PHYSICAL REVIEW A VOLUME 38, NUMBER 9 NOVEMBER 1, 1988

Nonadiabatic, momentum-dependent, and energy-dependent corrections in the effective-potential description for low-energy scattering of spinless systems: Their relations and validity

C. K. Au
Physics Department, University of South Carolina, Columbia, South Carolina 29208

(Received 23 July 1987; revised manuscript received 27 June 1988)

In the effective-potential description for low-energy scattering involving a spinless complex (a body with internal structure), the nonadiabatic corrections are sometimes disguised in momentum-dependent terms. These are distinct from energy-dependent corrections. A general procedure is given here by which all the momentum-dependent corrections can be converted into nonadiabatic corrections in truly local form. Circumstances under which an expansion of the effective potential, in terms of the adiabatic term plus nonadiabatic and energy-dependent corrections is allowed and forbidden, are discussed. An example for the latter is in the case of near degeneracy in the spectrum of the complex or in the extrapolation of the effective potential to short-distance behavior. This indicates that certain claims of "saturation effect" at short distances in low-energy electron-atom scattering are invalid.

I. INTRODUCTION

Two-body interaction and scattering processes are of wide interest in physics. In this paper, we confine our discussion to the scattering of a light spinless particle of mass m (the projectile) by an infinitely massive spinless complex (the target). We shall illustrate our discussion with the scattering of an electron (without spin) by a heavy spinless atom. Usually, the physical quantity of interest is the scattering amplitude, from which the scattering cross section can be computed. Very often, it is also desirable to have an effective potential in local form to describe the interaction. This potential V is conveniently defined as the Fourier transform of the on-shell scattering transition amplitude M (the T matrix) in the momentum transfer $\mathbf{Q}$ with respect to the distance vector $\mathbf{R}$ between the colliding particles.[1] Then the scattering amplitude is reproducible as the Born amplitude due to this effective potential. The scattering amplitude and the T matrix are related by a factor of $-m/2\pi$. Without fear of confusion, we shall use the scattering amplitude and the scattering transition amplitude interchangeably. A simple examination of the dimension is sufficient to make a distinction between the two. Since the spin-independent on-shell scattering amplitude is in general only a function of the collision energy and the magnitude of momentum transfer, the effective potential so defined possesses energy dependence. In all scattering processes, energy is conserved and so the energy dependence can be regarded as a parametric dependence. This is not so in bound-state problems where the energy levels are determined by the potential. Thus special care must be exercised when one extends an effective potential for scattering problems to bound-state problems, but we shall not be concerned with this issue any further in the present paper. Instead we examine the momentum-dependent terms in the effective potential that appear in some calculations.[2,3] These momentum-dependent terms occur because the scattering amplitude is being written as a function of the incident ($\mathbf{p}$) and emergent ($\mathbf{p}'$) momenta instead of as a function of the invariant scalars, namely, the center-of-mass-frame collision energy and the square of the momentum transfer. Off the energy shell, the scattering amplitude is a function of scalar quantities p^2, p'^2, and $\mathbf{p}\cdot\mathbf{p}'$, or equivalently of p^2, $\mathbf{p}\cdot\mathbf{Q}$, and Q^2 where $\mathbf{Q}=\mathbf{p}'-\mathbf{p}$ is the momentum transfer. On the energy shell, because $\mathbf{Q}\cdot(\mathbf{p}+\mathbf{p}')=0$ due to energy conservation, $\mathbf{Q}\cdot\mathbf{p}=-Q^2/2$. If one evaluates an effective potential $\bar{V}$ as the Fourier transform of the off-shell scattering amplitude $\bar{M}$, $\bar{V}$ appears as a function of p^2, R, and $\mathbf{p}\cdot\mathbf{R}$. Since $\bar{V}$ is derived from the off-shell amplitude $\bar{M}$, the momentum-dependent terms cannot be ignored even at threshold energy because zero energy does not imply zero momentum when the particle is off the energy shell.[4] In any case, whether it is used in a Schrödinger equation or in the evaluation of a scattering amplitude, the potential acts on a wave function corresponding to a state on the energy shell. Hence V, not $\bar{V}$, is the correct effective potential to use. Simple symmetry considerations would exclude terms proportional to odd powers of $\mathbf{p}\cdot\mathbf{R}$ since these violate time-reversal invariance. It is obvious that if the effective interaction is generated by Coulomb interactions, T invariance cannot be violated. Thus the momentum-dependent terms can appear only as functions of $i\mathbf{p}\cdot\mathbf{R}$. If left in this form, these momentum-dependent terms in the effective potential would give rise to non-Hermitian terms and are hence forbidden. A combination like $i\mathbf{p}\cdot\mathbf{R}-i\mathbf{R}\cdot\mathbf{p}$ is Hermitian but must be excluded because it is just a constant. Other combinations like $[i\mathbf{p}\cdot\mathbf{R}f(R)-if(R)\mathbf{R}\cdot\mathbf{p}]$, where $f(R)$ is a real function, can also be excluded because the momentum dependence can be eliminated by suitable use of commutation relations. If either or both of the colliding systems have spin then helicity-dependent terms appear in the scattering amplitude, leading to helicity-dependent effective potentials. However, in the absence of spin or any external vector that breaks the symmetry, these momentum-dependent terms in the effective potential are mathematical artifacts and should be transformed into truly local form. The mathematical procedure of transforming $\bar{V}$ into V upon imposition of the on-shell constraint (which is equivalent to setting $\mathbf{p}\cdot\mathbf{Q}$ equal to $-Q^2/2$) is given in Sec. III. The momentum-dependent terms in $\bar{V}$ reappear as nonadiabatic corrections in V. Nevertheless, there are circumstances under which it is invalid to expand the effective potential in terms of nonadiabatic and energy-dependent corrections. This occurs either when $R<[2m(E_n-E_0)]^{-1/2}$, where E_n-E_0 is the lowest excitation energy of the target complex, or when $p^2>2m(E_n-E_0)$, corresponding to the incident energy exceeding the lowest complex excitation threshold. For the scattering amplitude, this means a forbidden expansion in $Q^2/[2m(E_n-E_0)]$ or in $p^2/[2m(E_n-E_0)]$. Such situations can occur either when one tries to investigate the extremely-short-distance behavior of the effective scattering potential[2,3] or in the case of near degeneracy for the target complex.[2,5] In the infinite-mass limit, for both the target and the projectile, all the nonadiabatic corrections vanish. But for finite-mass projectile nonadiabatic corrections must be accounted for. It then becomes meaningless to extrapolate the effective potential to short distance while ignoring all momentum-dependent terms in $\bar{V}$ which transform into the nonadiabatic potentials in V. The invalidity to expand the effective potential in terms of nonadiabatic and energy-dependent corrections very likely excludes most calculational means by perturbation theory. This suggests that the most viable way of obtaining the effective potential at short distance is by means of variational calculations.

In Sec. II we discuss the general relation between the scattering amplitude and the effective potential defined by the Fourier transform of the former. In Sec. III we show that all momentum-dependent corrections in the effective potential $\bar{V}$ can be transformed into the nonadiabatic corrections in truly local form in the effective potential V upon imposition of the on-shell constraint and the general mathematical procedure for doing so is fully developed. The general discussions in Secs. II and III are applicable to both electron-atom and atom-atom scattering, ignoring spin effects. For finite-mass atoms, one replaces the projectile mass by the reduced mass and the vector $\mathbf{R}$ is then directed from the center of mass of the target to the center of mass of the projectile. In Sec. IV we study a situation in electron-atom scattering (both electron and atom taken to be spinless) where the nonadiabatic corrections can drastically alter the behavior of the effective potential indicated by the adiabatic term. This corresponds to a situation where it becomes invalid to seek an expansion of the effective potential in terms of nonadiabatic corrections. This happens under the circumstances described in the last paragraph. In Sec. V we add to our discussion on the validity of nonadiabatic and energy-dependent correction expansions in electron-atom scattering. $\hbar$ is set equal to 1 in this paper.

II. EFFECTIVE POTENTIAL: GENERAL PROPERTIES AND ITS RELATION TO THE SCATTERING AMPLITUDE

The amplitude of a two-body (spinless simple or complex particles) scattering process is a function of two Lorentz-invariant variables, usually taken to be s, the square of the energy in the center-of-mass frame, and t, the square of the four-momentum transfer. Under the present approximation, the scattering amplitude can only be a function of the atomic structure and the scalar quantities p^2 and Q^2. Within the physical region Q^2 is limited to be $\leq 4p^2$. The on-shell scattering amplitude is an analytic function in p^2 and Q^2 within its region of analyticity, which has nonzero measure as long as $p^2\neq 0$. An analytic continuation is then always possible to the unphysical region $Q^2>4p^2$. This analytic continuation in Q^2 into the unphysical region is necessary to obtain the effective potential as defined by Eq. (2.1) below.[6] The limiting behavior as $p\to 0$ can then be studied after the analytic continuation is carried out. In the covariant theory, that the scattering amplitude is an analytic function in s and t is a basic assumption in S-matrix theory, and this assumption is almost accepted as a fact. For elastic nonrelativistic scattering involving a heavy target, s reduces to the kinetic energy of the projectile plus the rest-mass energy of the scattering particles and t reduces to $-Q^2$.

The effective potential V is related to the scattering amplitude M by the Fourier transform in the momentum transfer $\mathbf{Q}$ with respect to the position vector $\mathbf{R}$,

$$V(R,p^2)\equiv\int\frac{d^3Q}{(2\pi)^3}e^{i\mathbf{Q}\cdot\mathbf{R}}M(Q^2,p^2)\ . \tag{2.1}$$

The scattering amplitude M depends on the structure of the target. Equation (2.1) clearly indicates that the effective potential should not have momentum-dependent terms. In a practical computation of the scattering amplitude, various approximation procedures, for example, a multipole expansion, are taken. To ensure that the subsequent scattering amplitude remains finite after taking these procedures, various cutoffs need to be introduced. However, if one is interested only in the effective potential as defined by Eq. (2.1), such cutoffs may be avoided by exchanging the orders of integration. The price one pays for this is that the Fourier transform in $\mathbf{Q}$ in Eq. (2.1) is taken before the completion of the evaluation of the scattering amplitude. In this event, one misses replacing $\mathbf{p}\cdot\mathbf{Q}$ by $-Q^2/2$ and the scattering amplitude is left off the energy shell and manifests itself as a function of the scalar quantities p^2, Q^2, and $\mathbf{p}\cdot\mathbf{Q}$. Consequently, the effective potential becomes a function of p^2, R, and $i\mathbf{p}\cdot\mathbf{R}$. Besides being ambiguous in the ordering of $\mathbf{p}$ and $\mathbf{R}$ since these variables do not commute, these ($i\mathbf{p}\cdot\mathbf{R}$)-dependent terms lead to non-Hermitian terms in the effective potential. It is possible to eliminate these non-Hermitian terms by a suitable transformation on the scattering wave function,[7–9] leading to effective local potentials. To see this from a slightly different angle, let us examine the term that goes like $i\mathbf{p}\cdot\mathbf{R}f(R)$. This resembles the coupling to a vector potential having a radial component only and whose dependence is entirely radial. Hence this vector potential seems not to lead to any physical magnetic field and such terms in the effective potential can be "gauged" away by a suitable gauge transformation. However, because of the factor i, the gauge function one needs to use is purely imaginary and the subsequent gauge transformation thus has a physical effect on the scattering wave function. Indeed, such a gauge transformation with a purely imaginary gauge function is equivalent to the scattering wave-function transformation that Norcross[8] employs to eliminate these non-Hermitian terms in the effective potential. However, such "gauge" transformations cannot be used to convert into local forms terms that depend on higher powers of $(i\mathbf{p}\cdot\mathbf{R})$.

These $(i\mathbf{p}\cdot\mathbf{R})$-dependent terms occur when one considers the nonadiabatic contributions to the effective potential, whose origin lies in the finite mass of the projectile. This makes $\mathbf{R}$, the position vector of the projectile relative to the target, a dynamical variable, not just a parameter; so is the momentum conjugate $\mathbf{p}$. Hence any projectile recoil effect and any nonadiabatic term have the same origin, and one must not emphasize one aspect while partially or completely neglecting the other. We shall return to this point later.

The momentum-dependent terms and the energy (p^2)-dependent terms are very different in origin since $\mathbf{p}\cdot\mathbf{Q}$ can be identified with $-Q^2/2$ and Q^2 and p^2 are independent scalar variables of the scattering amplitude. While all the p^2 and higher powers of (p^2)-dependent terms can be neglected at threshold energy, none of the $(i\mathbf{p}\cdot\mathbf{R})$-dependent terms which appear in the off-shell potential $\overline{V}$ can be neglected since threshold energy does not imply $\mathbf{p}=0$ when off the energy shell; they must be suitably converted into local forms. The mathematical prescription for such a procedure is given in Sec. III. Somewhat less general procedures, developed explicitly for the first and second nonadiabatic corrections, have been given previously.[10] The present paper deals with general nonadiabatic and energy-dependent corrections to any order.

III. NONADIABATIC AND MOMENTUM-DEPENDENT CORRECTIONS TO THE EFFECTIVE POTENTIAL AND THEIR TRANSFORMATION BETWEEN EACH OTHER

In this section, we would like to show that in the effective-potential description for the low-energy scattering of spinless particles, the momentum-dependent terms are mathematical artifacts and if these are expressed as a power series in $(i\mathbf{p}\cdot\mathbf{R})$, the truly local effective potential without momentum dependence can be recovered from the knowledge of the coefficients in this series. The result is expressed by Eq. (3.4), where the functions F_{kj} in Eq. (3.4) are determined by Eq. (3.17) and the functions $\overline{V}_{kj}$ in Eq. (3.17) are defined by a power series in Eq. (3.13). At threshold energy, the result is particularly simple and is given by Eq. (3.23).

In pursuing an effective interaction potential in the study of the scattering of a projectile by a target atom, one has, from the outset, classified the relevant variables into two groups: the atomic electron coordinates as the fast variables and the relative coordinates from the target to the projectile as the slow variables. For such an effective potential to be meaningful, one is necessarily confined to the low-projectile-energy region. We begin by assuming that the off-shell scattering amplitude $\overline{M}$ can be expressed as a power series in $\mathbf{p}\cdot\mathbf{Q}$ and p^2,

$$\overline{M}(Q^2, \mathbf{p}\cdot\mathbf{Q}, p^2) = \sum_{k,j} M_{kj}(Q^2)(\mathbf{p}\cdot\mathbf{Q})^k p^{2j} , \tag{3.1}$$

which on the energy shell reduces to

$$M(Q^2,p^2) = \sum_{k,j} M_{kj}(Q^2)(-Q^2/2)^k p^{2j} . \tag{3.2}$$

The truly local effective interaction potential is the Fourier transform of the on-shell scattering amplitude M in the variable Q with respect to $\mathbf{R}$,

$$V(R,p^2) \equiv \int \frac{d^3Q}{(2\pi)^3} e^{i\mathbf{Q}\cdot\mathbf{R}} M(Q^2,p^2) \tag{3.3}$$

$$= \sum_j p^{2j} \sum_k \left[\frac{\nabla^2}{2}\right]^k F_{kj}(R)$$

$$= \sum_j p^{2j} \sum_k \left[\frac{1}{2R^2}\frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R}\right]^k F_{kj}(R) , \tag{3.4}$$

where

$$F_{kj}(R) \equiv \int \frac{d^3Q}{(2\pi)^3} e^{i\mathbf{Q}\cdot\mathbf{R}} M_{kj}(Q^2) \tag{3.5}$$

is a function of $R=|\mathbf{R}|$ only. At threshold energy $p^2=0$ and only the $j=0$ terms survive in the double sum in Eq. (3.4),

$$V(R,p^2=0) = \sum_k \left[\frac{1}{2R^2}\frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R}\right]^k F_{k0}(R) . \tag{3.6}$$

The $k=0$ term in Eq. (3.6) reproduces the adiabatic potential and the $k\neq 0$, $j=0$ terms give the nonadiabatic corrections to the effective potential at threshold energy. Thus a very convenient interpretation is that k is the nonadiabatic correction index and j is the energy-dependence index.

If one had taken an effective potential as the Fourier transform of the off-shell scattering amplitude $\overline{M}$ as given in Eq. (3.1), the off-shell effective potential $\overline{V}$ would have an $(i\mathbf{p}\cdot\mathbf{R})$ dependence,

$$\overline{V}(R, \mathbf{p}\cdot\mathbf{R}, p^2) \equiv \int \frac{d^3Q}{(2\pi)^3} e^{i\mathbf{Q}\cdot\mathbf{R}} \overline{M}(Q^2, \mathbf{p}\cdot\mathbf{Q}, p^2) \tag{3.7}$$

$$= \sum_j p^{2j} \sum_k \int \frac{d^3Q}{(2\pi)^3} e^{i\mathbf{Q}\cdot\mathbf{R}} M_{kj}(Q^2)(\mathbf{p}\cdot\mathbf{Q})^k . \tag{3.8}$$

A tedious but straightforward computation leads to

$$\int \frac{d^3Q}{(2\pi)^3} e^{i\mathbf{Q}\cdot\mathbf{R}} M_{kj}(Q^2)(\mathbf{p}\cdot\mathbf{Q})^k$$

$$= \sum_{m=0}^{[k/2]} (-i\mathbf{p}\cdot\mathbf{R})^{k-2m} p^{2m} C^k_{2m} \frac{(2m+1)!!}{(2m+1)} (-i)^{2m}$$

$$\times \left[\frac{1}{R}\frac{\partial}{\partial R}\right]^{k-m} F_{kj} , \tag{3.9}$$

where

$$[k/2]=\begin{cases} k/2 & \text{if } k \text{ is even} \\ (k-1)/2 & \text{if } k \text{ is odd} \end{cases} \tag{3.10}$$

and

$$C_{2m}^{k}=\frac{k!}{(2m)!(k-2m)!} \tag{3.11}$$

is the usual combinatorics factor. Because this combinatoric factor is automatically zero when $m>[k/2]$, the upper limit in the summation in Eq. (3.9) can be removed. Then Eq. (3.8), in conjunction with Eq. (3.9), can be written as

$$\begin{aligned}\bar{V}(R,\,\mathbf{p}\cdot\mathbf{R},\,p^2)&=\bar{V}(\mathbf{R},\mathbf{p})\\ &=\sum_{j,k,m} p^{2(j+m)}(-i\mathbf{p}\cdot\mathbf{R})^{k-2m}C_{2m}^{k}\\ &\quad\times\frac{(2m+1)!!}{(2m+1)}(-i)^{2m}\\ &\quad\times\left[\frac{1}{R}\frac{\partial}{\partial R}\right]^{k-m}F_{kj}(R)\ . \end{aligned} \tag{3.12}$$

We now proceed to show how all the F_{kj}'s can be obtained from a knowledge of $\bar{V}(R,\,\mathbf{p}\cdot\mathbf{R},\,p^2)$ as a power series expansion in $(-i\mathbf{p}\cdot\mathbf{R})$ and p^2. We have

$$\bar{V}(R,\,\mathbf{p}\cdot\mathbf{R},\,p^2)=\sum_{k,j}\bar{V}_{kj}(R)(-i\mathbf{p}\cdot\mathbf{R})^k p^{2j}\ . \tag{3.13}$$

For convenience, we define the differential operator

$$D\equiv\frac{1}{R}\frac{d}{dR} \tag{3.14}$$

and its inverse $I\equiv D^{-1}$ such that for any function $f(R)$

$$If(R)\equiv\int_{\infty}^{R}xf(x)dx\ . \tag{3.15}$$

Then on comparing Eqs. (3.12) and (3.13), we obtain

$$\begin{aligned}\bar{V}_{kj}(R)=&\sum_{m=0}^{j}C_{2m}^{k+2m}\frac{(2m+1)!!}{(2m+1)}(-i)^{2m}D^{k+m}\\ &\times F_{k+2m,\,j-m}(R)\ . \end{aligned} \tag{3.16}$$

In general, Eq. (3.16) can be inverted in sequence and a general solution can be written in recurrent form

$$\begin{aligned}F_{kj}=I^k\bar{V}_{kj}-&\sum_{m=1}^{j}C_{2m}^{k+2m}\frac{(2m+1)!!}{(2m+!)}(-i)^{2m}D^{m}\\ &\times F_{k+2m,\,j-m}\ . \end{aligned} \tag{3.17}$$

It is clear that by substituting Eq. (3.17) into itself, F_{kj} can be expressed in terms of $\bar{V}_{k+2m,\,j-m}$ for $m=0,1,\ldots,j$. We write down the solutions explicitly for $j=0,1$, and 2,

$$F_{k0}(R)=I^k\bar{V}_{k0}(R)\ , \tag{3.18}$$

$$F_{k1}(R)=I^k\bar{V}_{k1}(R)+C_2^{k+2}I^{k+1}\bar{V}_{k+2,0}(R)\ , \tag{3.19}$$

and

$$\begin{aligned}F_{k2}=&I^k\bar{V}_{k2}+C_2^{k+2}I^{k+1}\bar{V}_{k+2,\,1}\\ &+(C_2^{k+2}C_2^{k+2}-3C_2^{k+4})I^{k+2}\bar{V}_{k+4,\,0}\ . \end{aligned} \tag{3.20}$$

Then the energy-dependent effective potential in a truly local form, when expanded as a power series in p^2 (the collision energy), is

$$V(R,p^2)=\sum_{j}p^{2j}V_j(R)\ , \tag{3.21}$$

with $V_j(R)$ given by

$$V_j(R)=\sum_{k}\left[\frac{\nabla^2}{2}\right]^{k}F_{kj}(R)\equiv\sum_{k}V_{kj}(R)\ , \tag{3.22}$$

according to Eq. (3.4). The function F_{kj} is determined by Eq. (3.17), where the function $\bar{V}_{kj}$ is in turn determined by the power series in Eq. (3.13). Here V_{kj} is the kth-order nonadiabatic correction to the effective-potential jth order in the collision energy (in p^{2j}). At threshold energy, the effective potential is given by $V_0(R)=\sum_k V_{k0}(R)$, that is, all the V_{k0} terms survive, not just V_{00} (which is identical to $\bar{V}_{00}$). Thus we have, from either Eq. (3.22) or Eq. (3.6),

$$V(R,p^2=0)=V_0(R)=\sum_{k}\left[\frac{\nabla^2}{2}\right]^{k}I^k\bar{V}_{k0}(R)\ . \tag{3.23}$$

The operator I, when acted on by the Laplacian operator ∇^2, obeys the equation

$$\begin{aligned}\nabla^2R^nI^k=&n(n+1)R^{n-2}I^k+(3+2n)R^nI^{k-1}\\ &+R^{n+2}I^{k-2}\ . \end{aligned} \tag{3.24}$$

This equation can be used iteratively to generate $(\nabla^2)^kI^k$ needed in Eq. (3.23). As an illustration, we write down the explicit results for the first few cases:

$$\nabla^2I^k=3I^{k-1}+R^2I^{k-2}\ , \tag{3.25}$$

$$\nabla^2\nabla^2I^k=15I^{k-2}+10R^2I^{k-3}+R^4I^{k-4}\ , \tag{3.26}$$

and

$$(\nabla^2)^3I^k=105I^{k-3}+105R^2I^{k-4}+21R^4I^{k-5}+R^6I^{k-6}\ . \tag{3.27}$$

This will enable us to obtain nonadiabatic corrections up to the third order. In general $(\nabla^2)^kI^k$ has the form $\sum_{j=0}^{k}C_jI^{-j}$, where the coefficients C_j can be determined from the repeated applications of Eq. (3.24). We remind our readers that

$$I^{-N}=(I^{-1})^N=D^N=\left[\frac{1}{R}\frac{d}{dR}\right]^{N} \tag{3.28}$$

and the operator I is defined in Eq. (3.15).

We conclude this section by pointing out that in the usual cases where an expansion in nonadiabatic corrections and collisional energy dependence is valid, the effective potential $V_{kj}(R)$ usually decreases as the order of k and j increase. But, as we show below, there exist exceptions where these corrections become important compared to $V_{00}(R)$, even at threshold energy, thus making the effective potential $V_0(R)=\sum_k V_{k0}(R)$ drastically different from $V_{00}(R)$. In fact, we give an example where $V_0(R)$ becomes divergent whereas $V_{00}(R)$ appears well behaved. This corresponds to a breakdown of the decomposition of the effective potential into its adiabatic approximation plus nonadiabatic correction. We emphasize again that the nonadiabatic corrections and projectile recoil corrections in the effective potential have the same origin, namely, the finite mass of the colliding particles. Hence any conclusion drawn from emphasizing projectile recoil effects in the evaluation of $V_{00}(R)$ while ignoring part or all of the nonadiabatic corrections is quite meaningless.

IV. WHERE NONADIABATIC CORRECTION EXPANSIONS FAIL: THE CASE OF NEAR DEGENERACY OR EXTRAPOLATION TO SHORT-DISTANCE BEHAVIOR IN ELECTRON ATOM SCATTERING

In this section, we study a situation where the nonadiabatic corrections cannot be ignored, even at threshold energy. We consider the scattering of a light and spinless charged projectile such as an electron or a positron, ignoring spin, from a momentum state $|\mathbf{p}\rangle$ to $|\mathbf{p}'\rangle$ by a heavy target atom in a rotationally invariant state $|0\rangle$ (for example, in a spin-averaged state). We assume that the dipole approximation is valid and shall return to discuss its validity later. Moreover, we confine ourselves to the discussion of the effect due to two instantaneous Coulomb photon exchange only and ignore any transverse photon-exchange effects. The two Coulomb photon-exchange scattering amplitude is given by

$$\overline{M}(\mathbf{p},\mathbf{p}')=\frac{4me^4}{\pi}\int d^3k\,d^3q\,d^3l\,\frac{k_\sigma q_\rho}{k^2q^2}\times\sum_n\frac{\langle 0|r_\sigma|n\rangle\langle n|r_\rho|0\rangle}{\Delta_n+l^2-p^2}\times\delta(\mathbf{p}'-\mathbf{q}-\mathbf{l})\delta(\mathbf{l}-\mathbf{k}-\mathbf{p})\,, \tag{4.1}$$

where

$$\Delta_n\equiv 2m(E_n-E_0)\,, \tag{4.2}$$

m is the mass of the charged projectile, e is the charge, $|n\rangle$ and $|\mathbf{l}\rangle$ are the intermediate states of the target atom and of the scattered particle, and E_n is the energy of the target atom in the state $|n\rangle$. Using $\mathbf{Q}=\mathbf{p}'-\mathbf{p}$ and writing $\overline{M}(\mathbf{p},\mathbf{p}')\equiv\sum_n\overline{M}^{(n)}(\mathbf{p},\mathbf{p}')$, where the index (n) indicates the contribution to the scattering amplitude from the atomic target intermediate state $|n\rangle$, we have

$$\overline{M}^{(n)}(\mathbf{p},\mathbf{p}')=\frac{4me^4}{\pi}\int\frac{d^3k}{k^2}k_\sigma\int\frac{d^3q}{q^2}q_\sigma\delta(\mathbf{Q}-\mathbf{k}-\mathbf{q})\times\frac{|\langle 0|z|n\rangle|^2}{\Delta_n+k^2+2\mathbf{p}\cdot\mathbf{k}}\,, \tag{4.3}$$

where we have carried out the integration over $\mathbf{l}$ in Eq. (4.1) and have made use of the rotational invariance of the state $|0\rangle$. If the integrals over $\mathbf{k}$ and $\mathbf{q}$ are performed in Eq. (4.3), the scattering amplitude $\overline{M}$ is a function of p^2, Q^2, and $\mathbf{p}\cdot\mathbf{Q}$, and is valid off-shell. On the energy shell, $\mathbf{p}\cdot\mathbf{Q}$ should be replaced by $-Q^2/2$. However, if the $\mathbf{k}$ and $\mathbf{q}$ integrals are postponed and the effective potential $\overline{V}$ is obtained as the Fourier transform of the off-shell amplitude $\overline{M}$ given by Eq. (4.3), on first carrying out the $\mathbf{Q}$ integral, we have a momentum-dependent effective potential

$$\overline{V}(\mathbf{R},\mathbf{p})=\sum_n\overline{V}^{(n)}(\mathbf{R},\mathbf{p})\,, \tag{4.4}$$

where

$$\overline{V}^{(n)}(\mathbf{R},\mathbf{p})=\frac{me^4}{2\pi^4}\int\frac{d^3k}{k^2}e^{i\mathbf{k}\cdot\mathbf{R}}k_\sigma\times\int\frac{d^3q}{q^2}e^{i\mathbf{q}\cdot\mathbf{R}}q_\sigma\frac{|\langle 0|z|n\rangle|^2}{\Delta_n+k^2+2\mathbf{p}\cdot\mathbf{k}}\,. \tag{4.5}$$

By exchanging the order of integration, the on-shell constraint has not been imposed and the potential expressed by Eq. (4.5) only corresponds to an off-shell potential. This potential must be transformed to the on-shell potential V according to the prescription given in Sec. III. The effective two-Coulomb exchange potential as given in Eqs. (4.4) and (4.5) is in agreement with that given by Kirzhnits and Pen'kov[2] and by Manson and Ritchie[3] in the limit of infinitely massive atoms after taking into account the rotational invariance of the initial state of the target atom. Kirzhnits and Pen'kov[2] arrive at the effective potential along a line similar to the procedure adopted here, whereas Manson and Ritchie[3] obtain their effective potential by a "complex single-particle self-energy" method. On carrying out the $\mathbf{q}$ integration, Eq. (4.5) becomes

$$\overline{V}^{(n)}(\mathbf{R},\mathbf{p})=\frac{ime^4R_\sigma}{\pi^2R^3}\int\frac{d^3k}{k^2}k_\sigma e^{i\mathbf{k}\cdot\mathbf{R}}\frac{|\langle 0|z|n\rangle|^2}{\Delta_n+k^2+2\mathbf{p}\cdot\mathbf{k}}\,. \tag{4.6}$$

In a previous analysis[10] where we were primarily concerned with the behavior of $\overline{V}(\mathbf{R},\mathbf{p})$ at large distances at threshold energy, we expanded the energy denominator in powers of $(k^2+2\mathbf{p}\cdot\mathbf{k})/\Delta_n$. Once in the numerator, terms proportional to k^2 and powers of k^2 can be neglected because they only lead to short-range terms. This is then equivalent to dropping k^2 in the energy denominator and then expanding it in powers of $2\mathbf{p}\cdot\mathbf{k}/\Delta_n$. This leads to the $(-i\mathbf{p}\cdot\mathbf{R})$- and p^2-dependent terms which are then subsequently converted into local form according to the prescription given in Sec. III. At threshold energy, all the terms proportional to p^2 and powers of p^2 can be neglected. In the present paper, we keep the k^2 term in the energy denominator. This allows us to study the mathematical property of $V^{(n)}(R)$ as either Δ_n or R approach zero. The results are interesting and we shall address the physical significance later on in this paper.

We expand the energy denominator in Eq. (4.6) as

$$(\Delta_n + k^2 + 2\mathbf{p}\cdot\mathbf{k})^{-1} = (\Delta_n + k^2)^{-1} \sum_{j=0}^{\infty} \left[\frac{-2\mathbf{p}\cdot\mathbf{k}}{\Delta_n + k^2} \right]^j \tag{4.7}$$

and define the following:

$$\langle z \rangle_n^2 \equiv |\langle 0 | z | n \rangle|^2 , \tag{4.8}$$

and

$$x_n \equiv R\sqrt{\Delta_n} = R\sqrt{2m(E_n - E_0)} . \tag{4.9}$$

Then if we expand $\bar{V}^{(n)}(\mathbf{R}\cdot\mathbf{p})$ as a power series in $(-i\mathbf{p}\cdot\mathbf{R})$ and in p^2 as we indicated in Sec. III, we have

$$\bar{V}^{(n)}(\mathbf{R},\mathbf{p}) = \sum_{k,j} \bar{V}^{(n)}{}_{kj}(R)(-i\mathbf{p}\cdot\mathbf{R})^k p^{2j} . \tag{4.10}$$

On using Eq. (4.7) in Eq. (4.6) and comparing with Eq. (4.10), we can obtain the $\bar{V}_{kj}^{(n)}(R)$ after the integration is performed. We get

$$\bar{V}_{00}^{(n)} = \frac{-2me^4\langle z \rangle_n^2}{R^2 x_n^2}[1-(1+x_n)\exp(-x_n)] , \tag{4.11}$$

$$\bar{V}_{10}^{(n)} = \frac{-4me^4\langle z \rangle_n^2}{R^2 x_n^4}[2-(2+x_n+x_n^2+x_n^3/2)\exp(-x_n)] , \tag{4.12}$$

$$\bar{V}_{20}^{(n)} = \frac{-4me^4\langle z \rangle_n^2}{R^2 x_n^6}\left[18 - \left[18 + 18x_n + 9x_n^2 + 3x_n^3 + \tfrac{3}{4}x_n^4 + \frac{x_n^5}{4}\right]\exp(-x_n)\right] , \tag{4.13}$$

and

$$\bar{V}_{01}^{(n)} = \frac{-4me^2\langle z \rangle_n^2}{x_n^6}\left[6 - \left[6 + 6x_n + 3x_n^2 + x_n^3 + \frac{x_n^4}{4}\right]\exp(-x_n)\right] , \tag{4.14}$$

where we have only written out the first few $\bar{V}_{kj}^{(n)}$ explicitly. The momentum-dependent potential can be transformed into truly local form according to the prescription in Sec. IIII. We get

$$V_{00}^{(n)}(R) = \bar{V}_{00}^{(n)}(R) = \frac{-2me^4\langle z \rangle_n^2}{R^2 x_n^2} \times [1-(1+x_n)\exp(-x_n)] , \tag{4.15}$$

$$V_{10}^{(n)}(R) = \frac{2me^4\langle z \rangle_n^2}{R^2 x_n^4}[6-(6+6x_n+3x_n^2+x_n^3 \times x_n^4/2)\exp(-x_n)] , \tag{4.16}$$

$$V_{20}^{(n)}(R) = \frac{-2me^4\langle z \rangle_n^2}{R^2 x_n^6} \times \left[135 - \left[135 + 135x_n + \tfrac{135}{2} + x_n^2 + \tfrac{45}{2}x_n^3 + \tfrac{45}{8}x_n^4 + \frac{9}{8}x_n^5 + \frac{x_n^7}{8}\right] \times \exp(-x_n)\right] , \tag{4.17}$$

and

$$V_{01}^{(n)}(R) = \frac{-2me^4\langle z \rangle_n^2}{x_n^6} \times \left[6 - \left[6 + 6x_n + 3x_n^2 + x_n^3 + \frac{x_n^4}{4} + \frac{x_n^5}{4}\right] \times e^{-x_n} + \frac{x_n^6}{4}\mathrm{Ei}(-x_n)\right] , \tag{4.18}$$

where

$$\mathrm{Ei}(-x) \equiv \int_{\infty}^{x} \frac{e^{-t}}{t} dt \tag{4.19}$$

is the exponential integral function and the truly local on-shell effective potential is represented by

$$V(R,p^2) = \sum_n V^{(n)}(R,P^2) , \tag{4.20}$$

where

$$V^{(n)}(R,p^2) = \sum_{k,j} V_{kj}^{(n)}(R)p^{2j} \equiv \sum_j V_j^{(n)}(R)p^{2j} . \tag{4.21}$$

For large values of x_n, Eqs. (4.11) to (4.18) agree with the results obtained previously[10] since all the exponential terms can be dropped. At threshold energy, the effective potential is given by

$$V^{(n)}(R, p^2=0) = \sum_k V_{k0}^{(n)}(R) , \tag{4.22}$$

which is the sum of the classical polarization (adiabatic) potential and its nonadiabatic corrections. We notice that all the functions $V_{k0}^{(n)}(R)$ are of the form

$$V_{k0}^{(n)}(R) = \frac{-me^4\langle z \rangle_n^2}{R^2} f_k(x_n) , \tag{4.23}$$

where the function $f_k(x_n)$ is displayed explicitly for $k=0$, 1, and 2 in Eqs. (4.15)–(4.17), and can be evaluated in a straightforward but tedious manner for all finite integral values of k. As x_n goes to zero, $f_k(x_n)$ becomes

$$\lim_{x_n \to 0} f_k(x_n) = C_k^{-1/2}(-1)^k , \tag{4.24}$$

where $C_k^{-1/2}$ is the generalized combinatoric factor. This can be verified in a straightforward way for $k=0$, 1, and 2 from Eqs. (4.15)–(4.17). For higher values of k, it can be verified by the expansion of Eq. (4.6) and then following the procedure described in Sec. III. Equation (4.24) has very interesting implications. It shows that as x_n goes to zero, we have

$$\lim_{x_n \to 0} V^{(n)}(R, p^2=0) = \frac{-me^4\langle z\rangle_n^2}{R^2} \sum_k C_k^{-1/2}(-1)^k . \tag{4.25}$$

The sum in Eq. (4.25) diverges as $(1-\mathcal{X})^{-1/2}$ in the limit $\mathcal{X} \to -1$ and indicates that the usual classification into the polarization potential and its nonadiabatic correction breaks down as x_n approaches zero. The equivalence of the result of Eq. (4.25) and that of Kirshnitz and Pen'kov will be demonstrated below in Eq. (4.29) and Eq. (4.33). The equivalent singular behavior is exhibited in Eq. (4.38). Note that if one ignores all the nonadiabatic corrections and keeps only the polarization potential, one gets

$$\lim_{x_n \to 0} V_{00}^{(n)}(R) \sim \frac{-me^4\langle z\rangle_n^2}{R^2} . \tag{4.26}$$

This has been noticed by Manson and Ritchie and has led them to conclude incorrectly that recoil effects of the electron "saturate" the usual dipole polarization R^{-4} potential to a R^{-2} potential at short distances.[3] As we have seen, recoil effects of the electron and nonadiabatic corrections have the same origin in the finite mass of the projectile. One cannot emphasize one while ignoring part or all of the other. An extrapolation to short-distance behavior cannot be made once the effective potential is expressed in terms of nonadiabatic corrections (or equivalently momentum-dependent corrections which are nondiabatic corrections in disguise). Alternately, we can say that the limiting procedure of $R \to 0$ and the sums over k and j (the nonadiabatic and energy correction indices) in Eqs. (4.20) and (4.21) do not commute.

Next, we observe that for x_n to approach zero, it is possible to have either R going to zero or Δ_n going to zero. The latter corresponds to the existence of a closely degenerate state in the spectrum of the target atom to which the initial state can couple.[5] One way of understanding the equivalence between R going to zero and Δ_n going to zero is to examine Eq. (4.6). From the Fourier integral, at short distances, the major contribution to the integral comes from large k and, in this case, Δ_n can be dropped relative to k^2. In this event, the integral in Eq. (4.6) can be done exactly by means of the Feynman parametric integral and we have

$$\lim_{R \sim 0} \bar{V}^{(n)}(\mathbf{R},\mathbf{p}) = \lim_{\Delta_n \sim 0} \bar{V}^{(n)}(\mathbf{R},\mathbf{p}) = \bar{V}^{(n)}(\mathbf{R},\mathbf{p}, \Delta_n = 0)$$

$$= \frac{me^4\langle z\rangle_n^2}{\pi^2 R^3} \int \frac{d^3k}{\partial R} e^{i\mathbf{k}\cdot\mathbf{R}} \frac{i\mathbf{k}\cdot\mathbf{R}}{k^2+2\mathbf{p}\cdot\mathbf{k}} \tag{4.27}$$

$$= \frac{me^4\langle z\rangle_n^2}{R^3} \int_0^1 d\alpha\, R_\sigma \frac{\partial}{\partial R_\sigma} \frac{\sin(\alpha p R)}{\alpha p} \exp(-i\alpha\mathbf{p}\cdot\mathbf{R}) \tag{4.28}$$

$$= \frac{-me^4\langle z\rangle_n^2}{R^3} \frac{\sin(pR)}{p} \exp(-i\mathbf{p}\cdot\mathbf{R}) , \tag{4.29}$$

which agrees with the result of Kirzhnits and Pen'kov[2] for short distances [their Eq. (3.2)]. If one were to replace $\sin(pR)/p$ by R and $\exp(-i\mathbf{p}\cdot\mathbf{R})$ by unity in Eq. (4.29), one would recover Eq. (4.26), the Manson-Ritchie result. However, since the potential $\bar{V}^{(n)}$ as given by Eq. (4.29) is the off-shell potential, the momentum-dependence cannot be ignored even at threshold energy. Equation (4.29) can be shown to be equivalent to the results in Eq. (4.25) if the momentum-dependent exponential factor in Eq. (4.29) can be expanded in a power series, as we shall show shortly in Eq. (4.33). In the analysis of Kirzhnits and Pen'kov,[2] the momentum dependence in the exponential factor in Eq. (4.29) is retained. Equation (4.29) is in a very convenient form for expansion in $(-i\mathbf{p}\cdot\mathbf{R})$ and p^2. According to Eq. (3.13),

$$\bar{V}^{(n)}(\mathbf{R},\mathbf{p}) = \sum_{k,j}^{(n)} \bar{V}_{kj}(R)(-i\mathbf{p}\cdot\mathbf{R})^k p^{2j} ,$$

we have

$$\lim_{\Delta_n \to 0} \bar{V}_{kj}^{(n)}(R) = \frac{-(-1)^j R^{2j-2}}{k!(2j+1)!} me^4\langle z\rangle_n^2 . \tag{4.30}$$

In particular, at threshold energy, $p^2=0$, only the $j=0$ terms survive and we have

$$\lim_{\Delta_n \to 0} \bar{V}_{k0}^{(n)}(R) = \frac{-me^4\langle z\rangle_n^2}{R^2 k!} . \tag{4.31}$$

This simple form of $\bar{V}_{k0}^{(n)}(R)$ can then be used in Eq. (3.23) to obtain the effective potential at threshold energy in a truly local form. By an explicit calculation, we obtain

$$\left[\frac{\nabla^2}{2}\right]^k I^k R^{-2}/k! = \frac{(-1)^k}{R^2} C_k^{-1/2} . \tag{4.32}$$

On substituting Eq. (4.31) into Eq. (3.23) and using the property in Eq. (4.32), we have

$$V^{(n)}(R,p^2=0,\ \Delta_n=0)=\frac{-me^4\langle z\rangle_n^2}{R^2}\sum_k C_k^{-1/2}(-1)^k\ , \tag{4.33}$$

in agreement with Eq. (4.25). We already notice that the sum in Eq. (4.33) or in Eq. (4.25) is divergent. The present analysis indicates that in the simultaneous limits $p^2\rightarrow 0$ and $\Delta_n\rightarrow 0$, the usual decomposition of the effective potential into the polarization potential and nonadiabatic and energy-dependent corrections breaks down.

A question that needs to be raised at this point is that since Eq. (4.6) can be evaluated exactly for $\Delta_n=0$, what, if anything, then is wrong with the momentum-dependent potential as given in Eq. (4.29). A momentum-dependent effective potential is a mathematical artifact corresponding to the Fourier transform of the off-shell scattering amplitude instead of the on-shell amplitude. In any physical process, the scattering amplitude is the physically relevant quantity and the effective potential is a mathematical convenience. Therefore we next try to recover the scattering amplitude from the momentum-dependent effective potential and from there understand the nature of the divergence that occurs in the effective potential when expressed as a decomposition into the polarization potential plus nonadiabatic and energy-dependent corrections. The scattering amplitude corresponding to the momentum-dependent effective potential is

$$M^{(n)}(\mathbf{Q},\mathbf{p},\ \Delta_n=0)=\int d^3R\ e^{-i\mathbf{Q}\cdot\mathbf{R}}\bar{V}^{(n)}(\mathbf{R},\mathbf{p},\ \Delta_n=0)\ . \tag{4.34}$$

On substituting Eq. (4.29) into Eq. (4.34), we have

$$M^{(n)}(\mathbf{Q},\mathbf{p},\Delta_n=0) =-me^4\langle z\rangle_n^2 4\pi\int_0^\infty \frac{\sin(pR)}{pR}\frac{\sin(p'R)}{p'R}dR \tag{4.35}$$

after carrying out the angular integration and using $\mathbf{p}'=\mathbf{p}+\mathbf{Q}$. The remaining integral is given in the literature[11] and on using the fact that $p=p'$ in elastic collisions, we have

$$M^{(n)}(\mathbf{Q},\mathbf{p},\ \Delta_n=0)=-2me^4\langle z\rangle_n^2\pi^2/p\ . \tag{4.36}$$

We observe the interesting result that the scattering amplitude is a function of the energy only, independent of the momentum transfer. Then if one still insists on an effective potential defined as the Fourier transform of the scattering amplitude in Eq. (4.36), we have

$$\begin{aligned}V^{(n)}(R,p^2,\ \Delta_n=0)&=\int\frac{d^3Q}{(2\pi)^3}e^{i\mathbf{Q}\cdot\mathbf{R}}\\&\quad\times M^{(n)}(Q^2,p^2,\ \Delta_n=0)\\&=-2\pi^2me^4\langle z\rangle_n^2\delta(\mathbf{R})/p &(4.37)\\&=\frac{-\pi me^4\langle z\rangle_n^2}{2pR^2}\delta(R)\ . &(4.38)\end{aligned}$$

Equation (4.38) indicates that as R and p^2 both approach zero, the effective potential diverges as $\pi\delta(R)/(2p)$. This accounts for the divergence of the sum in Eq. (4.33) or Eq. (4.25). Kirzhnits and Pen'kov[2] note that the momentum-dependent effective potential given in Eq. (4.29) only acts on S wave. Our transformation into truly local form as indicated by Eq. (4.38) explains why. We would also like to point out that the scattering amplitude evaluated in Eq. (4.36) is consistent with the real part of the low-energy electron-atom scattering amplitude evaluated by Feinberg, Sucher, and Amado[5] for the case of near degeneracy [see Eqs. (6), (10), and (12) of their paper]. In their work, they only examine the $Q^2\rightarrow 0$ limit for the real part of the scattering amplitude. Equation (4.36) in the present paper shows that because the real part of the scattering amplitude is independent of Q, the Feinberg-Sucher-Amado[5] result is valid for all Q.

The present method of reobtaining the scattering amplitude from the momentum-dependent effective potential is equivalent to taking the principal value only in the evaluation of the scattering amplitude given in Eq. (4.1). At threshold energy, $p^2=0$, and for Δ_n small but nonzero, the energy denominator in Eq. (4.1) is free from zero. In this case an expansion in nonadiabatic and energy-dependent corrections is valid provided we have $p^2/\Delta_n<1$ and $x_n=R\sqrt{\Delta_n}>1$. When either of these conditions is violated, the expansion breaks down. Then the only meaningful physical quantity one should be concerned with is the scattering amplitude. For $p^2/\Delta_n>1$, there appears a cut in the p plane in the scattering amplitude as is evident from the structure of Eq. (4.1). In this event, the scattering amplitude possesses both a real part and an imaginary part. The real part is given by the principal value and is given by Eq. (4.36). The imaginary part has been studied by Feinberg, Sucher, and Amado and can be evaluated exactly in certain limits.[5] The general solution is still lacking.

For the readers who may wonder why the momentum transfer and momentum $(\mathbf{Q},\mathbf{p})$-independent scattering amplitude, as given in Eq. (4.36), can give rise to a momentum-dependent potential, we conclude this section by briefly discussing the underlying mathematics involved. The energy p in the denominator of Eq. (4.36) can be written as, because of energy conservation,

$$\begin{aligned}p^{-1}&=|\mathbf{p}+\mathbf{Q}|^{-1} &(4.39)\\&=p^{-1}\left[1+\frac{2\mathbf{p}\cdot\mathbf{Q}+Q^2}{p^2}\right]^{-1/2}\ . &(4.40)\end{aligned}$$

the quantity $(2\mathbf{p}\cdot\mathbf{Q}+Q^2)/p^2$ should be set equal to zero for whatever value of p^2. If p^2 is preset to be zero at threshold, then the quantity $(2\mathbf{p}\cdot\mathbf{Q}+Q^2)/p^2$ becomes indeterminate and would approach any value if the incorrect limit is taken. In particular, it may take on the value $-(Q^2-Q^2)/p^2$ as $p^2\rightarrow 0$ and becomes -1. Indeed the sum

$$\sum_k C_k^{-1/2}(-1)^k$$

that appears in both Eqs. (4.33) and (4.25) behaves like

$(1+\mathcal{X})^{-1/2}$ in the limit $\mathcal{X}$ approaches -1. On the other hand, Eq. (4.39) can be rewritten as

$$p^{-1}=Q^{-1}\left[1+\frac{p^2}{Q^2}\right]^{-1/2}\times\left[1+\frac{2\mathbf{p}\cdot\mathbf{Q}}{Q^2}\left[1+\frac{p^2}{Q^2}\right]^{-1}\right]^{-1/2}, \tag{4.41}$$

which can be expanded to give a power series in $\mathbf{p}\cdot\mathbf{Q}$ and p^2. On Fourier transformation of this power series, one recovers the momentum-dependent effective potential expressed as a power series in $(-i\mathbf{p}\cdot\mathbf{R})$ and p^2. If one goes to the threshold limit $p^2=0$ in Eq. (4.41), one arrives at the "inconsistent" identity

$$\lim_{p^2\to 0} p^{-1}=Q^{-1}\left[1+\frac{2\mathbf{p}\cdot\mathbf{Q}}{Q^2}\right]^{1/2}. \tag{4.42}$$

Then when one expands the right-hand side of Eq. (4.42) and uses it in Eq. (4.36) and then in Eq. (2.1) in conjunction with a suitable converging factor one recovers Eq. (4.33). Furthermore, if one ignores all the nonadiabatic terms [$k>0$ terms in Eq. (4.33)], one would arrive at the result of Manson and Ritchie.[3] As we have seen, all these procedures are invalid in the simulations limits $p^2\to 0$ and $\Delta_n\to 0$.

When Δ_n is different from zero, then there exist regions in the p plane and Q plane in which the scattering amplitude can be expanded in powers of p^2/Δ_n, Q^2/Δ_n, and $\mathbf{p}\cdot\mathbf{Q}/\Delta_n$. The first corresponds to an energy dependence correction and is valid only when the incident energy is below the lowest threshold for resonance. Since $\mathbf{p}\cdot\mathbf{Q}$ is the same as $-Q^2/2$, the second and third expansions are the same and they correspond to the nonadiabatic corrections. Such an expansion is valid when Q^2/Δ_n is small or when $(\Delta_n R^2)^{-1}$ is small. This is equivalent to having $R>[2m(E_n-E_0)]^{-1/2}$. In the ordinary case without degeneracy, this reduces to the same condition as R greater than the size of the atom. Thus we see that the usual expression of the effective interaction potential in terms of the classical polarization and its nonadiabatic corrections is only valid at large distances (with the distances scale set by the atomic excitation energy) and the expansion in terms of energy dependence is valid only at energies small compared to the resonance excitation threshold energy. Therefore one cannot extrapolate the effective potential to short distances once an expansion in nonadiabatic corrections is made. This is precisely why the claim of a saturation behavior[3] in the effective potential is invalid.

V. FURTHER DISCUSSIONS ON THE NONADIABATIC CORRECTIONS

In case our discussion centered on the use of the dipole approximation brings out the worry among some of our readers, that the breakdown of the validity of the decomposition of the effective potential in terms of nonadiabatic corrections at short distances is primarily due to the fault of the multipole expansion applied to short distance, we reassure them it is not. This can be seen by going back to the scattering amplitude in Eq. (4.1), without using the dipole approximation. Then the scattering amplitude is

$$\overline{M}(\mathbf{p}\cdot\mathbf{p}')=\sum_n \overline{M}^{(n)}(\mathbf{p},\mathbf{p}')\ , \tag{5.1}$$

$$\overline{M}^{(n)}(\mathbf{p},\mathbf{p})=\frac{-4me^4}{\pi}\int\frac{d^3k}{k^2}\frac{d^3q}{q^2}d^3l\frac{\langle 0|(e^{i\mathbf{k}\cdot\mathbf{r}}-1)|n\rangle\langle n|(e^{i\mathbf{q}\cdot\mathbf{r}}-1)|0\rangle}{\Delta_n+l^2-p^2}\delta(\mathbf{p}'-\mathbf{q}-\boldsymbol{l})\delta(\boldsymbol{l}-\mathbf{k}-\mathbf{p}) \tag{5.2}$$

$$=\frac{-4me^4}{\pi}\int\frac{d^3k}{k^2}\frac{d^3q}{q^2}\frac{\langle 0|(e^{i\mathbf{k}\cdot\mathbf{r}}-1)|n\rangle\langle n|(e^{i\mathbf{q}\cdot\mathbf{r}}-1)|0\rangle}{\Delta_n+2\mathbf{p}\cdot\mathbf{k}+k^2}\delta(\mathbf{Q}-\mathbf{k}-\mathbf{q})\ . \tag{5.3}$$

For $p^2>\Delta_n$, the existence of the cut structure in the p plane is evident from Eq. (5.2). That the on-shell scattering amplitude is a function of p^2 and Q^2 is evident from Eq. (5.3) upon using the constraint $\mathbf{p}\cdot\mathbf{Q}=-Q^2/2$ and the rotational invariance of the state $|0\rangle$. The key lies in the fact that an expansion of the effective potential in terms of nonadiabatic corrections is equivalent to an expansion in Q^2 of the scattering amplitude. At threshold energy $p^2=0$ and an expansion in Q^2/p^2 is forbidden. The only other parameter in which a Q^2 expansion can be carried out is Q^2/Δ_n. If Δ_n goes to zero, such an expansion is also forbidden. An expansion in Q^2/Δ_n is always equivalent to an expansion in $(\Delta_n R^2)^{-1}$. For such an expansion to be meaningful, we must have $(\Delta_n R^2)^{-1}<1$ or $R>\Delta_n^{-1/2}$.

In the infinite-projectile-mass limit Δ_n approaches infinity except in the case of exact degeneracy. In this case, all Q^2/Δ_n corrections in the scattering amplitude vanish and so do all the nonadiabatic corrections to the effective potential. In the infinite-projectile-mass limit and in the absence of degeneracy, $R>\Delta_n^{-1/2}$ is always valid. Then it is meaningful to examine the behavior of the polarization potential at short distances, including all multipoles. This then reduces to the Dalgarno-Lynn solution.[12] In this case, the projectile and the target are held fixed with respect to each other and their separation distance R is strictly a parameter and not a dynamical variable. Then the effective potential is just the energy shift of the system due to the target and the projectile in the presence of each other, separated by a distance R.

The discussion presented in this paper does not forbid one from asking about the short-distance behavior of the effective potential provided an expansion in nonadiabatic corrections is *not* made. Since we have proven in this paper that all momentum-dependent corrections in the effective potential are in fact nonadiabatic corrections, one cannot extrapolate the effective potential to short distances when the effective potential is in momentum-dependent form unless all the momentum-dependent terms are retained. The restriction imposed on the validity of a nonadiabatic correction expansion excludes most perturbational approaches to the present problem. However, variational calculations have been done and they do indicate that the finite mass of the projectile modifies the Dalgarno-Lynn solution. According to Dalgarno and Lynn, the effective potential approaches a constant as R goes to zero in the infinite-projectile- and target-mass limit. Numerical variational calculations provided by Drachman[13] indicate that the effective potential goes quadratically in R to zero when the finite mass of the projectile is taken into account, with perhaps a very weak linear dependence.

Next, we would like to reexamine the effective potential in the dipole approximation at threshold energy $p^2=0$ via the scattering amplitude. We return to Eq. (4.1) and concentrate on the contribution from the intermediate target atom state $|n\rangle$. On performing the $\mathbf{k},\mathbf{q}$ integrals and the integration over the angular variables in $|l\rangle$, we have

$$M^{(n)}(Q,p^2=0)=8me^4\langle z\rangle_n^2 \times\int_0^\infty dl\,\frac{Q}{(\Delta_n+l^2)} \times\frac{\{\ln[Q+(l^2+Q^2)]^{1/2}-\ln l\}}{(l^2+Q^2)^{1/2}} \; . \tag{5.4}$$

The integral cannot be done analytically for arbitrary values of Δ_n and Q. However, we can examine the behavior of $M^{(n)}(Q,p^2=0)$ for low, intermediate, and high values of Q. It can be seen that

$$M^{(n)}(Q,p^2=0)\sim Q \quad \text{for } Q^2 \ll \Delta_n \tag{5.5}$$

$$\sim Q \quad \text{for } Q\le\Delta_n \tag{5.6}$$

$$\sim \ln Q \quad \text{for } Q \gg \Delta_n \; , \tag{5.7}$$

bearing in mind that the major contribution to the integral cannot come from high values of l. Equations (5.5)–(5.7) indicate that the effective potential $V^{(n)}(R,p^2=0)$ behave as

$$V^{(n)}(R,p^2=0)$$

$$R^{-4} \quad \text{for } R \gg \Delta_n^{-1/2} \; , \tag{5.8}$$

$$R^{-4} \quad \text{for } R \ge \Delta_n^{-1/2} \; , \tag{5.9}$$

$$\sim R^{-3} \quad \text{for } R \ll \Delta_n^{-1/2} \quad \text{(if at all meaningful)} \; . \tag{5.10}$$

Equations (5.8) and (5.9) are consistent with previous results.[10] Equation (5.10) indicates that the effective potential would have behaved as R^{-3} for $R \ll \Delta_n^{-1/2}$ if the dipole approximation was assumed to be valid and if the result was at all meaningful. If the potential were to behave as R^{-2} as exerted by Manson and Ritchie,[3] the scattering amplitude had to behave as Q^{-1} for large Q. It is obvious from Eq. (5.4) that this cannot be the case. The incorrect conclusion of Manson and Ritchie is based on their examination of a divergent series and erroneously taking the first term (which is also the leading term) to represent the entire sum.

Finally, we would like to address the question of recovering the scattering amplitude from the effective potential. It is obvious that if no approximation has been made in the evaluation of the effective potential defined as the Fourier transform of the scattering amplitude, then in reversing the process the scattering amplitude is recovered as the inverse Fourier transform of the effective potential. This follows from a trivial identity and is valid regardless of whether the dipole approximation is taken or the full Coulombic interaction is kept. To illustrate this point in the dipole approximation, one can return to the potential $V(R,p^2)$ defined in Eqs. (4.20) and (4.21), where the potential $V_{kj}^{(n)}$ is explicitly displayed from Eqs. (4.15)–(4.18) for the lowest k,j's. If one calculates the scattering amplitude from this set of $V_{kj}^{(n)}$'s, one recovers the scattering amplitude in Eq. (4.3) provided one also imposes the on-shell constraint $Q^2=-\mathbf{p}\cdot\mathbf{Q}/2$, and that an expansion in Q^2/Δ_n can be made. If one goes to the limit of large x_n in Eqs. (4.15)–(4.18) the effective potential is expressed in terms of its adiabatic approximation plus nonadiabatic corrections in the usual form. All this corresponds to making a small-Q^2 expansion in the scattering amplitude, which has a finite radius of convergence. This series expansion cannot be arbitrarily extended to the region of large Q^2. For the potential, this means its validity is limited to the region $R > \Delta_n^{-1/2}$. This is precisely the reason why the effective potential, when expressed in terms of nonadiabatic corrections, cannot be extrapolated to small distances ($R < \Delta_n^{-1/2}$). In this paper, we have shown that if such an extrapolation was indeed carried out in the dipole approximation, a singular potential would have resulted for the short-distance behavior. However, the extrapolation is not valid in the first place and so the resulting extrapolated effective potential is not at all meaningful and hence not usable in the recalculation of the scattering amplitude. That the extrapolation to short distance is forbidden when a nonadiabatic expansion has been made is regardless of whether the dipole approximation is taken or the full Coulomb interaction is kept. Obviously, the effective potential, so extrapolated to short distance, cannot reproduce the scattering amplitude correctly at large Q^2. Similarly, an effective potential that is valid only at very small distances cannot be extrapolated to large distance to give the correct behavior of the scattering amplitude at small Q^2. If one divides the interaction distance R into the large- and small-distance regions and uses the corresponding effective potential in the respective regions, then one certainly expects to recover a fairly close approximation to the scattering amplitude. It should be emphasized that within the physical region of p^2 and Q^2, the scattering amplitude is always finite when the full Coulomb interaction is taken into account. When the dipole approximation is employed, it reduces to Eq. (5.4), which shows that the scattering amplitude is finite at threshold energy.

An investigation into the very-short-distance behavior of the effective potential is equivalent to the investigation of the scattering amplitude at high momentum transfer. In the physical region Q^2 is always limited to be less than or equal to $4p^2$. At threshold energies, when p^2 goes to zero, Q^2 also goes to zero within the physical region. Therefore it is not surprising that it turns out not to be physically meaningful to inquire about the short-distance behavior of the effective potential. The word "atom" has been used in a general context in this paper. It refers to any particle with an internal structure.

ACKNOWLEDGMENTS

This work is supported in part by the National Science Foundation under Grant Nos. PHY-85-10642 and PHY-87-10118. Part of this work was done while the author received support from the Smithsonian Institution while visiting the Harvard-Smithsonian Center for Astrophysics. Hospitality of the Smithsonian Institution is gratefully acknowledged. Much of the final revision of this paper was carried out at the Santa Barbara Institute for Theoretical Physics while the author was supported in part by the National Science Foundation under Grant No. PHY-82-17853, supplemented by funds from the National Aeronautics and Space Administration. The author also thanks G. Feinberg, R. Drachman, J. Sucher, and A. Dalgarno for discussions related to the present paper in the past few years.

---

[1] G. Feinberg and J. Sucher, Phys. Rev. A **2**, 2395 (1970).

[2] D. A. Kirzhnits and F. M. Pen'kov, Zh. Eksp. Teor. Fiz. **85**, 80 (1983) [Sov. Phys.—JETP **58**, 46 (1983)].

[3] J. R. Manson and R. H. Ritchie, Phys. Rev. A **32**, 3782 (1985).

[4] C. K. Au and R. J. Drachman, Phys. Rev. Lett. **57**, 262 (1986).

[5] G. Feinberg, J. Sucher, and R. Amado, Phys. Rev. Lett. **57**, 416 (1986).

[6] G. Feinberg and J. Sucher (unpublished).

[7] C. J. Kleinman, Y. Hahn, and L. Spruch, Phys. Rev. **165**, 53 (1968).

[8] D. W. Norcross, Phys. Rev. A **28**, 3095 (1983).

[9] C. K. Au and R. J. Drachman, Phys. Rev. Lett. **56**, 324 (1986).

[10] C. K. Au, Phys. Rev. A **34**, 3568 (1986).

[11] I. S. Gradshtyn and I. M. Ryzhik, *Tables of Integrals Series and Products* (Academic, New York, 1965).

[12] A. Dalgarno and N. Lynn, Proc. Phys. Soc., London, Sec. A **70**, 223 (1957).

[13] R. J. Drachman (private communication). Also see R. J. Drachman and A. Tenkin, in *Case Studies in Atomic Collision Physics,* edited by E. W. McDaniel and M. R. C. McDowell (North-Holland, Amsterdam, 1972, Vol. 2, p. 399.