New Scattering Approximation*

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The spherical-harmonics decomposition of the wave equation for scattering of a plane wave by a potential of arbitrary space dependence is derived from the Green's function formulation. An approximation is then introduced which reduces the scattering problem to the solution of a set of coupled linear equations for the partial-wave amplitudes. The numerical coefficients in these equations involve Clebsch-Gordan coefficients and integrals over all space of a product of a spherical-harmonic component of the potential with a pair of Bessel functions. For central potentials (U), the equations decouple, and the phase shifts reduce to

$$\tan\delta_l = \frac{-k\int_0^\infty r^2dr\, j_l^2(kr)U(r)}{1-k\int_0^\infty r^2dr\, j_l(kr)y_l(kr)U(r)}.$$

While the manipulations involved resemble those in the Born approximation (the numerator above is the Born δ_l), the concept of the new approximation is quite different and the results can be very dissimilar. Exact and approximate phase shifts are exhibited for various spherical wells and barriers. For repulsive potentials, the approximation works well for short to moderate ranges ($ka\lesssim 2$) regardless of barrier height. For attractive potentials, comparable results are obtained for the "potential scattering," but the resonances are ignored.

I. EXACT FORMULATION

THE wave equation,

$$\nabla^2\Psi+[k^2-U(r,\theta,\phi)]\Psi=0, \tag{1}$$

for the scattering of a plane wave $\exp(ikz)$ by a potential U (in appropriate units) has the formal solution in terms of a Green's function,[1]

$$\Psi(r,\theta,\phi)=\exp(ikr\cos\theta)-(4\pi)^{-1}\int|\mathbf{r}-\mathbf{r}'|^{-1}\exp(ik|\mathbf{r}-\mathbf{r}'|)\times U(r',\theta',\phi')\Psi(r',\theta',\phi')d\tau'. \tag{2}$$

Since the cross section depends on the scattered part of the wave function, it is best to split off the plane wave from the start:

$$\Psi(r,\theta,\phi)=\exp(ikr\cos\theta)+\psi(r,\theta,\phi), \tag{3}$$

and deal with the equation

$$\psi(r,\theta,\phi)=-(4\pi)^{-1}\int|\mathbf{r}-\mathbf{r}'|^{-1}\times\exp(ik|\mathbf{r}-\mathbf{r}'|)U(r',\theta',\phi')\exp(ikr'\cos\theta')d\tau' -(4\pi)^{-1}\int|\mathbf{r}-\mathbf{r}'|^{-1}\exp(ik|\mathbf{r}-\mathbf{r}'|)U(r',\theta',\phi')\times\psi(r',\theta',\phi')d\tau'. \tag{4}$$

The first term on the right leads to the Born approximation (after the replacement of the Green's function by its asymptotic value for large r).

The wave function and the potential are next expanded in spherical harmonics,

$$\psi(r,\theta,\phi)=(4\pi)^{\frac{1}{2}}\sum_{ls}(2l+1)^{\frac{1}{2}}\psi_{ls}(r)Y_{ls}(\theta,\phi), \tag{5}$$

$$U(r,\theta,\phi)=(4\pi)^{\frac{1}{2}}\sum_{pq}(2p+1)^{\frac{1}{2}}U_{pq}(r)Y_{pq}(\theta,\phi). \tag{6}$$

For the plane wave, there is the Rayleigh expansion,

$$\exp(ikr\cos\theta)=(4\pi)^{\frac{1}{2}}\sum_l i^l(2l+1)^{\frac{1}{2}}j_l(kr)Y_{l0}(\theta,\phi), \tag{7}$$

and for the Green's function

$$|\mathbf{r}-\mathbf{r}'|^{-1}\exp(ik|\mathbf{r}-\mathbf{r}'|)=ik\sum_n(2n+1)P_n(\cos\Theta)j_n(kr_<)h_n^{(1)}(kr_>), \tag{8}$$

where $r_<$ and $r_>$ are the smaller and larger, respectively, of r and r', and Θ is the relative angle between the vectors $\mathbf{r}$ and $\mathbf{r}'$ (i.e., $\cos\Theta=\mathbf{r}\cdot\mathbf{r}'/rr'$). In turn, the addition theorem for spherical harmonics is

$$P_n(\cos\Theta)=4\pi(2n+1)^{-1}\sum_m Y_{nm}(\theta,\phi)Y_{nm}^*(\theta',\phi'). \tag{9}$$

The angular part of the integration yields[2]

$$\int d\Omega'\, Y_{nm}^*(\theta',\phi')Y_{ls}(\theta',\phi')Y_{pq}(\theta',\phi')=[(2p+1)(2l+1)/4\pi(2n+1)]^{\frac{1}{2}}C(pln;m-s\;s)C(pln;00)\delta_{q,m-s}, \tag{10}$$

where the C's are Clebsch-Gordan coefficients. Thus

$$(4\pi)^{\frac{1}{2}}\sum_{nm}(2n+1)^{\frac{1}{2}}\psi_{nm}(r)Y_{nm}(\theta,\phi)=-ik(4\pi)^{\frac{1}{2}}\sum_{nmlp}(2l+1)(2p+1)(2n+1)^{-\frac{1}{2}}C(pln;00)Y_{nm}(\theta,\phi)\times\left[i^lC(pln;m0)\int_0^\infty r'^2dr'\, j_n(kr_<)h_n^{(1)}(kr_>)j_l(kr')U_{pm}(r') +\sum_s C(pln;m-s\;s)\int_0^\infty r'^2dr'\, j_n(kr_<)h_n^{(1)}(kr_>)\psi_{ls}(r')U_{p\,m-s}(r')\right]. \tag{11}$$

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[1] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1950), 2nd ed.
[2] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

Using the orthogonality of the spherical harmonics (and the symmetry relation for the C's) this reduces to an equation involving the radial variables only:

$$\psi_{nm}(r)=-ik(-)^m\sum_{lp}(2p+1)C(pnl;00)\bigg[i^lC(pnl;m\ -m)\int_0^\infty r'^2dr'\ j_n(kr_<)h_n^{(1)}(kr_>)j_l(kr')U_{pm}(r')$$
$$+\sum_s(-)^sC(pnl;m-s,\ -m)\int_0^\infty r'^2dr'\ j_n(kr_<)h_n^{(1)}(kr_>)\psi_{ls}(r')U_{p\ m-s}(r')\bigg].\quad(12)$$

The range of integration of r' must be split at $r'=r$ in order to handle $r_<$ and $r_>$. No special care is required concerning $r'=r$ inasmuch as the pole of the Green's function is excluded from the volume integral. Indicating the Born approximation terms by a superscript B,

$$\psi_{nm}^B(r)=-ik(-)^m\sum_{lp}i^l(2p+1)C(pnl;m\ -m)C(pnl;00)\bigg[h_n^{(1)}(kr)\int_0^r r'^2dr'\ j_n(kr')j_l(kr')U_{pm}(r')$$
$$+j_n(kr)\int_r^\infty r'^2dr'\ h_n^{(1)}(kr')j_l(kr')U_{pm}(r')\bigg],\quad(13)$$

$$\psi_{nm}(r)-\psi_{nm}^B(r)=-ik(-)^m\sum_{lps}(-)^s(2p+1)C(pnl;m-s,\ -m)C(pnl;00)$$
$$\times\bigg[h_n^{(1)}(kr)\int_0^r r'^2dr'\ j_n(kr')\psi_{ls}(r')U_{p\ m-s}(r')+j_n(kr)\int_r^\infty r'^2dr'\ h_n^{(1)}(kr')\psi_{ls}(r')U_{p\ m-s}(r')\bigg].\quad(14)$$

A slight rearrangement leads to

$$\psi_{nm}^B(r)=-ik(-)^m\sum_{lp}i^l(2p+1)C(pnl;m\ -m)C(pnl;00)\bigg\{h_n^{(1)}(kr)\int_0^\infty r'^2dr'\ j_n(kr')j_l(kr')U_{pm}(r')$$
$$-\int_r^\infty r'^2dr'\ j_l(kr')U_{pm}(r')[h_n^{(1)}(kr)j_n(kr')-j_n(kr)h_n^{(1)}(kr')]\bigg\},\quad(15)$$

$$\psi_{nm}(r)-\psi_{nm}^B(r)=-ik(-)^m\sum_{lps}(-)^s(2p+1)C(pnl;m-s,\ -m)C(pnl;00)$$
$$\times\bigg\{h_n^{(1)}(kr)\int_0^\infty r'^2dr'\ j_n(kr')\psi_{ls}(r')U_{p\ m-s}(r')$$
$$-\int_r^\infty r'^2dr'\ \psi_{ls}(r')U_{p\ m-s}(r')[h_n^{(1)}(kr)j_n(kr')-j_n(kr)h_n^{(1)}(kr')]\bigg\}.\quad(16)$$

The cross section involves the value of $\psi_{nm}(r)$ for large r. The second integral in Eqs. (15) and (16) vanishes in the limit of large r, so that $\psi_{nm}(r)$ becomes a constant times $h_n^{(1)}(kr)$ whose asymptotic value is

$$h_n^{(1)}(kr)\sim(-i)^{n+1}(kr)^{-1}\exp(ikr),\quad(17)$$

an outgoing spherical wave as it should be. Asymptotically then,

$$\psi_{nm}^B(r)\sim(-i)^n(-)^{m+1}r^{-1}\exp(ikr)\sum_{lp}i^l(2p+1)C(pnl;m\ -m)C(pnl;00)$$
$$\times\int_0^\infty r'^2dr'\ j_n(kr')j_l(kr')U_{pm}(r'),\quad(18)$$

$$\psi_{nm}(r)-\psi_{nm}^B(r)\sim(-i)^n(-)^{m+1}r^{-1}\exp(ikr)\sum_{lps}(-)^s(2p+1)C(pnl;m-s,\ -m)C(pnl;00)$$
$$\times\int_0^\infty r'^2dr'\ j_n(kr')\psi_{ls}(r')U_{p\ m-s}(r').\quad(19)$$

If the potential has no azimuthal dependence, neither will the wave function by symmetry. The indices m and s will then be restricted to the value zero. The spherical harmonics break down to Legendre polynomials, so that

$$\psi(r,\theta)=\sum_l(2l+1)\psi_l(r)P_l(\cos\theta), \tag{20}$$

$$U(r,\theta)=\sum_p(2p+1)U_p(r)P_p(\cos\theta), \tag{21}$$

in view of

$$Y_{l0}(\theta,\phi)=[(2l+1)/4\pi]^{\frac{1}{2}}P_l(\cos\theta). \tag{22}$$

Equations (15), (16), (18), and (19) become

$$\psi_n{}^B(r)=-ik\sum_{lp}i^l(2p+1)C^2(pnl;00)\bigg\{h_n{}^{(1)}(kr)\int_0^\infty r'^2dr'\ j_n(kr')j_l(kr')U_p(r') - \int_r^\infty r'^2dr'\ j_l(kr')U_p(r')[h_n{}^{(1)}(kr)j_n(kr')-j_n(kr)h_n{}^{(1)}(kr')]\bigg\}, \tag{23}$$

$$\psi_n{}^B(r)\sim-(-i)^nr^{-1}\exp(ikr)\sum_{lp}i^l(2p+1)C^2(pnl;00)\int_0^\infty r'^2dr'\ j_n(kr')j_l(kr')U_p(r'), \tag{24}$$

$$\psi_n(r)-\psi_n{}^B(r)=-ik\sum_{lp}(2p+1)C^2(pnl;00)\bigg\{h_n{}^{(1)}(kr)\int_0^\infty r'^2dr'\ j_n(kr')\psi_l(r')U_p(r') - \int_r^\infty r'^2dr'\ \psi_l(r')U_p(r')[h_n{}^{(1)}(kr)j_n(kr')-j_n(kr)h_n{}^{(1)}(kr')]\bigg\}, \tag{25}$$

$$\psi_n(r)-\psi_n{}^B(r)\sim-(-i)^nr^{-1}\exp(ikr)\sum_{lp}(2p+1)C^2(pnl;00)\int_0^\infty r'^2dr'\ j_n(kr')\psi_l(r')U_p(r'). \tag{26}$$

For a central potential (spherically symmetric), there is only a $p=0$ term (i.e., $U=U_0$). The Clebsch-Gordan coefficient then reduces to δ_{ln}, so that the Legendre coefficients of the wave function are decoupled:

$$\psi_n{}^B(r)=-i^{n+1}k\bigg\{h_n{}^{(1)}(kr)\int_0^\infty r'^2dr'\ j_n{}^2(kr')U(r')-\int_r^\infty r'^2dr'\ j_n(kr')U(r')[h_n{}^{(1)}(kr)j_n(kr')-j_n(kr)h_n{}^{(1)}(kr')]\bigg\}, \tag{27}$$

$$\psi_n{}^B(r)\sim-r^{-1}\exp(ikr)\int_0^\infty r'^2dr'\ j_n{}^2(kr')U(r'), \tag{28}$$

$$\psi_n(r)-\psi_n{}^B(r)=-ik\bigg\{h_n{}^{(1)}(kr)\int_0^\infty r'^2dr'\ j_n(kr')\psi_n(r')U(r') - \int_r^\infty r'^2dr'\ \psi_n(r')U(r')[h_n{}^{(1)}(kr)j_n(kr')-j_n(kr)h_n{}^{(1)}(kr')]\bigg\}, \tag{29}$$

$$\psi_n(r)-\psi_n{}^B(r)\sim-(-i)^nr^{-1}\exp(ikr)\int_0^\infty r'^2dr'\ j_n(kr')\psi_n(r')U(r'). \tag{30}$$

II. APPROXIMATION

A. Statement

To within the Born approximation, the asymptotic values clearly suffice. In the non-Born part of $\psi_{nm}(r)$, however, $\psi_{ls}(r')$ in the integrand runs through all values of r' down to zero; hence it differs significantly from its asymptotic value over part of the range of integration. This difficulty arises even for the second Born approximation, i.e., if an iterative solution is attempted by using $\psi_{ls}{}^B(r')$ for $\psi_{ls}(r')$ in the integrand, this properly requires the knowledge of $\psi_{ls}{}^B(r')$ for all r', not just its asymptotic value. Since the second integral in Eqs. (15) and (16) [or their special cases (23), (25), (27), and (29)] has r as a lower limit, there results a complicated r dependence of the wave function, even in the Born approximation. This in turn means that the integrands in Eq. (16) are unwieldy already in the second Born approximation, and a complete formal solution of the integral equation is well-nigh hopeless. Furthermore, iteration converges satisfactorily only if the first-order expression is a fairly good approximation.

The approximation proposed in this paper is the neglect of the troublesome second integral in Eqs. (15) and (16). The effect of this approximation is a vast simplification, permitting a direct evaluation of the asymptotic value of $\psi_{nm}(r)$ with little more effort than is required for the Born approximation coefficients. Since only the infinite integrals are retained, the right-hand side of Eqs. (15) and (16) takes the form of a constant times $h_n^{(1)}(kr)$. Hence, $\psi_{nm}(r)$ itself is of the form

$$\psi_{nm}(r)=i^{n+1}(-)^m A_{nm}h_n^{(1)}(kr), \tag{31}$$

where A_{nm} is a numerical constant independent of r. Substituting Eq. (31) into the simplified Eqs. (15) and (16) [including the integrand of (16)],

$$A_{nm}=-k\sum_{lp} i^{l-n}(2p+1)C(pnl;m\ -m)C(pnl;00)\int_0^\infty r'^2dr'\ j_n(kr')j_l(kr')U_{pm}(r')$$
$$-ik\sum_{lps} i^{l-n}(2p+1)C(pnl;m-s,\ -m)C(pnl;00)A_{ls}\int_0^\infty r'^2dr'\ j_n(kr')h_l^{(1)}(kr')U_{p\ m-s}(r'), \tag{32}$$

a set of equations relating the numerical coefficients A_{nm} from which they can be individually evaluated. The asymptotic wave function is then

$$\psi(r,\theta,\phi)\sim(4\pi)^{\frac{1}{2}}(kr)^{-1}\exp(ikr)\sum_{nm}(2n+1)^{\frac{1}{2}}(-)^m A_{nm}Y_{nm}(\theta,\phi). \tag{33}$$

If there is azimuthal symmetry, $\psi_n(r)$ in Eqs. (23) and (25) becomes

$$\psi_n(r)=i^{n+1}A_nh_n^{(1)}(kr), \tag{34}$$

and Eq. (32) reduces to

$$A_n=-k\sum_{lp} i^{l-n}(2p+1)C^2(pnl;00)\int_0^\infty r'^2dr'\ j_n(kr')j_l(kr')U_p(r')$$
$$-ik\sum_{lp} i^{l-n}(2p+1)C^2(pnl;00)A_l\int_0^\infty r'^2dr'\ j_n(kr')h_l^{(1)}(kr')U_p(r'), \tag{35}$$

leading to the asymptotic wave function

$$\psi(r,\theta)\sim(kr)^{-1}\exp(ikr)\sum_n(2n+1)A_nP_n(\cos\theta). \tag{36}$$

For a spherically symmetric potential,

$$A_l=-k\int_0^\infty r'^2dr'\ j_l^2(kr')U(r')-ikA_l\int_0^\infty r'^2dr'\ j_l(kr')h_l^{(1)}(kr')U(r'), \tag{37}$$

from which

$$A_l=\frac{-k\int_0^\infty r'^2dr'\ j_l^2(kr')U(r')}{1+ik\int_0^\infty r'^2dr'\ j_l(kr')h_l^{(1)}(kr')U(r')}. \tag{38}$$

When there is azimuthal symmetry, the coefficients A_l can be written in terms of the phase shifts [comparing Eq. (36) with the usual phase-shift expression]:

$$A_l=(2i)^{-1}[\exp(2i\delta_l)-1]. \tag{39}$$

Since in practice it is usually $\tan\delta_l$ that is computed, a more convenient form of the relation is obtained by a bit of manipulation:

$$A_l=\tan\delta_l/(1-i\tan\delta_l), \tag{40}$$

which can be inverted to read

$$\tan\delta_l=A_l/(1+iA_l). \tag{41}$$

For a spherically symmetric potential, Eq. (38) leads directly to an equation for $\tan\delta_l$, namely,

$$\tan\delta_l=\frac{-k\int_0^\infty r'^2dr'\ j_l^2(kr')U(r')}{1-k\int_0^\infty r'^2dr'\ j_l(kr')y_l(kr')U(r')}, \tag{42}$$

where, in order to write the equation in terms of real quantities, the Hankel function has been split into a Bessel function and a Neumann function:

$$h_l^{(1)}(kr')=j_l(kr')+iy_l(kr'). \tag{43}$$

If the potential is sufficiently weak, the denominator in Eq. (42) reduces to unity and the numerator is small. Since the phase shift is then small:

$$\delta_l{}^B \approx -k\int_0^\infty r'^2 dr'\ j_l{}^2(kr')U(r'), \tag{44}$$

which is the Born-approximation result. While the weak-potential limit is the same in this procedure as in the usual derivation of the Born approximation, the way it is approached is not the same. The Born approximation is extended to moderately stronger potentials (up to $\delta_l{}^B \approx \pi/2$) by using Eq. (44) via Eq. (39) to obtain the asymptotic wave function [Eq. (36)].[1] This can give an answer markedly different from Eq. (38).

It is important to note that the two integrals in Eq. (42) need not be of the same order of magnitude; this depends on the shape of the potential. The Neumann function weights small values of r' more heavily than the Bessel function, large values of r' less heavily. For a strong potential, it is the 1 in Eq. (42) that is negligible. Even though the integrals be large (and the Born approximation phase shift accordingly large), their ratio will be small for a short-range potential and hence the phase shift will be small too.

B. Justification

To justify the use of the approximation, it is necessary to trace through just where it comes in. This involves maintaining a clear distinction between the asymptotic value of the wave function (which alone is required for the cross section) and the wave function itself (which concerns us insofar as it appears as a factor in the integrand for the non-Born part of the asymptotic value). The Eqs. (18) and (19) used for the asymptotic value are exact. The Born approximation part of the asymptotic value [Eq. (18)] is computed exactly. The approximation enters in the evaluation of the integral in Eq. (19)—in using the approximate value [Eq. (31)] for $\psi_{ls}(r')$ in the integrand. In a sense, then, the solution used is the asymptotic value of the wave function obtained by iteration on a trial function given by Eq. (31). To obtain the wave function itself by iteration, Eq. (31) would have to be substituted into Eq. (16) and the integrals in Eqs. (15) and (16) computed for arbitrary r—a far more onerous procedure. If this were done, the next iteration would be completed by inserting this wave function into Eq. (19).

The accuracy of the trial function [Eq. (31)] can be gauged from an examination of Eqs. (15) and (16). The discarded integral looks like a truncated version of the retained one (in fact, half of it is precisely that), and can thus be expected to be smaller (except possibly for very small r). The argument is reinforced by the fact that the integrand is zero at $r'=r$, so that the integral does not start to build up till a value of r' well above r. A detailed analysis of the integrals requires specification of the potential, but some further comments are possible if the potential is not strongly oscillatory. It appears that the integrand of the discarded integral is more oscillatory than the integrand of the retained integral, so that the relative magnitude of the discarded integral is further reduced.

The oscillatory behavior is most evident for a central potential. In the discarded integral, the Bessel functions can be replaced by their asymptotic values:

$$j_n(kr)\sim (kr)^{-1}\sin(kr-n\pi/2), \tag{45}$$

$$h_n{}^{(1)}(kr)\sim(-i)^{n+1}(kr)^{-1}\exp(ikr). \tag{17}$$

With a bit of trigonometric manipulation,

$$h_n{}^{(1)}(kr)j_n(kr')-j_n(kr)h_n{}^{(1)}(kr') \sim (i/k^2rr')\sin k(r'-r), \tag{46}$$

and the integrand for the Born term contains $j_n(kr')$ times this, or

$$\sin k(r'-r)\sin(kr'-n\pi/2) = 2\cos(2kr'-kr-n\pi/2)-2\cos(kr-n\pi/2). \tag{47}$$

The first term is oscillatory in the variable r', with mean value zero, as against $j_n{}^2(kr')\propto \sin^2(kr'-n\pi/2)$ appearing in the retained infinite integral—so its contribution is attenuated. The second term contributes to $\psi_n{}^B(r)$ the quantity

$$\delta\psi_n{}^B(r)\sim(2i/k^3r)\cos(kr-n\pi/2)\int_r^\infty dr'\ U(r'). \tag{48}$$

This expression is finally used in the integrand of Eq. (30), where it is multiplied by $j_n(kr)\propto\sin(kr-n\pi/2)$, leading again to an integral attenuated by oscillation as against the retained term. A parallel chain of reasoning leads to similar conclusions for the non-Born terms.

C. Assessment

The way the approximation is introduced does not lend itself to an *a priori* quantitative analysis of limits of validity and probable error. A couple of general remarks are nonetheless possible:

(1) The effect of the approximation is to distort the scattered wave function in the innermost region of the potential. The importance of this distortion grows in importance with the range of the potential, as the cumulative phase error builds up. Thus the approximation can be expected to work well with short- to moderate-range potentials (for which the phase shifts are not too large) and to break down for longer ranges, pretty much independently of the strength of the potential. (In contrast, the Born approximation gives erroneously large phase shifts for strong short-range potentials.)

(2) As the strength of the potential is increased (for fixed range), the scattering coefficients become nonlinear in the amplitude of the potential and ultimately

reach an asymptotic value independent of it. The approximation should be able to cope with strong potentials as well as weak. The exception to this is that, for attractive potentials, it will not reproduce the details of resonance behavior where the latter occurs; in that case, reasonable values for the "potential scattering" can be expected, but not the abrupt changes of phase shift (and cross section) at the individual resonances.

An incidental advantage of the present formulation is that it provides a more natural way of treating a continuously varying potential than the usual procedure of truncating the potential and then matching wave functions at the fictitious boundary.

III. SPHERICAL WELLS AND BARRIERS

To provide something of a calibration of the approximation, a detailed comparison of exact and approximate phase shifts has been carried out for a variety of spherical wells and barriers, i.e., spherically symmetric potentials of the form

$$\begin{aligned} U&=U_0, \quad r<a, \\ U&=0, \quad r>a, \end{aligned} \tag{49}$$

where U_0 can be a negative or positive constant. By varying U_0 and a, it is possible to map out the dependence of the accuracy of the approximation upon the strength and range of the potential; the conclusions thus arrived at should be applicable to any reasonable potential that falls off rapidly enough for large r (of course, just as in the Born approximation, the potential must fall off faster than $1/r$ for the integrals to converge).

To illustrate the results and sort out their pattern, some values of the $l=0$ phase shift are shown in Figs. 1–4. The display selected is to plot δ_0 versus U_0/k^2 (the ratio of the potential energy inside to the kinetic energy outside) for a fixed range, repeating for different ranges. Using absolute values, the results for attractive and repulsive potentials are superposed to save space. The values of $|U_0|/k^2$ run in each case from 1 to 100. The values of ka (the range in units of the reduced wavelength) used in the figures are 0.1, 0.5, 1.0, and 2.0, respectively. While the corresponding curves in Figs. 1–4 are qualitatively similar, the choice of values is such as to emphasize a different (partially overlapping) region of the curves in each figure.

Figure 1 depicts the state of affairs for small ka and correspondingly small phase shifts. For the stronger potentials shown, the Born approximation is appreciably in error, though not overwhelmingly. The present approximation does considerably better.

Figure 2, for $ka=0.5$, brings us into a region where the phase shift is no longer small. The Born approximation breaks down completely, and over much of this region it is doubtful that a second-order Born calculation would do any good. The present approximation gradually increases in error but remains in reasonable agreement with the exact values; a second-order calculation would undoubtedly come extremely close.

In discussing the effect of further increasing ka, it becomes necessary to distinguish between attractive and repulsive potentials. For the latter, the exact and approximate curves are similar, but the spread between them grows with ka. It is clear that as ka is increased this spread will reach an inadmissibly large value (for fixed U_0). To gauge where this occurs, the exact and

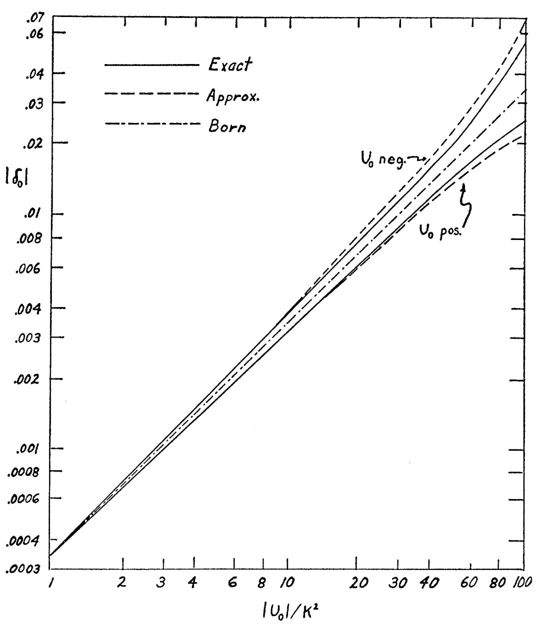

FIG. 1. Phase shift δ_0 for a spherical well or barrier of range $ka=0.1$.

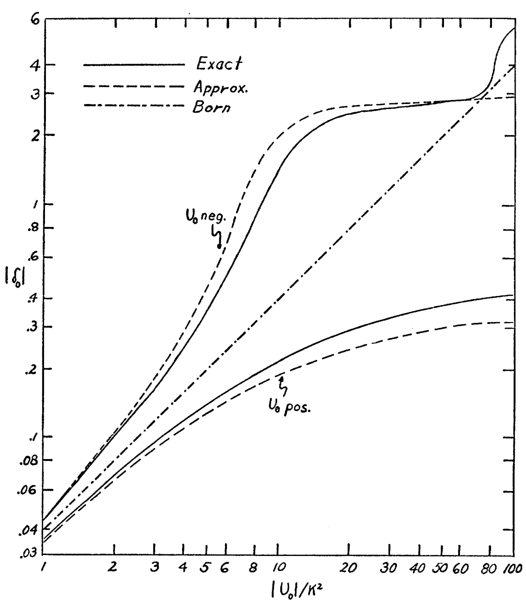

FIG. 2. Phase shift δ_0 for a spherical well or barrier of range $ka=0.5$.

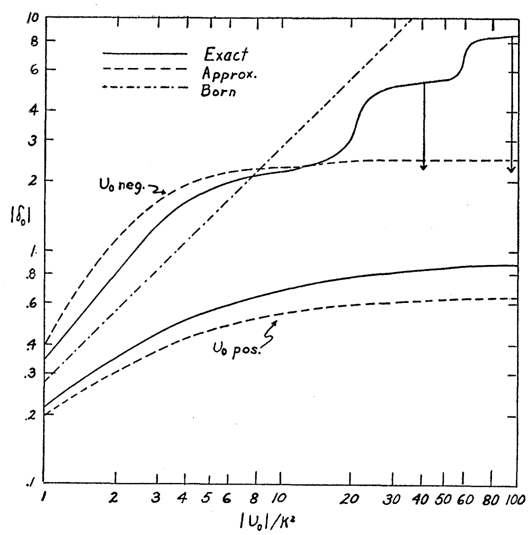

FIG. 3. Phase shift δ_0 for a spherical well or barrier of range $ka=1.0$. Arrows indicate displacement by $n\pi$ of plateau after nth resonance.

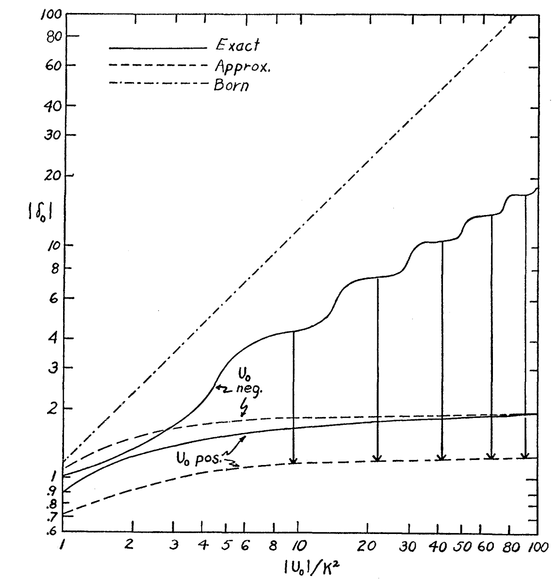

FIG. 4. Phase shift δ_0 for a spherical well or barrier of range $ka=2.0$. Arrows indicate displacement by $n\pi$ of plateau after nth resonance.

approximate values of $\sin\delta_0$ must be compared, inasmuch as the magnitude of the partial wave amplitude is proportional to $\sin\delta_0$. For the ka's illustrated, the values of $\sin\delta_0$ agree better than the values of δ_0; in fact, for $ka=2.0$ and strong potentials the agreement in $\sin\delta_0$ is excellent through the happenstance that the exact and approximate values of δ_0 straddle $-\pi/2$. For larger ka values this relationship quickly reverses, until for $ka=\pi$ a factor-of-two error in δ_0 leads to total disagreement (in the hard-sphere limit for $ka=\pi$, the exact δ_0 is $-\pi$, the approximate $-\pi/2$). For ka of the order of π or larger, the present approximation breaks down before the Born approximation does.

For attractive potentials, the exact and approximate curves part company when the exact curve begins the terrace pattern (a sequence of sharp rises in the magnitude of δ_0 followed by a plateau) characteristic of resonance behavior. The net effect after a resonance has been passed is an increase in $|\delta_0|$ by π. Since δ_0 enters in the partial wave amplitude only in the function $\exp(i2\delta_0)$, a shift in δ_0 by π is not observable. In Figs. 3 and 4, the arrows indicate where the plateau following the nth resonance would fall if $|\delta_0|$ were reduced by $n\pi$. If the arrow tips are connected, a smooth flat curve results which resembles the one for repulsive potentials, and which yields the partial-wave amplitude correctly except near the resonances. This is the "potential scattering," which is subtracted off in an analysis of resonances. It is evident that the approximate curve for attractive potentials follows the "potential scattering" curve, overshooting it by about the same amount as the approximate curve for repulsive potentials undershoots its exact counterpart (In both cases, a spurious positive phase shift is introduced, making the potential appear more repulsive than it actually is). On the other hand, it ignores the resonances altogether; the latter have to be found and treated in some other way.

Going back to Eq. (42), the spread between the exact and approximate curves (for repulsive potentials and for the "potential scattering" contribution for attractive potentials) can be ascribed to the integral in the denominator being too large. In fact, the exact and approximate curves can be made to coincide by scaling down the value of this integral (at least through $ka=1$), the scaling factor required decreasing as ka increases. The interpretation of this observation is that the approximation overestimates the effect of the scattering on the wave function in the innermost region of the potential, the more so the longer the range of the potential.