $\bar{v}(r) = V(r)$, there are obviously no differences between the low-energy predictions of the KG and S equations, even though there may be domains of very strong interaction. As in the D case, one can rely on effective-range theory rather than so restricting V_{KG}.

We have been assuming that the various potentials are short-ranged, but, in fact, it is well known[3] that for sufficiently low energies for electrons incident on neutral atoms, $\delta(l = 0)$ is significantly affected and $\delta(l > 0)$ is completely determined by the long-range $(1/r^4)$ polarization potential. (Effective-range theory must be modified.) To the extent that the electric-dipole polarizability, α, is taken to be an experimentally determined number, relativistic corrections to these contributions to scattering are entirely negligible, since the contributions originate from great distances where the effective potential is exceedingly weak. [Incidentally, since the potentials used in Ref. 1 largely ignore long-range effects, the very-low-energy δ's are surely bad. Thus, $\alpha = 16.6a_0^3$

for Kr, and for very low energies E (in eV), we have

$$\tan\delta(l=2)=(\pi/105)(16.6)(E/13.6)+O(E^2),$$

leading to values of $\delta(l=2)$ much larger than those obtained from Fig. 3 of Ref. 1.]

The basic argument, presupposing the existence of a bound state and considering only that δ for the given l and j, is a very specialized one and is not conclusive. It proves only that regions of strong interaction need not lead to significant R effects, not that they cannot. It would be difficult to give a conclusive argument without getting closer to first principles in discussing the equivalent one-body potential to be used. Cowardice inhibits us from making quick simple estimates of the R effects, while sloth and the absence of more compelling reasons for believing R effects to be really significant keep us from making a serious theoretical analysis. The results of Rotenberg and those presented here, combined with the feeling that $v_\lambda - V_\lambda$ will be large only in that region, near the origin, where the valence electron or the incident particle spend little time because of the Pauli principle and (for $l \neq 0$) the centrifugal barrier, suggest that it is highly unlikely that the S and D equations, properly used, can really lead to results differing by a factor of 10. In fact, one suspects that R effects are probably much smaller, in general, than present uncertainties in NR calculations.

*Work sponsored by the U. S. Office of Naval Research, the Advanced Research Projects Agency under Contract No. Nonr-285 (49), NRO12-109, and the National Aeronautics and Space Administration under Contract No. NSG699.

[1]H. N. Browne and E. Bauer, Phys. Rev. Letters 16, 495 (1966).

[2]M. Rotenberg, Phys. Rev. Letters 16, 969 (1966).

[3]L. Spruch, T. F. O'Malley, and L. Rosenberg, Phys. Rev. Letters 5, 375 (1960); T. F. O'Malley, L. Spruch, and L. Rosenberg, J. Math. Phys. 2, 491 (1961).

IMPORTANCE OF CORRELATION EFFECTS IN THE IONIZATION OF HELIUM BY ELECTRON IMPACT*

F. W. Byron, Jr.,† and C. J. Joachain
Department of Physics, University of California, Berkeley, California
(Received 16 May 1966)

The phenomena of single and double ionization of helium by electron impact have received much recent interest both from the theroetical[1] and experimental[2-5] points of view.

Perhaps a fruitful way of looking at the double-ionization process is to say that it proceeds via final- (initial-) state interactions between the atomic electrons, following (preceding) a single interaction with the projectile electron. If we use exact initial- and final-state helium wave functions in the Born approximation to first order in the interaction between the projectile and the atom, we are essentially including initial- and final-state interactions between the two atomic electrons to all orders. Figure 1(a) shows a typical perturbation-theory diagram which is important for double ionization while Fig. 1(b) shows a diagram which, being of second order in the interaction with the projectile electron, is unimportant at high incident energies.

We consider the case where the incoming electron, although nonrelativistic, has sufficiently high energy so that we may neglect exchange between the incident and bound electrons. Then, applying the first Born approximation, we get

$$\frac{d\sigma_{n+}}{d\Omega}=\frac{m^2e^4}{4\pi^2\hbar^4}\sum_f\frac{k_f}{k_i}\left|\left\langle\exp(i\vec{k}_f\cdot\vec{r}_0)\Psi_f(\vec{r}_1,\vec{r}_2)\right|\right.$$
$$\left.\times V\left|\exp(i\vec{k}_i\cdot\vec{r}_0)\Psi_i(\vec{r}_1,\vec{r}_2)\right\rangle\right|^2 \quad (n=1,2), \quad (1)$$

where $\vec{k}_i$ and $\vec{k}_f$ are the initial and final propagation vectors of the projectile electron and

$$V=-\frac{2}{r_0}+\frac{1}{r_{01}}+\frac{1}{r_{02}} \quad (2)$$

is the interaction potential. The coordinates $\vec{r}_0$, $\vec{r}_1$, and $\vec{r}_2$ denote the incoming and the two atomic electrons, respectively. The function $\Psi_i(\vec{r}_1,\vec{r}_2)$ is the exact ground-state helium wave