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PHYSICAL REVIEW A VOLUME 2, NUMBER 5 NOVEMBER 1970

Intermediate-Energy Electron-Atom Scattering. I

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The problem of electron-atom scattering in the energy range where both high- and low-energy methods are unreliable is considered. A previously proposed equation is made tractable by a separable approximation on the electron-electron correlation function. This results in a pair of coupled equations in which all inelastic channels are lumped into one effective one. The equations are then reduced to a tractable form by some drastic approximations and solved by an eikonal approximation. The results are good in a restricted angular range, and the restrictions are shown to be due to the "drastic approximations" and the eikonal approximation, neither of which is really necessary.

When a particle is scattered by a target with internal degrees of freedom, the energy scale can be set in terms of an average excitation energy of the medium. When the incident energy is smaller than, or of the order of, this excitation energy, so that only a few channels are open, then there are reliable calculational methods for obtaining scattering amplitudes. For example, for the problem of electron-atom scattering the close coupling method[1] or its modifications[2] gives good results with a reasonable expenditure of computing effort when only a few channels are open. As the energy goes up and the number of open channels increases, the amount of computing time necessary for any given accuracy of the results becomes prohibitively large.

At high energies the Born approximation or its modifications[3] give good results, but as the energy is lowered approaching, say, ten times the scale energy, these methods also become less reliable. There is then a large energy region where there is a need for more reliable methods.

Chase[4] seems to have been the first to have suggested an approximation in which the target particles are frozen in a given configuration, and then the amplitude for scattering from this configuration is calculated. If we denote this amplitude for scattering from P_i to P_f by $f(P_f, P_i; X)$, where X represents the (fixed) coordinates of the target particles, then the theory gives a result for the inelastic (or elastic) scattering amplitude:

$$f_{n',n}(P_f, P_i) = \int (dX)\varphi^*_{n'}(X) f(P_f, P_i; X)\varphi_n(X), \quad (1)$$

where the $\varphi_s(X)$ are the target wave functions. The method has been generalized,[5] so that not all the target degrees of freedom have to be treated by this approximation. This is particularly useful in electron-molecule scattering where rotational and electronic degrees of freedom have widely different time scales (or energy scales).

This is a high- or intermediate-energy method, and the corrections to it become important as the energy decreases. It is however a better approximation than would seem justified at first sight. This may be explained as follows. There are two collision times involved: the duration of the collision with the entire target τ_1 and the duration of the collision with a single particle τ_2. For many cases $\tau_2 \ll \tau_1$. The approximation seems to be one in which the motion of the target particles during τ_1 is neglected. This is not completely true. For example, if in the multiple scattering of the projectile on the target particles it escapes before returning to a previously struck particle, the fact that the target particles move during τ_1 (but not τ_2) is not important. Thus the approximation may be described as one neglecting the motion during τ_2, except for corrections introduced by the projectile scattering twice or more off the same target particle during τ_1.

Recently, Foldy and Walecka[6] have discussed this model with the additional assumption of separable two-body potentials. This allows an essentially analytic solution for $f(P_f, P_i; X)$. For more realistic cases it is difficult to obtain this function without additional approximations.

Some simple approximations yield previously obtained results. For example, if one obtains from the single-particle equation (for the frozen target) $f(P_f, P_i; X)$ by first Born approximation, then Eq. (1) is just the usual first Born approximation. If one obtains $f(P_f, P_i; X)$ by an eikonal approximation, then Eq. (1) is the same as the Glauber[7] approximation. Thus the Glauber approximation may be viewed as just an eikonal approximation in Chase's model.

At the energies in question here, one can investigate cross sections for excitation to particular states, elastic, or total cross sections. Since excitation cross sections are probably the most demanding of the theory, we avoid them here. On the other hand, total cross sections are not very critically dependent on the theory. We therefore look at elastic scattering to begin with.

Experience in nuclear scattering shows that even a small imaginary part of the potential may have large effects in the cross section. The equivalent potential for elastic scattering has an absorptive part, but this has been neglected previously in atomic scattering. We attempt to include it here.

It has been shown in electron-atom scattering[8] and in nuclear-nucleus[9] scattering that the Pauli Principle is negligible at higher energies. We neglect it here. This is probably the most serious error in the theory and the most difficult to correct. The elastic scattering part of the wave function can be obtained from[10]

$$P\left(E - H - H\,\frac{Q}{E^{\dagger} - QHQ}\,H\right)P\psi = 0, \tag{2}$$

where P projects onto the target ground state and Q is its complement. There are open channels in the Q part of space so that the propagator $(E + i\eta - QHQ)^{-1}$ has an absorptive imaginary part. If we neglect the coupling of the projectile to the target to the extent that it can cause transitions in the target, then this propagator may be approximated[11] by

$$\frac{Q}{E + i\eta - QHQ} \simeq \sum_{n \neq 0} \int \frac{d^3k}{(2\pi)^3}\; \frac{\Psi_{kn}(r)\Phi_n(x)\Phi_n^*(x')\Psi_{kn}^*(r')}{p^2 - k^2 + W_0 - W_n + i\eta}\;. \tag{3}$$

Here the $\Phi_n(x)$ and W_n are the target wave functions and energies, $\Psi_{kn}^{(r)}$ are projectile wave functions in the potential presented by the target in the nth state, and p^2 is the incident energy. The essential approximation now is to neglect the excitation energy of the target relative to the incident energy. Thus the pole in the k integration which occurs at

$$k = \pm[p^2 + (W_0 - W_n)]^{1/2} \tag{4}$$

is taken at $\pm p$. This is precisely the approximation which, when made in the Lippman-Schwinger equation for the wave function, yields Chase's model. Note that the approximation is made here in the equivalent potential instead. In addition, we neglect the n dependence of the Ψ, in effect neglecting the difference of the scattering potentials in the various target states. The fact that the kinetic energy of the projectile is large in the intermediate state should make the propagator insensitive to the potential in which it propagates; we shall choose it below for convenience.

The sum over n can then be done by completeness, yielding a result for the equivalent potential in Eq. (2) which then yields an equation for the elastic wave function

$$P\Psi = \Phi_0(x)\Psi_p(r) \tag{5}$$

of the form

$$[P^2 - T - V_0(r)]\,\Psi_p(r) - \int d^3r'\, G(r, r')A(r, r')\Psi_p(r') = 0, \tag{6}$$

where V_0 is the static potential of the ground state:

$$V_0(r) = \int (dx)\,|\,\Phi_0(x)|^2\, V(r, X) \tag{7}$$

and $V(r, X)$ is the interaction of the projectile with all the target particles. The function A is given by

$$A(r, r') = \int (dx)(dx')\,\Phi_0^*(x)V(r, X)[\delta(x, x') - \Phi_0(x)\Phi_0^*(x')]\,V(r', X')\Phi_0(x')\;. \tag{8}$$

In this form its relation to the electron-electron correlation function in the atom is evident. It will be discussed further below. G is the propagator for the projectile in the average potential of the target.

The last term of Eq. (6) came from the Q part of the space in Eq. (2). It is well known that this term in Eq. (2) also yields the r^{-4} polarization potential in the adiabatic limit. It is also well known that the r at which the adiabatic limit becomes applicable gets larger the larger the energy.[12] Since we are interested in moderately high energies, here the r^{-4} local form of the potential is only applicable at distances where it is negligible, so its omission is unimportant here.

This form has been suggested earlier,[12] but it presents serious difficulties, the most obvious of which is that for Coulomb interactions the total neglect of $W_0 - W_n$ in the denominator of Eq. (3) yields a spurious long-range interaction which gives a logarithmic divergence of the cross section in the forward direction. This may be avoided by replacing $W_0 - W_n$ by some average excitation energy Δ, a phenomenological parameter. The result in the cross section is to replace the $\ln(q)$ dependence in the amplitude (q is the momentum transfer) by $\frac{1}{2}\ln(q^2+\Delta^2)$, so that the modification is important only in the small angular region given by $q^2 < \Delta^2$. A more serious difficulty presents itself in the solution of Eq. (6). We anticipate its use for intermediate energies where eikonal or WKB techniques are usually useful. However, the nonlocal potential in (6) is rapidly varying (because of G) so that these methods are not applicable. Even a partial-wave decomposition is cumbersome because of the vector dependence on r and r' of both G and A. All this has so far prevented a numerical solution of (6).

We now return to a discussion of the function A. After the neglect of the excitation energy in the denominator of (3), the sum can be performed by completeness.[12,13] However, we need not allow all excitations into the intermediate state. For example, in the problem of electron scattering by a heavy atom, completeness would include excitation of the inner electrons. One would have to go to very high energies before such excitation energies were negligible. Instead, one could limit the sum over intermediate states to ones in which the core of the target is frozen and only the outer electrons are allowed to excite. This presupposes a product form for the target wave functions, which is usually as good as one can do anyway. This is entirely analogous to the remarks made above in relation to the generalization[5] of Chase's model[4] where not all degrees of freedom are "frozen."

We use these ideas for electron-helium scattering as follows: Let us limit the intermediate states in (3) to single-particle excitations only. In addition, we assume that the excitation and deexcitation takes place fast enough so that the spectator electron cannot relax. The intermediate states then take the form

$$\Phi_n(x_1,x_2)=2^{-1/2}[g_n(x_1)g_0(x_2)+g_0(x_1)g_n(x_2)]\ ,$$

where g_0 is ideally the Hartree-Fock ground-state orbital of He and the g_n are some complete set of orthogonal orbitals of which g_0 is a member. Note that this is not a good approximation to the excited states of He, but is instead dictated by intuition as to what kind of excitations will be important. It is not difficult to modify this step and, indeed, a similar approximation is available for more complicated atoms, so that the method is in no way restricted to simple targets. The function A may now be rewritten as

$$A(r,r')=8\left(\int\frac{d^3x g_0^2(x)}{|x-r||x-r'|}-s(r)s(r')\right)\ , \tag{9}$$

$$s(r)=\int\frac{d^3x\, g_0^2(x)}{|x-r|}\ . \tag{10}$$

Equation (9) is still no further toward solution of (6). The first term in (9) is still not analytically obtainable[14] for even the simplest form of g_0. However, A is not a very startling function. It is positive, everywhere finite, symmetric, and vanishes as r^{-2} for large r. With the hope that the results are not critically dependent upon the detailed form of A we make a separable approximation for A:

$$A(r,r')=v(r)v(r')\ , \tag{11}$$

where we may reasonably choose

$$v(r)=[A(r,r)]^{1/2}\ . \tag{12}$$

Note that this is not a separable potential approximation; correlation between r and r' is still contained in G. It is rather an approximation replacing all the inelastic channels by one average one as will be clear below.[13]

The propagator G has not been completely specified. We chose it *for convenience* by using the ground-state static potential V_0 as the one occurring in G. This is not very physical, but we anticipate that its choice is not very crucial. With these approximations (6) can be rewritten as

$$(P^2-T-V_0)\Psi(r)-v(r)\int G(r,r')v(r')\Psi(r')d^3r'=0\ . \tag{13}$$

We define

$$\lambda(r)=\int G(r,r')v(r')\Psi(r')d^3r'\ , \tag{14}$$

$$X_\pm(r)=\Psi(r)\pm\lambda(r)\ , \tag{15}$$

so that (13) may be rewritten as a pair of uncoupled equations:

$$[P^2-T-(V_0\pm v)]X_\pm=0\ . \tag{16}$$

Note that the choice of V_0 in G results in the uncoupling of the two equations, but it is an inessential approximation when we admit the possibility of numerical solution of the coupled differential equations.

The potentials in (16) are real and central, so that standard methods may be used to obtain the scattering amplitudes $f_\pm$ or the real phase shifts $\delta_{1\pm}$. The elastic amplitude which we set out to obtain is then obtained from

$$f = \tfrac{1}{2}(f_+ + f_-) \,, \tag{17}$$

and the phase shift from

$$e^{2i\delta_1} = \tfrac{1}{2}(e^{2i\delta_{1+}} + e^{2i\delta_{1-}}) \,. \tag{18}$$

Note that both $\delta_{1\pm}$ are real but the δ_1 is not and

$$\mathrm{Im}\,\delta_1 = -\tfrac{1}{4}\ln\cos^2(\delta_{1+} - \delta_{1-}) \geq 0 \,, \tag{19}$$

so the process is absorptive as it must be. Returning to Chase's model for the moment, the elastic scattering phase shift is obtained from

$$e^{2i\delta_1} = \int (dx)\, |\Phi_0(x)|^2 e^{2i\delta_1(X)} \,, \tag{20}$$

which is a generalization of (18), in which the average over two terms, ±, has been extended to a weighted average over a continuous number of terms. Again, the absorptive result $\mathrm{Im}\,\delta_1 \geq 0$ is implied by (20).

An eikonal approximation for (16) is straightforward, yielding

$$f(P_f, P_i) = -ip \int_0^\infty b\,db\,J_0(qb)\{e^{-iu_1(b)/p}$$

$$\times \cos[u_2(b)/p] - 1\} \,, \tag{21}$$

$$q = P_f - P_i \,, \quad u_1(b) = \int_0^\infty d\xi\; V_0(r) \,,$$

$$u_2(b) = \int_0^\infty d\xi\, v(r), \quad r = (b^2 + \xi^2)^{1/2} \,. \tag{22}$$

The effect of the absorptive potential is solely in the factor $\cos[u_2(b)/p]$. If we chose the simplest variational approximation

$$g_0(x) = (a/\pi)^{3/2} e^{-ax} \,; \quad a = \tfrac{27}{16} \,, \tag{23}$$

then

$$V_0(r) = -(4/r)e^{-2ar}(1 + ar) \,, \tag{24}$$

$$s(r) = (1/r)[1 - e^{-2ar}(1 + ar)] \,. \tag{25}$$

$v(r)$, given by (12), can be expressed in terms of Lommel functions, but its computation seems unwarranted in view of the approximation of Eq. (11). Instead we fit a simple function to (12) by noting that

$$v(0) = a \,,$$

$$\lim v(r) \rightarrow \frac{2\sqrt{2}}{a}\,\frac{1}{r^2} + \frac{9}{\sqrt{2}}\,\frac{1}{a^3 r^4} \,, \quad \text{as } r \rightarrow \infty \,.$$

A function which reproduces this is

$$v(r) = \frac{a}{(r^2 + \beta^2)} + \frac{c}{(r^2 + \beta^2)^2} \,, \tag{26}$$

where

$$a = 2\sqrt{2}a^{-1} \,,$$

$$\beta^2 = 2\sqrt{2}\,a^{-2}(1 + \gamma) \,,$$

$$c = 8a^{-3}\gamma(1 + \gamma) \,,$$

with

$$\gamma = (1 + \tfrac{9}{16}\sqrt{2})^{1/2} = 1.32 \,.$$

The functions u_1 and u_2 are then obtained as

$$\begin{aligned} u_1 &= -4[K_0(2ab) + abK_1(2ab)] \,, \\ u_2 &= \sqrt{2}\,\pi a^{-1}(b^2 + \beta^2)^{-1/2} + \tfrac{1}{4}c\pi(b^2 + \beta^2)^{-3/2} \,. \end{aligned} \tag{27}$$

The remaining integral in f was carried out numerically for several energies and angles with the results displayed in Figs. 1 and 2. The experimental data are those of Vriens, Kuyatt, and Mielczarek.[15]

The most obvious feature of the results in the large peak in the theoretical cross section at small angles, well above the experimental one. We attribute this to the logarithmic divergence of (21) in the forward direction. An estimate of the angle below which this error becomes important can be obtained from the relation $q \leq \Delta$, where Δ is the "average excitation energy" mentioned above. Taking this as about 1.5 Ry, one obtains angles of about 10° for 300–400 eV, which fits well with Fig. 1. At larger angles the fit with the data is reasonable at the higher energies shown here (200 eV and above), but there is a tendency for the agreement between theory and experiment to worsen as the angles in-

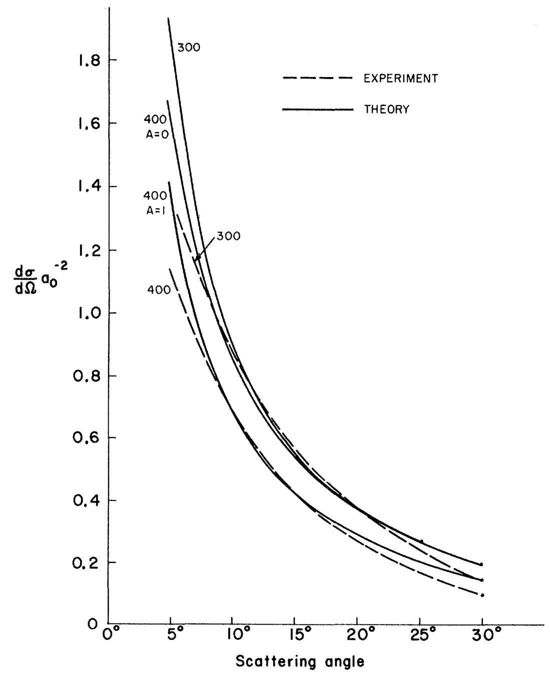

FIG. 1. $(d\sigma/d\omega)\, 1/a_0^2$ versus angle. The energy in eV is shown next to each curve. See the text for the meaning of $A=1$ or 0.

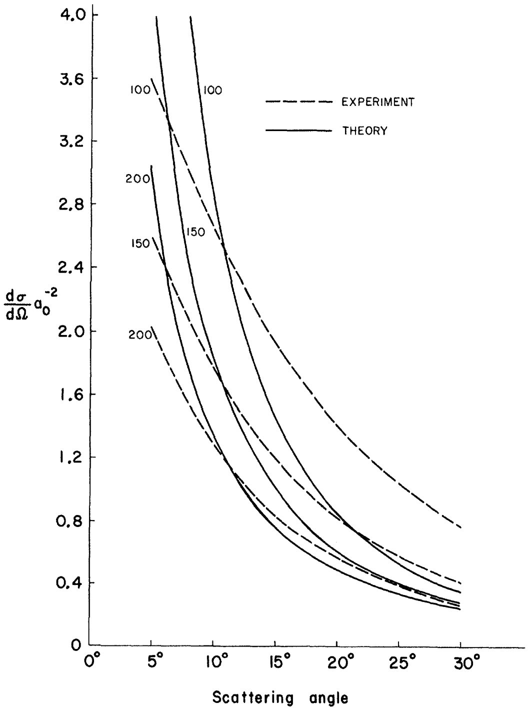

FIG. 2. $(d\sigma/d\omega)\ 1/a_0^2$ versus angle. The energy in eV is shown next to each curve.

crease. This may be attributed to a breakdown of the eikonal approximation to Eq. (16) at larger angles. At the lower energies in Fig. 2, the regions where the spurious logarithmic singularity is important and where the scattering angle is too large overlap, and the theory is totally unreliable.

In Fig. 1 we have also shown the result in which the inelastic channel is eliminated at only 400 eV. This result is just that obtained from an eikonal approximation on the static theory. It is clear that absorption is an important effect in elastic scattering.

There are many approaches for improving the eikonal approximation[16] at large scattering angles. Unfortunately, they all sacrifice the simplicity of Eq. (21) and result in multiple integrals instead. It therefore seems reasonable to abandon the approximate solutions to the uncoupled Eqs. (16) and instead solve the coupled equations which result from Eqs. (13) and (14). These are

$$\begin{aligned}(p^2 - T - V_0)\Psi(r) - v(r)\lambda(r) &= 0\ ,\\ (p'^2 - T - \overline{V})\lambda(r) - v(r)\Psi(r) &= 0\ ,\end{aligned}\qquad (28)$$

where $p'^2 = p^2 - \Delta$ and $\overline{V}$ is the average potential appearing in the intermediate-state propagator G. The inclusion of the phenomenological parameter Δ will eliminate the logarithmic divergence in the forward direction, and the potential $\overline{V}$ may consistently be set equal to zero. The resultant pair of coupled equations may then be solved with the aid of a partial-wave decomposition and a fast computer. Indeed, at this stage one can think of improving the separable approximation (11) to A. A simple generalization which seems reasonable is

$$A(r, r') = v(r)v(r') + u(r)\mathbf{r}\cdot\mathbf{r}'u(r'), \qquad (29)$$

which results in three coupled equations rather than the two of Eq. (28). These calculations will be described in a later publication.

Finally, we remark on Chase's model. The function $f(P_f, P_i; X)$ is not obtainable exactly except for electron-hydrogen scattering, in which case it can be obtained as the amplitude for scattering from an extended dipole. This case then provides a unique situation for checking some aspects of the Glauber approximation. This will also be discussed subsequently.

The content of this paper may be summarized by listing the approximations made.

(a) The Pauli Principle between the incident and target particles is neglected.

(b) The state changing coupling between target and projectile is neglected in the propagator $(E - QHQ)^{-1}$ of Eq. (2). This may also be viewed as a second-order evaluation of the equivalent potential.[12,13]

(c) The excitation energies are replaced by an average value Δ and the potential in which the projectile propagates in the intermediate state is made independent of the target state. This allows some completeness evaluation of Eq. (3).

(d) The Function A is replaced by some separable superposition such as (11) or (29) which makes the nonlocal rapidly varying Eq. (5) equivalent to a set of coupled local differential equations.

(e) The separability is specialized to one term, Δ is set equal to zero, and the potential that the projectile sees in the intermediate state is set equal to the static potential. This allows the decoupling of the pair of differential equation.

(f) The eikonal approximation is used to solve the equations.

We have tentatively attributed the deviation of the theory and experiment at large and small angles and low energies solely to approximations (5) and (6), neither of which are really necessary and both of which will be removed. The first three approximations seem absolutely necessary to yield any remotely tractable form for the theory. However, the fourth may not be necessary, that is, Eq. (6) may yet be solvable.

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Single-Electron Capture by C^{4+} in Helium, Neon, and Argon below 40 keV*

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Total cross sections for single-electron capture by C^{4+} from the target gases He, Ne, and Ar were measured at laboratory energies between 400 eV and 40 keV. The fast-collision products that scattered less than 1° were charge analyzed after single collision in a gas cell. Experimental results are interpreted in terms of pseudocrossings of the adiabatic potential curves for the initial and final states. The cross sections for $C^{4+}+\mathrm{He}$ and $C^{4+}+\mathrm{Ne}$ are consistent with the second maximum predicted for distant pseudocrossings by a numerical solution of the two-state semiclassical approximation by Bates, Johnson, and Stewart. Electron capture with an Auger-type ionization of the target is exothermic for $C^{4+}+\mathrm{Ne}$ and $C^{4+}+\mathrm{Ar}$ and is considered as the explanation of the large (50 Å^2) and slowly varying cross section measured for $C^{4+}+\mathrm{Ar}$.

I. INTRODUCTION

Low-velocity collisions between heavy particles frequently are described by the adiabatic potential-energy curves of the quasimolecule formed by the colliding atoms. The adiabatic description is appropriate when the relative velocity (V_R) of approach is small compared to the orbital velocity of internal electron motion. An electron transfer between collision partners is viewed in this model as a transition between states of the quasimolecule in a region of internuclear separation (R) where the adiabatic potential curves for the states are sufficiently close for an appreciable transition probability to exist. Collisions of multiply charged ions with neutral atoms are particularly interesting because the phenomenon of pseudocrossing of the adiabatic potential-energy curves significantly effects the transition probability.

The dominant process in multiply charged ion-atom collisions is usually single-electron capture, e.g.,

$$C^{4+}+\mathrm{He}\rightarrow C^{3+}+\mathrm{He}^{+}+\Delta E_i\ , \qquad (1.1)$$

where ΔE_i is the energy defect between the ith pair of initial and final states at infinite R. In the present experiment, a beam of C^{4+} ions was directed through a thin gas target under single-collision conditions, and the fast-collision products were separated and measured according to their charge. The ratio of C^{3+} to incident C^{4+} (ground state) provided the total cross section for single-electron capture without regard for the excitation state of the products. Since the relative collisions velocities were in the range of $(1-8)\times 10^7$ cm/sec, consideration of the adiabatic curves is appropriate. [For a carbon projectile, we have $E_{\mathrm{lab}}^{1/2}=25.2V_R$, where E_{lab} is in eV, and V_R in units of 10^7 cm/sec.]

Potential-energy curves for process (1.1) that include only the target polarization in the initial state and the Coulomb repulsion in the final state are good classical approximations for $R\gtrsim 2.5a_0$. If ΔE is positive (exothermic) and the states have the same symmetry, their adiabatic potential curves