Limiting behaviors of off-shell scattering wave functions and T matrices for centrally modified Coulomb potentials

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In the formal theory of scattering, the limiting behavior of off-energy-shell scattering wave functions and T matrices as the energy shell is approached is of considerable importance in deriving an impulse approximation to the full scattering amplitudes. On-shell limits do not exist for the pure Coulomb potential, but sufficiently near the shell the off-shell wave function and T matrix are approximated by the continuum eigenstate and scattering amplitude, respectively, multiplied by certain "off-shell" factors. For central potentials which are Coulomb-like at large distances, but modified at smaller radii, it is shown that the on-shell limits again do not exist and the near-shell approximations mimic the pure Coulomb case with the asymptotic charge appearing in the off-shell factors. Numerical results for a realistic atomic potential covering a broad range of defects from the energy shell give a picture of the approximations involved and show that the errors arising from the use of near-shell forms are comparable in magnitude to the energy defects divided by the energy.

I. INTRODUCTION

The impulse approximation was introduced into formal scattering theory by Chew in 1950 in an attempt to treat the inelastic collisions of neutrons with protons.[1] Subsequent applications have been numerous in both atomic[2] and nuclear[3] physics. For many-body collisions in general and rearrangement processes in particular, so-called binding effects lead to the introduction of off-energy-shell scattering wave functions and T matrices.[4] When such effects are small and negligible, the impulse approximation is derived by a consequent reduction of the sum over intermediate states to a single dominant term. This is usually the case if the process occurs near the energy shell.

The limit to the energy shell of the off-shell wave function and T matrix is a uniform one for short-range potentials like the Yukawa or inverse-power ones other than Coulomb. For the pure Coulomb case, on the other hand, the limit does not exist, but near the energy shell the off-shell wave function and T matrix are approximated by the continuum eigenfunction and scattering amplitude, respectively, multiplied by "off-shell" factors.[5,6] Correction terms are of the order of the defect from the energy shell. The near-shell form of the off-shell Coulomb wave function is limited to a finite region of coordinate space. This follows since asymptotically the continuum eigenfunction contains logarithmic terms, while the exact off-shell function does not.

The situation is not as clear for the large class of potentials involving a short-range modification of a Coulomb potential, and, although a statement of the wave-function limit[7] and work on Jost functions for the addition of some separable potentials[8] exists, a detailed look at the problem seems to be warranted. The modified Coulomb potential has particular recent relevance to the theory of the capture of an inner-shell electron of a target atom by a fast, heavy, charged projectile, where a controversy exists as to the precise form of the near-shell behavior.[9] Also, for symmetric capture at high velocities, e.g., for protons incident on hydrogen at MeV energies, the near-shell behavior is needed in distorted-wave or Faddeev-Watson approaches to the transfer process.[10]

In this article we use the simple device of adding and subtracting the asymptotic forms of the full regular and irregular continuum eigenfunctions in the coordinate (and partial-wave) representation to show that the near-shell approximation for a central, modified Coulomb potential mimics that of the pure Coulomb case with the asymptotic charge appearing in the off-shell factors. The near-shell wave-function approximation is valid for a limited region of coordinate space and the on-shell limit again is not well defined. We work within a standard potential scattering formalism[4] and place no restrictions on the potential beyond normal boundedness requirements on integrals involving it.

A numerical example having application to the above-mentioned electron-capture problem and employing a realistic atomic potential is also presented. Results of calculations give a general picture of the magnitude of the errors expected when the near-shell wave function or T matrix is used; errors are seen to indeed be determined by the size of the defect from the energy shell. The numerical study extends recent work[6] on short-range and Coulomb potentials, but it is directed more at presenting average wave-function deviations than at deviations versus the radial coordinate.

In the rest of the article, we consider in Secs. II and III, respectively, the off-shell wave function and T matrix. Section IV contains results from an atomic potential calculation. A conclusion appears at the end. Our notation follows, to a certain extent, that of a previous arti-

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cle.[6] In general, lower-case letters will denote wave functions and upper-case ones integrals containing the wave functions. Atomic units ($m_e=\hbar=e=1$) are used.

II. NEAR-SHELL BEHAVIOR OF THE OFF-SHELL SCATTERING WAVE FUNCTION

We first define the off-shell state for a general potential V and make a partial-wave decomposition of it, after which the limiting behavior of the radial wave function is derived. Finally, the various waves are resummed to give the limit for the full wave function.

The off-energy-shell, single-particle scattering state satisfying an outgoing-wave boundary condition is defined by

$$\psi^+_{\mathbf{k},E}=[1+(E-\mathcal{H}_0-V+i\eta)^{-1}V]\,|\,\mathbf{k}\rangle\ , \tag{2.1}$$

where $\mathcal{H}_0$ is the free-particle Hamiltonian, E is the energy, and η is an infinitesimal quantity. The state is off the energy shell by virtue of $k^2/2$ not being equal to E. The form of the potential V, other than it being central, is left open at this point. The notation is such that $\langle\mathbf{r}\,|\,\mathbf{k}\rangle=\exp(i\mathbf{k}\cdot\mathbf{r})$. We introduce a partial-wave analysis in the coordinate representation,

$$\psi^+_{\mathbf{k},E}(\mathbf{r})=(kr)^{-1}\sum_{l=0}^{\infty} i^l(2l+1)u_l(k,p,r)P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})\ , \tag{2.2}$$

with $E=p^2/2$, but henceforth suppress the l dependence on the radial wave function, i.e., $u=u_l$, as this is not crucial to our arguments. On most later notations l will also not be indicated.

The lth radial Green function for V (outgoing wave) is defined as

$$-p^{-1}f(pr_<)[g(pr_>)+if(pr_>)]\ , \tag{2.3}$$

where f and g are regular and irregular positive-energy solutions of the radial Schrödinger equation possessing the asymptotic forms:

$$f(pr)\sim\sin[pr-\nu\ln(2pr)+l\pi/2+\sigma+\delta]\ \text{ as } r\to\infty\ , \tag{2.4a}$$

$$g(pr)\sim\cos[pr-\nu\ln(2pr)+l\pi/2+\sigma+\delta]\ \text{ as } r\to\infty\ . \tag{2.4b}$$

Z is the charge for (i.e., strength of) the Coulomb potential; it is negative for the attractive case and zero for a short-range potential. The Coulomb phase shift σ is defined to be $\arg\Gamma(l+1+i\nu)$ and ν equals Z/p, the Sommerfeld parameter. The phase shift δ arises from the short-range part of the potential. When Z is nonzero, δ represents scattering relative to (and in addition to) that from the Coulomb potential. The greater (lesser) of the two radial variables r and r' is denoted by $r_>$ ($r_<$).

Use of Eq. (2.3) in the radial integral equation which u satisfies leads, after some rearrangement, to the following expression:

$$u(k,p,r)=j(kr)-p^{-1}\{[F(k,r)g(pr)-G(k,r)f(pr)]+[G(k,\infty)+iF(k,\infty)]f(pr)\}\ .$$

Here, $j(kr)$ [$\equiv krj_l(kr)$] is the Riccati-Bessel function and F and G are the following integrals:

$$F(k,b)=2\int_0^b dr\,j(kr)V(r)f(pr),\quad G(k,b)=2\int_0^b dr\,j(kr)V(r)g(pr)\ .$$

It is useful to rewrite F and G by using the differential equations which f, g, and j satisfy and then partially integrating the ensuing derivative terms twice. Hence, the radial wave function can be put into the form

$$u(k,p,r)=d_k(k+p)[\mathcal{F}(k,r)g(pr)-\mathcal{G}(k,r)f(pr)]-p^{-1}H(k,p)f(pr)\ , \tag{2.5}$$

where

$$H(k,p)\equiv G(k,\infty)+iF(k,\infty)-\{W[g(pr),j(kr)]\}_{r=0}\ . \tag{2.6}$$

The scaled wave-vector defect $(k-p)/p$ is denoted by d_k. We have introduced the additional functions

$$\mathcal{F}(k,b)=\int_0^b dr\,j(kr)f(pr)$$

and

$$\mathcal{G}(k,b)=\int_0^b dr\,j(kr)g(pr)\ .$$

The Wronskian of two functions f and g and is denoted by $W[f,g]$. We now consider Eqs. (2.5) and (2.6) for short-range, pure Coulomb, and modified Coulomb potentials.

In the case of a potential that falls off faster than r^{-1} at large radii, it is well known[4,6] that the corresponding short-range form of Eq. (2.6), $H^{\rm sr}(k,p)$, reduces to $-pe^{i\delta}$ with δ a function of p. The superscript sr stands for short range. Equation (2.5) explicitly isolates terms proportional to the off-shell energy defect. Since $\mathcal{F}$ and $\mathcal{G}$ are, in general, analytic at $k=p$, and a change of variable in Eq. (2.5) implies the essentially dimensionless and constant nature of $k+p$ times $\mathcal{F}$ and $\mathcal{G}$, it follows that

$$u^{\rm sr}(k,p,r)=e^{i\delta}f^{\rm sr}(pr)+O(d_k)\ ; \tag{2.7}$$

a uniform limit to the shell is obtained. O is short for "terms of the order of."

For the Coulomb potential, a closed-form expression for the function, $H^c(Z,k,p)$, of Eq. (2.6) has been obtained;[11] however, $H^c(Z,k,k)$ is not well defined. A superscript c will denote Coulomb quantities and the Z dependence of H^c has been made explicit. From the form

in Ref. 11, the leading term in H^c can be derived when d_k is small. For the sake of completeness, we present a derivation showing this in an Appendix. The result, for $k>p$, is

$$H^c(Z,k,p)=-pQ(Z,k,p)e^{i\sigma}+O(d_k)\ . \tag{2.8}$$

Thus, one can write

$$u^c(k,p,r)=Q(Z,k,p)e^{i\sigma}f^c(pr)+O(d_k)\ . \tag{2.9}$$

The off-shell factor Q has the form

$$Q(Z,k,p)=e^{-\pi\nu/2}\Gamma(1-i\nu)[(k-p)/(k+p)]^{i\nu}\ . \tag{2.10}$$

The analyticity of $\mathcal{F}^c$ and $\mathcal{G}^c$ on shell for *finite* r is again implicit in the derivation of Eq. (2.9). Equation (2.9) must, however, eventually become invalid for large r since f^c contains a logarithmic term in its asymptotic form, while u^c does not (because an inhomogeneous plane-wave term determines this). The Coulomb near-shell relation has been derived before by several authors.[6,12] Its statement here serves as a reference point and allows the introduction of needed notation.

In order to derive a relation for the modified Coulomb potential similar to Eq. (2.9), and something similar might be expected since the potential's asymptotic form is Coulombic with charge Z_a, we expand f and g in terms of the Coulomb functions f^c and g^c:

$$f(pr)=\cos\delta\, f^c(pr)+\sin\delta\, g^c(pr)=f^a(pr)\ , \tag{2.11a}$$

$$g(pr)=\cos\delta\, g^c(pr)-\sin\delta\, f^c(pr)=g^a(pr)\ . \tag{2.11b}$$

It is assumed here that r is greater than the cutoff radius of the short-range modification of the Coulomb potential, or, if no such radius is easily identifiable, that r is large enough for these forms to be as accurate as desired. A superscript a will, in general, denote the use of the functions f^a and g^a in an equation. Asymptotic forms for f^a and g^a are readily deduced from Eq. (2.4).

It is now convenient to define two difference integrals,

$$D_f(k,b)=\int_0^b dr\, j(kr)[f(pr)-f^a(pr)]\ ,$$

$$D_g(k,b)=\int_0^b dr\, j(kr)[g(pr)-g^a(pr)]\ ,$$

that remain well defined for $k=p$, even for b going to infinity. Using these and the differential equations which f, g, f^a, g^a, and j satisfy, we can write

$$-p^{-1}[H(k,p)-H^a(k,p)] =d_k(k+p)[D_g(k,\infty)+iD_f(k,\infty)] \tag{2.12}$$

by partially integrating the derivative terms twice.

Consequently, if we add and subtract $H^a(k,p)$ in Eq. (2.5) and replace H^a by the equivalent form $e^{i\delta}H^c$, we obtain

$$u(k,p,r)=d_k(k+p)\{[\mathcal{F}(k,r)g(pr)-\mathcal{G}(k,r)f(pr)]+[D_g(k,\infty)+iD_f(k,\infty)]f(pr)\}-p^{-1}e^{i\delta}H^c(Z_a,k,p)f(pr)\ . \tag{2.13}$$

The near-shell approximation to u is now seen, with use of Eq. (2.13), to be

$$u(k,p,r)=Q(Z_a,k,p)e^{i(\sigma+\delta)}f(pr)+O(d_k)\ . \tag{2.14}$$

This relation, in which the asymptotic charge Z_a appears, has precisely the same *form* as for a pure Coulomb potential [Eq. (2.9)], even though the function f on the right-hand side represents scattering from the full potential and not just the Coulomb part. The validity of Eq. (2.14) relies critically on the appearance of D_f and D_g in Eq. (2.13). Note the implicit dependence of σ on Z_a.

Let us denote a continuum eigenstate satisfying the outgoing-wave boundary condition by $\phi_{\mathbf{k}}^+$. Since Q is partial-wave independent, the near-shell approximation to $\psi_{\mathbf{k},E}^+$ can be readily derived from the above equation by summing the partial waves. Gathering together here the expressions for the various potentials, we have

$$\psi_{\mathbf{k},E}^{\mathrm{sr}\,+}(\mathbf{r})=\phi_{\mathbf{k}}^{\mathrm{sr}\,+}(\mathbf{r})+O(d_k)\ \text{(short range)}\ , \tag{2.15a}$$

$$\psi_{\mathbf{k},E}^{c\,+}(\mathbf{r})=Q(Z,k,p)\phi_{\mathbf{k}}^{c\,+}(\mathbf{r})+O(d_k)\ \text{(pure Coulomb)}\ , \tag{2.15b}$$

$$\psi_{\mathbf{k},E}^{+}(\mathbf{r})=Q(Z_a,k,p)\phi_{\mathbf{k}}^{+}(\mathbf{r})+O(d_k)\ \text{(modified Coulomb)}\ . \tag{2.15c}$$

The derivation of Eq. (2.15c) has assumed no special requirements of the potential beyond the boundedness of the integrals involved, which, in any event, is also required of the short-range and pure Coulomb cases. The appearance of Z_a in Q and the fact that Q multiplies the full wave function is clearly a result of the validity of Eq. (2.11): the "pathological" asymptotic behavior of the Coulomb potential leads to the presence of Q. Although the above derivation is limited to positive energies, $E>0$, a generalization to negative energies should be possible if the appropriate negative-energy Green function is introduced. We do not pursue this point here.

III. NEAR-SHELL BEHAVIOR OF THE OFF-SHELL T MATRIX

In this section the full T matrix is first introduced and then partial-wave analyzed. Manipulations involving f^a and g^a similar to those of the preceding section are carried out next, leading to the near-shell limit for the partial T matrix. Summation of the partial-wave components once again gives the result for the full T matrix.

The full T matrix is defined, using the off-shell scattering state, as

$$T_{\mathbf{k}',\mathbf{k}}(E)=\langle\mathbf{k}'\mid V\mid\psi_{\mathbf{k},E}^+\rangle\ . \tag{3.1}$$

The form of the potential in Eq. (3.1) is as yet unspecified. A partial-wave analysis

$$T_{\mathbf{k}',\mathbf{k}}(E)=(2\pi/kk')\sum_{l=0}^{\infty}(2l+1)T_l(k',k,p)P_l(\hat{\mathbf{k}}'\cdot\hat{\mathbf{k}}) \quad (3.2)$$

gives

$$T_l(k',k,p)=2\int_0^{\infty}dr\,j(k'r)V(r)u(k,p,r) \quad (3.3)$$

for the partial T matrix. When Eq. (2.13) is inserted for u, we find

$$T_l(k',k,p)=d_k(k+p)\left[2\int_0^{\infty}dr\,j(k'r)V(r)[\mathcal{F}(k,r)g(pr)-\mathcal{G}(k,r)f(pr)]\right.$$
$$\left.+[D_g(k,\infty)+iD_f(k,\infty)]F(k',\infty)\right]-p^{-1}e^{i\delta}H^c(Z_a,k,p)F(k',\infty)\ .$$

From this equation, an expression for the pure Coulomb, partial T matrix T_l^c can easily be derived. Noting that the D functions and δ vanish in this case, we find

$$T_l^c(k,k',p)=2d_k(k+p)\int_0^{\infty}dr\,j(k'r)V^c(r)[\mathcal{F}^c(k,r)g^c(pr)-\mathcal{G}^c(k,r)f^c(pr)]-p^{-1}H^c(Z,k,p)F^c(k',\infty)\ . \quad (3.4)$$

A relation between asymptotic and Coulomb wave functions, useful in performing some further manipulations, is

$$g^a(pr)f^a(pr')-f^a(pr)g^a(pr')=g^c(pr)f^c(pr')-f^c(pr)g^c(pr')\ , \quad (3.5)$$

an equation obtained with the use of Eq. (2.11).

We now consider the difference of the modified and pure Coulomb partial T matrices. Our aim, as in the preceding section, is to produce an equation which isolates terms proportional to d_k or $d_{k'}$. Inserting Eq. (3.5) into the T-matrix difference and rearranging, we get

$$T_l-T_l^c=2d_k(k+p)\int_0^{\infty}dr\,j(k'r)((Vg-V^cg^a)\mathcal{F}(k,r)-(Vf-V^cf^a)\mathcal{G}(k,r)$$
$$+V^c\{g^a[D_f(k,r)-D_f(k,\infty)]-f^a[D_g(k,r)-D_g(k,\infty)]\})$$
$$+p^{-1}([F(k',\infty)-F^a(k',\infty)]\{(k^2-p^2)[D_g(k,\infty)+iD_f(k,\infty)]-e^{i\delta}H^c(Z_a,k,p)\}$$
$$-H^c(Z_a,k,p)[e^{i\delta}F^a(k',\infty)-F^c(k',\infty)])+d_k(k+p)[\mathcal{G}^a(k',\infty)+i\mathcal{F}^a(k',\infty)]D_f(k,\infty)\ .$$

Some further tedious manipulations involving the use of Eq. (2.12) and the replacement of H^a by its equivalent form $e^{i\delta}H^c$ lead to the final form,

$$T_l-T_l^c=d_k(k+p)\left[2\int_0^{\infty}dr\,j(k'r)((Vg-V^cg^a)\mathcal{F}(k,r)-(Vf-V^cf^a)\mathcal{G}(k,r)\right.$$
$$+V^c\{g^a[D_f(k,r)-D_f(k,\infty)]-f^a[D_g(k,r)-D_g(k,\infty)]\})$$
$$\left.-[D_g(k,\infty)\sin\delta-D_f(k,\infty)\cos\delta]\{W[g^c(pr),j(k'r)]\}_{r=0}+e^{i\delta}H^c(Z_a,k',p)D_f(k,\infty)\right]$$
$$+d_{k'}(k'+p)H(k,p)D_f(k',\infty)-H^c(Z_a,k',p)H^c(Z_a,k,p)p^{-1}e^{i\delta}\sin\delta\ . \quad (3.6)$$

As k,k' approach p, the terms containing $d_k,d_{k'}$ go to zero. Note further, in particular, that the integrand of the r integral decreases sufficiently fast enough at large r to allow a convergent integral. The one term which does not contain any energy-difference factor is the last one. It provides the leading term for small energy defects.

Before writing the near-shell approximation down, we first recall the form of the lth component of the short-range part of the full (on-shell) modified Coulomb scattering amplitude,[4] namely,

$$f_l^{sr}(p)=p^{-1}(e^{i\delta}\sin\delta)e^{2i\sigma}\ . \quad (3.7)$$

f_l^{sr} measures the extra scattering due to the short-range potential beyond that arising from the Coulomb potential. When there is no Coulomb part, δ becomes the phase shift for a strictly short-range potential.

Finally, considering Eq. (3.6) and assuming that d_k and $d_{k'}$ are small, we find, upon inserting the previously stated near-shell result for H^c [Eq. (2.8)], the desired relation

$$[T_l(k',k,p)-T_l^c(k',k,p)]/kk'=-Q(Z_a,k',p)Q(Z_a,kp)f_l^{sr}(p)+O(d_k)+O(d_{k'})\ . \quad (3.8)$$

Since Q is not l dependent, we can sum the partial waves to obtain the full T-matrix relation: Q multiplies the full amplitude.

Combining Eqs. (3.2) and (3.8) with the limiting form[5] for the full Coulomb T matrix [Eq. (3.9b) below], we can write down the limiting behaviors of the full T matrix for all three types of potential considered here. Collecting the results,

we find

$$T^{sr}_{k',k}(E) = -2\pi \mathscr{f}^{sr}_{k',k}(E) + O(d_k) \quad \text{(short range)}, \tag{3.9a}$$

$$T^{c}_{k',k}(E) = -2\pi Q(Z,k',p) Q(Z,k,p) \mathscr{f}^{c}_{k',k}(E) + O(d_k) \quad \text{(pure Coulomb)}, \tag{3.9b}$$

$$T_{k',k}(E) = -2\pi Q(Z_a,k',p) Q(Z_a,k,p) [\mathscr{f}^{c}_{k',k}(E) + \mathscr{f}^{sr}_{k',k}(E)] + O(d_k) + O(d_{k'}) \quad \text{(modified Coulomb)}. \tag{3.9c}$$

Equation (3.9c) reduces to Eq. (3.9b) when there is no short-range modification and to Eq. (3.9a) if there is no Coulomb part ($Z_a = 0$). The full Coulomb scattering amplitude, in a generalized form,[13] is given by

$$\mathscr{f}^{c}_{k',k}(E) = (2Z/|\mathbf{k}'-\mathbf{k}|^2) e^{2i\sigma_0} [|\mathbf{k}'-\mathbf{k}|/(k'+k)]^{-2i\nu},$$

with σ_0 denoting $\arg\Gamma(1+i\nu)$.

In Eqs. (3.9a) and (3.9b) we note that only d_k is assumed small. The derivations of the near-shell approximation to the full Coulomb T matrix given in Refs. 5 and 9 show explicitly using analytic representations that either d_k or $d_{k'}$ alone need to be small. We have chosen the former to be the case here. The same is true of the short-range case in Eq. (3.9a). For Eq. (3.9c), on the other hand, both $d_{k'}$ and d_k need to be small. The $d_{k'}$ term in Eq. (3.6) is multiplied by D_f and thus it vanishes for the cases (3.9a) and (3.9b).

IV. APPLICATION TO A REALISTIC ATOMIC POTENTIAL

We present in this section a specific study of the off-shell wave function and T matrix near the energy shell. Basically, we consider in Eqs. (2.13) and (3.6) the magnitude of the correction terms proportional to d_k and $d_{k'}$. While there are very many interesting modified Coulomb potentials, one that is of particular importance[9] is the Hartree-Fock-Slater (e.g., Hermann-Skillman) potential.[14] It is an approximation to the true Hartree-Fock potential in which an atomic electron moves; the approximate character of the potential derives from a local treatment of exchange effects following Slater.[15]

We choose, in particular, to use the K-shell potential in neon as this has application to electron capture from a target atom by a fast, heavy projectile ion. In the case of an incident proton, the final binding energy of the captured electron is one-half of an atomic unit. For impact energies from 400 keV to 5 MeV the scaled wave-vector defect $d_k = (k-p)/p$ in the off-shell wave function typically assumes values from 10^{-2}–10^{-3}. Results in the range 10^{-1}–10^{-4} for p values of 2, 6, 10, and 14 a.u. are presented here to provide a somewhat broader perspective on the approximate forms.

An explicit numerical construction of u runs as follows. The Numerov method is used to obtain f, g, f^c, and g^c. The lth radial Green function is formed from the first two functions and then u is generated using Eq. (2.13) by a Simpson's integration. A further Simpson's integration provides for the wave-function averaging. Actually, only terms in Eqs. (2.13) and (3.6) *linear* in d_k are kept in calculating[16] u and T_l and therefore the results for $d_k \approx 0.1$ are to be viewed cautiously as concerns accuracy. We have employed also a linear approximation to H^c (see Appendix). Equations (2.13) and (3.6) are especially conducive to numerical calculation involving as they do functions which go to zero at large radii or are even zero beyond the finite-range modification of the Coulomb part of the potential. A double-precision (15 significant digits) program written in BASIC was used for the calculations. The program was checked by comparing the present u for short-range and Coulomb potentials with selected results from Ref. 6. Regular and irregular wave functions were checked for reproduction of Manson's phase shifts[17] and for correctness of the Wronskian. Generally, f, g, f^c, and g^c were accurate to five digits, leading to errors in u and T_l of 1%. All calculations were performed on a Zenith ZF-148-42 personal computer.

Since we are interested in an average picture of the magnitude of the correction terms in Eq. (2.13), it is not especially useful to show wave-function plots. Rather, we consider the difference of the lth off-shell and near-shell radial wave functions divided by the near-shell one integrated from zero to some finite radius r_0. We use a finite upper limit since the near-shell approximation to u eventually breaks down at larger r (because the asymptotic forms of the two wave functions are different). The capture problem provides us with a convenient choice of radius, namely, that for which the neon K-shell bound-state wave function has significant amplitude, say, 1% of its maximum value. This occurs at 0.882 bohr or at roughly 8 times the Bohr radius of the K shell in neon. Although our definition of wave-function defect is necessarily arbitrary, we note that the majority of the contributions to a matrix element involving the continuum and ground-state wave functions would, in general, come from radii less than the chosen value.

The integral is, in addition, divided by the length of the radial integration interval and scaled by the wave-vector defect. Our scaled, averaged wave-function defect is thus defined as

$$|r_0 d_k|^{-1} \mathcal{P} \int_0^{r_0} dr \{ |\mathrm{Re}[I(r)]| + i |\mathrm{Im}[I(r)]| \}, \tag{4.1}$$

where

$$I(r) = \frac{u(k,p,r) - Q(Z_a,k,p) e^{i(\sigma+\delta)} f(kr)}{Q e^{i(\sigma+\delta)} f(kr)}.$$

$\mathcal{P}$ denotes a principal-part integration which is necessary due to the zeros of $f(pr)$. We recall the implicit l dependence of u and f.

Figures 1 and 2 show the scaled averaged absolute values of the real and imaginary parts of the wave-function defects versus the wave-vector defect d_k for various p. The bulk of the oscillations seen in these

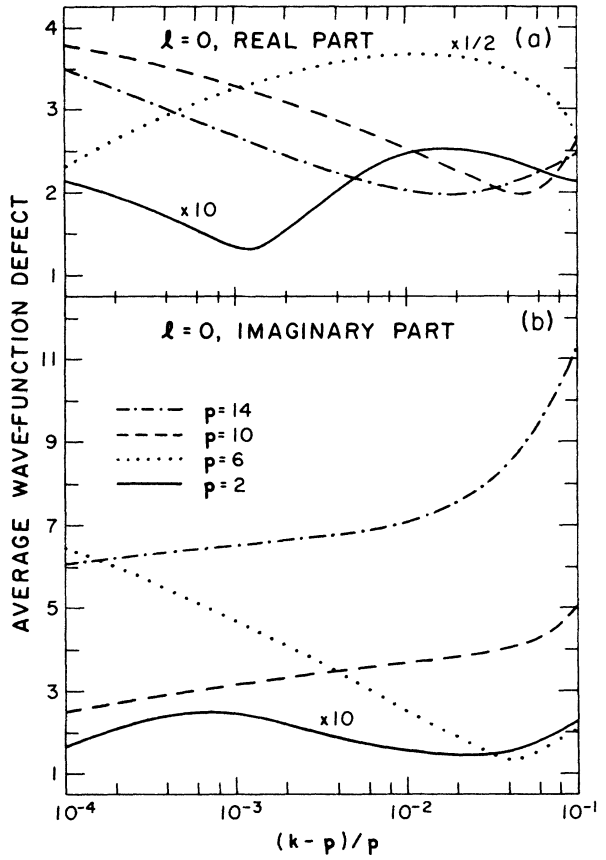

FIG. 1. Average absolute values of the (a) real and (b) imaginary components of the *scaled*, $l=0$ defect of the radial off-shell wave function from the near-shell wave function divided by the near-shell wave function are shown vs the scaled wave-vector defect. A complete definition of the defect is given in Eq. (4.1).

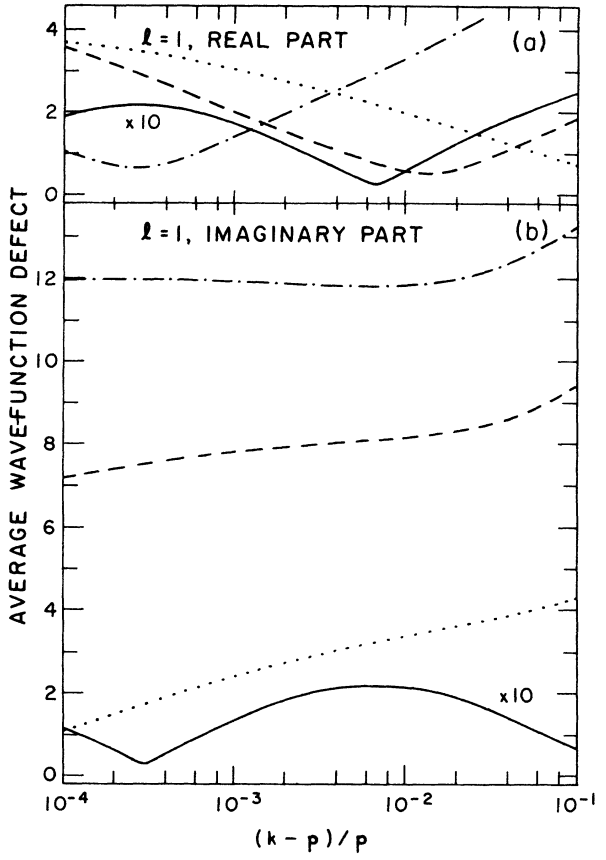

FIG. 2. Average absolute values of the (a) real and (b) imaginary components of the *scaled*, $l=1$ defect of the radial off-shell wave function from the near-shell wave function divided by the near-shell wave function are shown vs the scaled wave-vector defect. A complete definition of the defect is given in Eq. (4.1). Curve designations are as in Fig. 1.

figures and in Figs. 3 and 4 are a result of the phase factor $[(k-p)/(k+p)]^{i\nu}$ in Q. For low energies, $p=2$, the rapidity of the oscillations is greater because ν is larger and the off-shell contributions are very small indeed. With increasing energy, i.e., for $p=6,10,14$, the oscillations slow and the errors grow. The imaginary parts are rather smoother, except at the lowest energies, and increase faster at higher energy due to the irregular function contribution in D_g. The $p=6$ curve in Fig. 1(a) shows that in certain energy ranges a more pronounced error can occur. Overall, though, the deviations are relatively small and roughly of the magnitude of d_k. In an actual application smaller deviations can be expected because of cancellation effects, i.e., the worst-case situation presented here is not likely to be realized in practice. When accuracy of a few percent is desired, as in the capture problem, the approximate forms should prove adequate. Higher partial waves could be problematic, but they have smaller overlaps with the ground-state wave function.

We next consider the partial T matrix $T_l(k,k',p)$. The pure Coulomb term has been studied elsewhere[6] and need not be considered further here. In order to keep the discussion relatively simple, we restrict k and k' to be equal and consider the difference of the short-range part of the partial T matrix with the corresponding component of the near-shell scattering amplitude divided by that component. This quotient is once again scaled by the wave-vector defect d_k. Explicitly, we have

$$d_k^{-1}\{[T_l(k,k,p)-T_l^c(k,k,p)] + p^2[Q(Z_a,k,p)]^2 \mathcal{F}_l^{sr}(p)\}/(p^2Q^2\mathcal{F}_l^{sr}) \quad (4.2)$$

for the partial T-matrix defect.

In Figs. 3 and 4 we show, respectively, the absolute values of the real and imaginary parts of the $l=0$ and 1 scaled defects of the short-range part of the partial T matrix. The oscillatory nature and zeros of the defects are even more apparent in these figures, with the smaller periods reflecting the appearance of Q^2 in Eq. (4.2). The partial T matrix for the pure Coulomb problem also has zeros, but unlike that case the zeros in the real and imaginary parts of $T_l-T_l^c$ here do not occur at the same energies. Consequently, the case of no effective scattering cannot occur though scattering could possibly be due solely to the short-range part of the potential. Lastly, an envelope function determines the magnitude of the oscil-

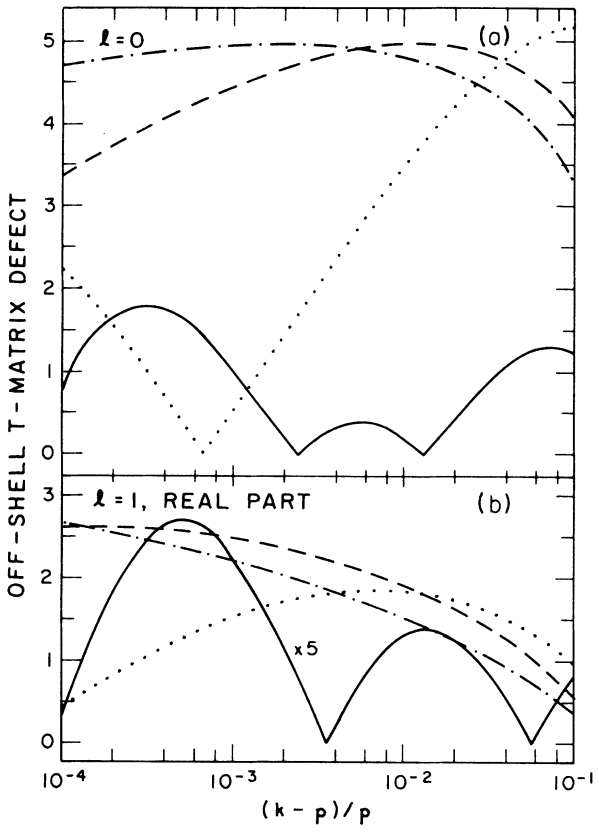

FIG. 3. Absolute values of the real part of the *scaled* defects of the (a) $l=0$ and (b) $l=1$ short-range, partial T matrices from the corresponding components of the near-shell scattering amplitude divided by the respective components are shown vs the scaled wave-vector defect. A complete definition of the defect is given in Eq. (4.2). Curve designations are as in Fig. 1.

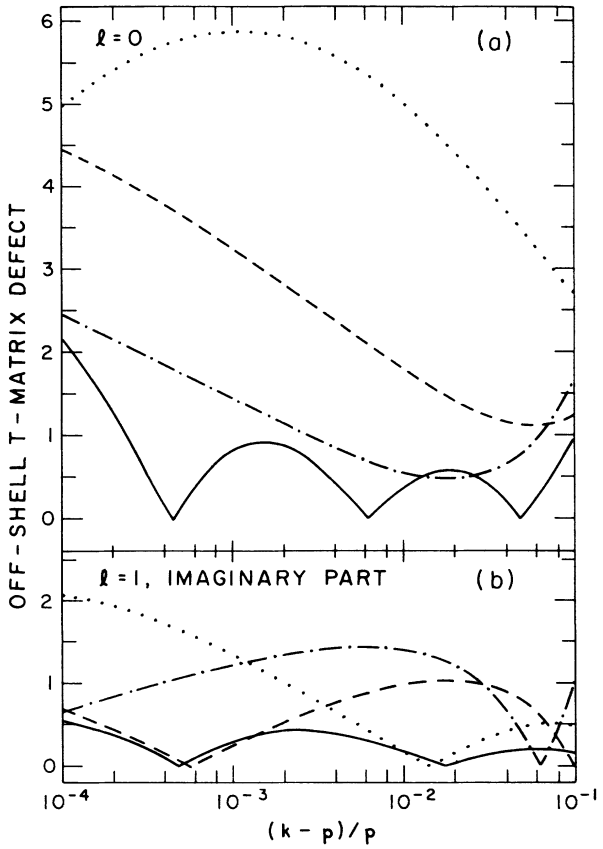

FIG. 4. Absolute values of the imaginary part of the *scaled* defects of the (a) $l=0$ and (b) $l=1$ short-range, partial T matrices from the corresponding components of the near-shell scattering amplitude divided by the respective components are shown vs the scaled wave-vector defect. A complete definition of the defect is given in Eq. (4.2). Curve designations are as in Fig. 1.

lations and the $l=1$ terms are generally smaller than the $l=0$ ones. Comparison of Figs. 3(a) and 4(a) shows a more slowly varying contribution to be present also. The defects for the T matrices are smaller than for the wave functions and of the size of d_k. For high-energy electron capture,[10] defects of the order of 0.001 arise; limiting forms for the two partial waves discussed here would be applicable in this range.

V. CONCLUSION

In this paper we have derived another link between off-shell and on-shell scattering. By separating the short-range part of the potential from the pure Coulomb part and adding and subtracting the asymptotic forms of the continuum eigenfunctions, the near-shell behaviors of the off-shell wave function and T matrix for a modified Coulomb potential have been shown to mimic those already known to exist for the pure Coulomb case. The limiting forms for a much wider class of potential is thus established. Our method, though not employing a first-principles two-potential formalism, is nevertheless oriented in this direction and indicates the need for more work along this line, particularly in regard to placing bounds on the factors multiplying the energy defects. Establishing such bounds would offer a broader statement of the near-shell errors which we have described briefly here from a numerical point of view.

ACKNOWLEDGMENTS

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APPENDIX

We derive here an approximation for the function $H^c(Z,k,p)$ [Eq. (2.6) for a Coulomb potential] containing the leading term and terms linear in d_k. Our starting point is Eq. (20) of Ref. 11, which in our notation assumes the form

$$G^c(k,\infty)+iF^c(k,\infty)=[p(l!)e^{\pi\nu/2}\,|\,\Gamma(l+1+i\nu)\,|\,^{-1}]\{X_l(1+d_k)+\mathrm{Im}[P_l^{(i\nu,-i\nu)}(u)]+{}_2F_1(1,i\nu,1+i\nu,a)P_l^{(-i\nu,i\nu)}(u) - {}_2F_1(1,i\nu,1+i\nu,1/a)P_l^{(i\nu,-i\nu)}(u)\}\ .$$

The variables in this equation are defined

$$a=d_k/(2+d_k),\quad u=[1+d_k+1/(1+d_k)]/2\ .$$

$P_l^{(a,c)}(u)$ is a Jacobi polynomial and $X_l(1+d_k)$ is another polynomial which is defined in Ref. 11, the first few of which are $X_0=X_1=0$, $X_2=\nu^2(1+d_k)/2$, and $X_3=\nu^2[7(1+d_k)^2+5]/12$.

For d_k small, we introduce the first-order approximations $a\approx d_k/2$ and $u\approx 1$. Using these we obtain

$${}_2F_1(1,i\nu,1+i\nu,a)\approx 1+i\nu d_k/2(1+i\nu)\ ,$$

$$P_l^{(i\nu,-i\nu)}(u)\approx P_l^{(i\nu,-i\nu)}(1)=\Gamma(l+1+i\nu)/\Gamma(1+i\nu)(l!)\ ,$$

$$X_l(1+d_k)\approx X_l(1)+X_l'(1)d_k=1-\mathrm{Re}[P_l^{(i\nu,-i\nu)}(1)]+X_l'(1)d_k$$

and, by analytic continuation,

$${}_2F_1(1,i\nu,1+i\nu,1/a)\approx\,|\,\Gamma(1+i\nu)\,|\,^2e^{-\pi\nu}[(k-p)/(k+p)]^{i\nu}+i\nu d_k/2(1-i\nu)\ .$$

It has been assumed that $k>p$ in deriving the latter expression.

Combining the approximate forms, we find

$$G^c+iF^c\approx p(l!)e^{\pi\nu/2}\,|\,\Gamma(l+1+i\nu)\,|\,^{-1}-pe^{-\pi\nu/2}\Gamma(1-i\nu)[(k-p)/(k+p)]^{i\nu}e^{i\sigma} + d_k(pe^{\pi\nu/2}\,|\,\Gamma(l+1+i\nu)\,|\,^{-1}\{(l!)X_l'(1)+\mathrm{Re}[i\nu\Gamma(l+1-i\nu)/(1+i\nu)\Gamma(1-i\nu)]\})\ .$$

The Wronskian of the irregular Coulomb function g^c and j is

$$\{W[g^c(pr),j(kr)]\}_{r=0}=[p(l!)e^{\pi\nu/2}\,|\,\Gamma(l+1+i\nu)\,|\,^{-1}](k/p)^{l+1}\approx p(l!)e^{\pi\nu/2}\,|\,\Gamma(l+1+i\nu)\,|\,^{-1}[1+(l+1)d_k]\ .$$

Thus, the final result for H^c is seen to be

$$H^c(Z,k,p)=G^c+iF^c-\{W[g^c,j]\}_{r=0} \approx -pQ(Z,k,p)e^{i\sigma}+d_k[pe^{\pi\nu/2}\,|\,\Gamma(l+1+i\nu)\,|\,^{-1}] \times\{(l!)[X_l'(1)-(l+1)]+\mathrm{Re}[i\nu\Gamma(l+1-i\nu)/(1+i\nu)\Gamma(1-i\nu)]\}\ ,$$

where Q is defined in Eq. (2.10). Note the entirely real contribution of the linear terms.

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