Formulation of High-Energy Potential Scattering Problems*

DAVID S. SAXON†
Institute of Theoretical Physics, Copenhagen, Denmark
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A method is presented for treating high-energy potential scattering in which the zero-order result is essentially the WKB approximation. The correction terms which appear involve the rate of change of the local wave number and the curvature of the classical trajectory. Unlike the usual WKB procedure which is only asymptotically correct, the formulation remains exact, but not necessarily convenient, even if the corrections are large. The improvement over the WKB approximation is demonstrated explicitly for one-dimensional scattering and for the calculation of phase shifts for scattering from a central potential. It is also shown that this prescription reduces to the Born approximation when the conditions for the validity of that approximation are satisfied. Thus the proposed formulation contains both the WKB and Born approximations as simple limiting cases.

IN the following a new method is briefly discussed for treating high-energy potential scattering. The essential idea is to construct a Green's function in which the customary free-space propagation is replaced by propagation with nearly correct local wave number. The resulting formulation is such that the zero-order result is essentially the WKB approximation.[1] The correction terms which appear involve the rate of change of wave number and the curvature of the classical trajectory. Unlike the usual WKB procedure which is only asymptotically correct, the formulation remains exact, but not necessarily convenient, even if the corrections are large. The motivation for the development of the method lies, on the one hand, with the need for analyzing the rapidly accumulating experimental data on elastic scattering of high-energy particles from nuclei and, on the other, with the hope of generalizing the recent approximation method of Schiff.[2]

We begin by treating one-dimensional scattering. In addition to whatever intrinsic interest this may have (e.g., propagation in a stratified medium), it serves as a suitable introduction because of its simplicity.

I. ONE-DIMENSIONAL SCATTERING

We write Schrödinger's equation in the form

$$d^2\psi/dx^2+\kappa^2(x)\psi=0, \tag{1}$$

where the local wave number $\kappa(x)$ is given by

$$\kappa^2(x)=(2m/\hbar^2)[E-V(x)]\equiv k^2+U(x). \tag{2}$$

For simplicity, we assume that $U(x)$ is real and that it approaches zero faster than $1/x$ as $|x|$ approaches infinity. We seek solutions of (1) subject to the boundary conditions

$$x\rightarrow-\infty,\quad \psi(x)\simeq e^{ikx}+Re^{-ikx};$$
$$x\rightarrow\infty,\quad \psi(x)\simeq Te^{ikx}.$$

The usual integral-equation formulation of this problem is obtained by using the free-space Green's function,

$$G(x,x')=(i/2k)e^{ik|x-x'|}.$$

However, instead we introduce the Green's function

$$F(x,x')=F(x',x)=\tfrac{1}{2}i\exp\{i[Z(x_>)-Z(x_<)]\}, \tag{3}$$

where

$$Z(x)=\int_0^x\kappa(x)dx;$$
$$Z(x_>)-Z(x_<)=k|x-x'|+\int_{x_<}^{x_>}(\kappa-k)dx, \tag{4}$$

and where $x_>$ is the greater of x and x', $x_<$ the lesser. F, which is just the one-dimensional Green's function in the variables $Z=Z(x)$ and $Z'=Z(x')$, is easily seen to satisfy the differential equation

$$\frac{d^2F}{dx^2}+\kappa^2(x)F=-\kappa(x)\delta(x-x')+\frac{d\kappa}{dx}\frac{dF}{dZ}. \tag{5}$$

To derive an integral equation for ψ, we begin with the identity

$$\frac{d}{dx}\left(\psi\frac{dF}{dx}-F\frac{d\psi}{dx}\right)=\psi\frac{d^2F}{dx^2}-F\frac{d^2\psi}{dx^2}.$$

Using (1) and (5) to eliminate the second derivatives on the right hand side and then integrating the result from x equal minus infinity to plus infinity, we obtain the integral equation

$$\psi(x)=\frac{k}{\kappa(x)}\exp\left[ikx+i\int_{-\infty}^x(\kappa-k)dx\right]+\frac{1}{\kappa(x)}\int_{-\infty}^{\infty}\frac{d\kappa(x')}{dx'}\frac{dF(Z,Z')}{dZ'}\psi(x')dx'. \tag{6}$$

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† Permanent address: University of California, Los Angeles, California.

[1] See H. J. Groenewold, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **30**, No. 19 (1956), in which the general problem of expansions with semiclassical zero-order terms is discussed by methods quite different from ours.

[2] L. I. Schiff, Phys. Rev. **103**, 443 (1956). I would like to thank Professor Schiff for a prepublication copy of his paper and for some illuminating discussions on the topic.

Letting x approach $\pm\infty$, respectively, we then find for the amplitudes of the transmitted and reflected waves

$$T=\exp\left[i\int_{-\infty}^{\infty}(\kappa-k)dx\right]+\frac{1}{2k}\int_{-\infty}^{\infty}\frac{d\kappa}{dx}\times\exp\left[i\int_{x}^{\infty}(\kappa-k)dx-ikx\right]\psi(x)dx; \quad (7)$$

$$R=-\frac{1}{2k}\int_{-\infty}^{\infty}\frac{d\kappa}{dx}\exp\left[ikx+i\int_{-\infty}^{x}(\kappa-k)dx\right]\psi(x)dx.$$

So far these expressions are exact. If $d\kappa/dx$ varies sufficiently slowly however, the integral in (6) is small and $\psi(x)$ can be found to any desired order in $d\kappa/dx$ by iteration. If we denote by $T^{(n)}$ and $R^{(n)}$ the resulting approximations to T and R valid up to terms of order $(d\kappa/dx)^n$, we then find

$$T^{(0)}=\exp\left[i\int_{-\infty}^{\infty}(\kappa-k)dx\right], \quad R^{(0)}=0;$$

$$T^{(1)}=T^{(0)}, \quad R^{(1)}=-\frac{1}{2}\int_{-\infty}^{\infty}\frac{1}{\kappa}\frac{d\kappa}{dx}\times\exp\left[2ikx+2i\int_{-\infty}^{x}(\kappa-k)dx\right]dx; \quad (8)$$

$\cdots$,

in agreement with the asymptotic result of Gol'dman and Migdal.[3] If one calculates $T^{(2)}$ and $R^{(2)}$, it is easily verified that the unitary character of the scattering is correctly preserved up to and including terms of order $(d\kappa/dx)^2$.

The resemblance of these results to those obtained by the WKB method[3] is quite apparent. It should be noted that even though the zero-order result for the transmission and reflection coefficients are exactly those obtained in the usual WKB approach, the zero-order wave function does not have the usual WKB amplitude dependence.[4] It should also be noted that in no sense is this formulation an asymptotic one. It remains valid even if κ is small or if it changes suddenly. As a matter of fact, the integral equation is trivially soluble in the extreme case of a square well. To outline the procedure in this case, let $U(x)=0$, $|x|>\frac{1}{2}a$ and $U(x)=U_0$, $|x|<\frac{1}{2}a$. Then,

$$d\kappa/dx=\Delta\kappa\delta(x+\tfrac{1}{2}a)-\Delta\kappa\delta(x-\tfrac{1}{2}a),$$

where $\Delta\kappa=(k^2+U_0)^{\frac{1}{2}}-k$. The integral in (6) can thus be evaluated exactly and $\psi(x)$ is then expressed in terms of $\psi(\frac{1}{2}a)$ and $\psi(-\frac{1}{2}a)$. Setting $x=\frac{1}{2}a$ and $-\frac{1}{2}a$, respectively, leads to a pair of algebraic equations for the unknown fields at these points. Solution of these equations then determines the wave function everywhere and the result obtained is exact. This suggests that whenever κ changes suddenly in a distance small compared to a wavelength, the integral in (6) should be approximately evaluated by treating all other factors in the integral as slowly varying over each such region. This leads to a kind of equivalent step-well result which can be iterated to find the relatively small corrections associated with any regions in which κ changes slowly. An example of a problem which could be treated this way would be a square well with a sloping or curved bottom.

A more interesting example is a potential which is flat over an extended region and which then decreases smoothly to zero, like the nuclear optical-model potential. At energies low enough that this decrease occurs in a fraction of a wavelength, the procedure above could be followed. On the other hand, at energies high enough that κ changes little in a wavelength, the problem is again easily treated by straight iteration, Eq. (8). Thus, the integral equation (6) has the remarkable property that it leads in this case to simple results in both the high- and low-energy limits.

The integral equation also has the interesting property that it reduces to the Born approximation when the conditions for the validity of that approximation are satisfied. The proof is not difficult but we omit it here since we shall shortly give an equivalent proof in the similar treatment of partial waves which follows.

II. PARTIAL WAVES

We next consider scattering in three dimensions. We begin by treating expansions in partial waves for spherically symmetrical potentials. Writing

$$\psi=\sum(1/r)u_l(r)P_l(\cos\theta),$$

we obtain (in the same notation as before) the radial equations

$$d^2u_l/dr^2+[\kappa^2(r)-l(l+1)/r^2]u_l=0; \quad u_l(0)=0. \quad (9)$$

Again we introduce a modified Green's function,

$$F_l(r,r')=F_l(r',r)=Z(r)Z(r')j_l[Z(r_<)]y_l[Z(r_>)]. \quad (10)$$

For the moment, we leave the precise definition of Z open except for the assumption that it is a single-valued function of r which vanishes at the origin and which has the asymptotic behavior

$$r\to\infty, \quad Z(r)\simeq kr+\epsilon_l. \quad (11)$$

It is not difficult to show that F_l satisfies the differential

[3] I. I. Gol'dman and A. B. Migdal, J. Exptl. Theoret. Phys. U.S.S.R. **28**, 463 (1955); translation: Soviet Phys. JETP **1**, 304 (1955).

[4] This is a matter of choice; a corresponding treatment which incorporates the WKB amplitude dependence can easily be developed. It leads to a more complicated integral equation than here but converges more rapidly in the WKB limit. The question of amplitude dependence, among others, will be treated in a forthcoming paper by J. Nodvik. In this connection, see also reference 1.

equation

$$\frac{d^2F_l}{dr^2}+\left(\frac{dZ}{dr}\right)^2\left[1-\frac{l(l+1)}{Z^2}\right]F_l=\frac{dZ}{dr}\delta(r-r')+\frac{d^2Z}{dr^2}\left(\frac{dF_l}{dZ}\right).$$

Applying Green's theorem to F_l and u_l, we then obtain

$$u_l(r)\frac{dZ}{dr}=\left[u_l(r')\frac{dF_l}{dr'}-F_l\frac{du_l}{dr'}\right]_{r'=0}^{\infty}-\int_0^\infty u_l(r')\frac{d^2Z(r')}{dr'^2}\frac{dF_l}{dZ'}dr'-\int_0^\infty u_l(r')F_l\times\left[\kappa^2(r')-\frac{l(l+1)}{r'^2}-\left(\frac{dZ'}{dr'}\right)^2\left(1-\frac{l(l+1)}{Z'^2}\right)\right]dr'.$$

Recalling our assumption that $Z(r)=0$ for $r=0$, the first term is seen to vanish at the lower limit. Recalling also that $Z(r)\simeq kr+\epsilon_l$ for large r, the upper limit is most easily treated by taking the asymptotic form of u_l to be

$$u_l\simeq Z[j_l(Z)-\tan\gamma_l y_l(Z)]\simeq A_l kr[j_l(kr)-\tan\delta_l y_l(kr)],$$

so that the true phase shift δ_l is given by

$$\delta_l=\gamma_l+\epsilon_l, \tag{12}$$

with ϵ_l defined by Eq. (11). We then find

$$u_l(r)\frac{dZ}{dr}=kZj_l(Z)-\int_0^\infty u_l(r')\frac{d^2Z'}{dr'^2}\frac{dF_l}{dZ'}dr'-\int_0^\infty u_l(r')F_l\left[\kappa^2(r')-\frac{l(l+1)}{r'^2}-\left(\frac{dZ'}{dr'}\right)^2\left(1-\frac{l(l+1)}{Z'^2}\right)\right]dr'.$$

If Z is taken to be kr the first integral on the right vanishes, and this reduces to the usual free-space Green's function formulation. Instead we choose Z by requiring that the last integral vanish identically; i.e., we write

$$(dZ/dr)^2[1-l(l+1)/Z^2]=\kappa^2(r)-l(l+1)/r^2, \tag{13}$$

and hence our integral equation is finally

$$u_l=\frac{kZj_l(Z)}{dZ/dr}-\frac{1}{dZ/dr}\int_0^\infty u_l(r')\frac{d^2Z'}{dr'^2}\frac{dF_l}{dZ'}dr'. \tag{14}$$

$Z(r)$ is determined up to a constant by (13) and it is easily verified that it has the required behavior at the origin and at infinity. Assuming for simplicity that $\kappa(r)$ is such that there is only one classical turning point r_l, we now choose this constant in the definition of Z by requiring that $Z(r_l)$ be the turning point for Z, i.e., that $Z(r_l)=[l(l+1)]^{\frac{1}{2}}\equiv Z_l$. Hence we have

$$\begin{aligned} r\le r_l;\quad &\int_r^{r_l} dr\left[\frac{l(l+1)}{r^2}-\kappa^2(r)\right]^{\frac{1}{2}} \\ &=Z_l\ln\left[\frac{Z_l+(Z_l^2-Z^2)^{\frac{1}{2}}}{Z}\right]-(Z_l^2-Z^2)^{\frac{1}{2}}, \\ r\ge r_l;\quad &\int_{r_l}^{r} dr\left[\kappa^2(r)-\frac{l(l+1)}{r^2}\right]^{\frac{1}{2}} \\ &=(Z^2-Z_l^2)^{\frac{1}{2}}-Z_l\cos^{-1}\left(\frac{Z_l}{Z}\right). \end{aligned} \tag{15}$$

Letting r approach ∞ in this last equation (after subtracting and adding $\int^r_{Z_l/k} dr[k^2-l(l+1)/r^2]^{\frac{1}{2}}$), we then find that ϵ_l is just the familiar Jeffries WKB phase shift,

$$\epsilon_l=\int_{r_l}^\infty dr\left[\kappa^2-\frac{l(l+1)}{r^2}\right]^{\frac{1}{2}}-\int_{Z_l/k}^\infty dr\left[k^2-\frac{l(l+1)}{r^2}\right]^{\frac{1}{2}}. \tag{16}$$

Finally, letting r and therefore $Z(r)$ approach infinity in the integral equation (14), we find

$$\tan\gamma_l=\frac{1}{k}\int_0^\infty u_l(r)\frac{d^2Z}{dr^2}\frac{d}{dZ}[Zj_l(Z)]dr, \tag{17}$$

with the actual phase shift δ_l given according to (12) by $\delta_l=\epsilon_l+\gamma_l$. Thus once again we have arrived at a formulation, more complicated to be sure, in which the scattering is determined in zero approximation by its WKB value and to higher approximation is corrected by terms involving the rate of change of the local wave number. Assuming these corrections to be small, $u_l(r)$ will be given adequately by the first term in the integral equation, and to this approximation we thus obtain

$$\tan\gamma_l\simeq\frac{1}{2}\int_0^\infty\frac{1}{dZ/dr}\left(\frac{d^2Z}{dr^2}\right)\frac{d}{dZ}[Zj_l(Z)]^2dr. \tag{18}$$

In the past there have been two difficulties associated with the use of WKB phase shifts even for potentials which are properly slowly varying. First, because a large number of phase shifts is generally required, each must be very precisely determined if the cross section is to be given with any accuracy. It is hoped that the correction represented by (18) will effectively correct the WKB values to the required precision. Secondly, it is well known[5] that as l increases, the WKB phase shifts eventually become somewhat inaccurate and indeed become a poorer approximation than the Born to the actual phase shifts. In connection with this latter point, we now show that our approximation reduces to the Born approximation for large enough l, or more gener-

[5] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, 1950).

ally, whenever the conditions for the validity of the Born approximation are satisfied. To show this, we first integrate Eq. (18) by parts, obtaining,

$$\tan\gamma_l=-\frac{1}{2}\int_0^\infty \ln\left(\frac{1}{k}\frac{dZ}{dr}\right)\frac{dZ}{dr}\frac{d^2}{dZ^2}[Zj_l(Z)]^2dr.$$

Next we use the identity

$$\frac{1}{2}\frac{d^2}{dZ^2}[Zj_l(Z)]^2=1-2\left[1-\frac{l(l+1)}{Z^2}\right][Zj_l(Z)]^2 -2\int_Z^\infty \frac{l(l+1)}{Z}j_l^2(Z)dZ,$$

which is easily verified by differentiating once with respect to Z and then using the differential equation satisfied by $Zj_l(Z)$ to replace the higher order derivatives on the left. In any case, we thus have

$$\tan\gamma_l=-\int_0^\infty \frac{dZ}{dr}\ln\left(\frac{1}{k}\frac{dZ}{dr}\right)\left\{1-2\left[1-\frac{l(l+1)}{Z^2}\right]\times[Zj_l(Z)]^2-2l(l+1)\int_Z^\infty dZ\frac{j_l^2(Z)}{Z}\right\}dr.$$

Thus far, no additional approximations have been made. We now assume however that l is sufficiently large, or U sufficiently small that Z deviates only slightly from kr. In this case, writing

$$\frac{1}{k}\frac{dZ}{dr}=1+\left(\frac{1}{k}\frac{dZ}{dr}-1\right),$$

we obtain, neglecting second-order terms,

$$\frac{dZ}{dr}\ln\left(\frac{1}{k}\frac{dZ}{dr}\right)\simeq\frac{dZ}{dr}-k.$$

Hence, to this order,

$$\tan\gamma_l\simeq-\int_0^\infty\left(\frac{dZ}{dr}-k\right)dr+2k^2\int_0^\infty\left(\frac{dZ}{dr}-k\right)\times\left[1-\frac{l(l+1)}{k^2r^2}\right]j_l^2(kr)r^2dr+(2l(l+1)\times\int_0^\infty\left(\frac{dZ}{dr}-k\right)\left\{\int_r^\infty dr\frac{j_l^2(kr)}{r}\right\}dr.$$

The first term is easily evaluated and gives $-\epsilon_l$. Turning now to the second term, we find a more explicit expression for $dZ/dr-k$ using the defining Eq. (13). We thus write, to the same order as above

$$\frac{dZ}{dr}-k\simeq\frac{1}{2k}\left[\left(\frac{dZ}{dr}\right)^2-k^2\right]\simeq\frac{1}{2k}\left(\frac{U(r)-k^2l(l+1)[(1/k^2r^2)-(1/Z^2)]}{1-[l(l+1)/k^2r^2]}\right),$$

or,

$$2\left[1-\frac{l(l+1)}{k^2r^2}\right]\left(\frac{dZ}{dr}-k\right)\simeq\frac{U(r)}{k}-2kl(l+1)\frac{(Z-kr)}{k^3r^3}.$$

Hence

$$\tan\gamma_l\simeq-\epsilon_l+k\int_0^\infty U(r)j_l^2(kr)r^2dr-2l(l+1)\times\int_0^\infty\left\{(Z-kr)\frac{j_l^2}{r}-\left(\frac{dZ}{dr}-k\right)\int_r^\infty dr\frac{j_l^2}{r}\right\}dr.$$

The integrand in the last term is now recognized as a perfect differential which integrates to zero. Since γ_l is small, we thus have

$$\gamma_l\simeq-\epsilon_l+k\int_0^\infty U(r)j_l^2(kr)r^2dr,$$

and hence finally that

$$\delta_l=\gamma_l+\epsilon_l\simeq k\int_0^\infty U(r)j_l^2(kr)r^2dr,$$

which is indeed the Born approximation. We regard this as a rather illuminating illustration of how the WKB phase shifts can be effectively corrected in this formulation.

As a test of our method, we have calculated the S-wave phase shift for a triangular well,

$$U(r)=U_0(1-r/a),\quad r\leq a;$$
$$U(r)=0,\quad r\geq a.$$

Admittedly, this test is quite incomplete, since for higher l values the entire procedure is more complicated and to some extent, more uncertain. In any case, the S-wave phase shift for such a potential can be found exactly and is given by

$$\tan(ka+\delta)=\pm\frac{J_{\frac{1}{3}}(y_a)J_{-\frac{1}{3}}(y_0)-J_{\frac{1}{3}}(y_0)J_{-\frac{1}{3}}(y_a)}{J_{-\frac{2}{3}}(y_a)J_{-\frac{1}{3}}(y_0)-J_{\frac{1}{3}}(y_0)J_{\frac{2}{3}}(y_a)},\quad(19)$$

where the upper sign applies for repulsive, the lower for attractive potentials, and where

$$y_0=\tfrac{2}{3}(U_0+k^2)^{\frac{3}{2}}a/|U_0|,\quad y_a=\tfrac{2}{3}k^3a/|U_0|.$$

The corresponding result derived from our integral equation approximation, Eqs. (12), (16), and (18) with

$l=0$, is easily found to be

$$\delta=|y_0-y_a|-ka\pm\tan^{-1}\tfrac{1}{6}\{\sin 2y_0[\mathrm{Ci}(2y_0)-\mathrm{Ci}(2y_a)] -\cos 2y_0[\mathrm{Si}(2y_0)-\mathrm{Si}(2y_a)]\}, \quad (20)$$

where the same sign convention holds as in Eq. (19) and where

$$\mathrm{Ci}(x)\equiv\int_\infty^x \frac{\cos x}{x}dx,\quad \mathrm{Si}(x)\equiv\int_0^x \frac{\sin x}{x}dx.$$

The inverse tangent term in (20) is the correction to the WKB result,

$$\delta_{\mathrm{WKB}}=|y_0-y_a|-ka. \quad (21)$$

In Table I, the exact phase shifts computed from (19), our approximate values (20) and the WKB values (21) are given for a wide range of the parameters y_0 and y_a. As seen from this table, the WKB phase shifts are effectively corrected even in the limit of small values of y_0 and/or y_a when the WKB approximation is not valid. The explicit behavior of the results in the opposite limit, in which y_0 and y_a are both large, is easily exhibited. In this case the exact result can be asymptotically expanded to yield

$$\delta\simeq|y_0-y_a|-ka\pm\left[\frac{5}{72}\left(\frac{1}{y_0}-\frac{1}{y_a}\right) -\frac{1}{6y_a}\sin^2(y_0-y_a)\right]+\cdots.$$

The corresponding asymptotic expansion of the approximate Eq. (20), is found to be identical except that the coefficient 5/72 is replaced by 6/72. The error in this approximation is thus about one order of magnitude less than the error in the WKB approximation.

Detailed comparison of the results obtained using the formulation outlined above with exact results are planned for a variety of potentials, both real and complex, for many different energies and for many partial waves. Potentials containing a Coulomb part will also be studied. Until such comparisons are made, it is difficult to assess the precise range of validity of this treatment. It is hoped that the method will sufficiently extend the range of validity of the usual WKB approximation that it can be applied for example to the optical-model analysis of nuclear scattering at energies which are quite moderate by present standards.

TABLE I. Comparison of exact and approximate S-wave phase shifts for a triangular potential.

y_0	y_a	ka	U_0a^2	WKB	Exact	Approx.
1	$\frac{1}{4}$	0.5700	0.49	0.18	0.0237	0.0134
	$\frac{1}{2}$	0.4406	0.11	0.0594	0.0041	0.0008
	1	···	0	0	0	0
	2	1.1102	−0.46	−0.1102	−0.0345	−0.0355
	4	3.6189	−7.9	−0.6189	−0.5797	−0.5715
	8	9.0000	−60.8	−2.000	−1.9438	−1.9356
4	$\frac{1}{4}$	2.0061	21.5	1.7440	1.6569	1.6685
	$\frac{1}{2}$	2.2500	15.2	1.2500	1.2543	1.2702
	1	2.2797	7.9	0.7203	0.7604	0.7706
	2	1.7621	1.8	0.2379	0.1933	0.1989
	4	···	0	0	0	0
	8	4.406	−7.3	−0.4406	−0.4207	−0.4196
16	$\frac{1}{4}$	5.6250	475	10.1250	10.2101	10.2526
	$\frac{1}{2}$	6.8097	421	8.6903	8.7808	8.8025
	1	8.0244	344	6.9756	6.9926	7.0046
	2	9.0000	243	5.0000	4.9504	4.9560
	4	9.1191	126	2.8809	2.8840	2.8869
	8	7.0488	30	0.9512	0.9354	0.9362

III. THREE-DIMENSIONAL FORMULATION

We conclude with a few remarks on the corresponding formulation in three dimensions. Here we want to solve

$$[\nabla^2+\kappa^2(\mathbf{r})]\psi(\mathbf{r})=0,$$

subject to

$$\mathbf{r}=\mathbf{n}r\to\infty,$$
$$\psi(\mathbf{n}r)\simeq\exp(ik\mathbf{n}_0\cdot\mathbf{n}r)+f(\mathbf{n}_0,\mathbf{n})e^{ikr}/r. \quad (22)$$

As before, we introduce a modified Green's function

$$F(\mathbf{r},\mathbf{r}')=F(\mathbf{r}',\mathbf{r})=e^{iS(\mathbf{r},\mathbf{r}')}/4\pi|\mathbf{r}-\mathbf{r}'|. \quad (23)$$

For the moment we leave the precise definition of $S(\mathbf{r},\mathbf{r}')$ open except to assume that it represents some approximation to the "correct" propagator between $\mathbf{r}$ and $\mathbf{r}'$. Thus we shall assume that $S(\mathbf{r},\mathbf{r})=0$, or more precisely, that

$$\lim_{\mathbf{r}\to\mathbf{r}'}\frac{S(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}=c(r).$$

We further assume that as $\mathbf{r}=\mathbf{n}r\to\infty$ with $\mathbf{r}'$ finite, the propagation proceeds along $\mathbf{n}$ with the free-space propagation constant, i.e., that

$$\mathbf{r}=\mathbf{n}r\to\infty,\quad \nabla S=k\mathbf{n}+O(1/r). \quad (24)$$

It is easily verified that F satisfies the differential equation

$$\nabla^2F+(\nabla S)^2F=-\delta(\mathbf{r}-\mathbf{r}')+iF|\mathbf{r}-\mathbf{r}'|^2\nabla\cdot\frac{\nabla S}{|\mathbf{r}-\mathbf{r}'|^2}.$$

Applying Green's theorem to ψ and F, we then find

$$\psi(\mathbf{r})=\lim_{\mathbf{r}'=\mathbf{n}r'\to\infty}\int r'^2d\Omega\mathbf{n}\cdot[F\nabla'\psi(\mathbf{r}')-\psi(\mathbf{r}')\nabla'F] +\int\left\{\kappa^2(\mathbf{r}')-(\nabla'S)^2+i|\mathbf{r}-\mathbf{r}'|^2\nabla'\cdot\frac{\nabla'S}{|\mathbf{r}-\mathbf{r}'|^2}\right\}\psi(\mathbf{r}')Fd^3r'.$$

When we utilize the known asymptotic form of ψ, given in Eq. (22), and the assumed properties of S, given in Eq. (24), the surface integral is easily evaluated and we find

$$\psi(\mathbf{r})=\exp[ik\mathbf{n}_0\cdot\mathbf{r}+i\delta(\mathbf{n}_0,\mathbf{r})]$$
$$+\int\left\{\kappa^2-(\nabla'S)^2+i|\mathbf{r}-\mathbf{r}'|^2\nabla'\cdot\frac{\nabla'S}{|\mathbf{r}-\mathbf{r}'|^2}\right\}\psi F d^3r',$$

where $\delta(\mathbf{n}_0,\mathbf{r})$ is defined by

$$\lim_{r'\to\infty} S(\mathbf{r},-\mathbf{n}_0r')-k|\mathbf{r}+\mathbf{n}_0r'|=\delta(\mathbf{n}_0,\mathbf{r}).$$

Thus δ represents the change in the phase of a ray incident along $\mathbf{n}_0$ and arriving at $\mathbf{r}$ compared to its value for free propagation.

For the customary choice of S as the free-space propagator $k|\mathbf{r}-\mathbf{r}'|$, this formulation reduces to the familiar one in terms of the free-space Green's function. However, we shall choose S to be the classical action function (in units of $\hbar$) which means, of course, that

$$(\nabla S)^2=\kappa^2(\mathbf{r}),$$

with the orthogonal trajectories to the surfaces of constant S giving the classical-mechanical trajectories or geometrical-optical ray paths. Hence if these are known, S can be regarded as known.[6] With this choice the integral equation becomes finally

$$\psi(\mathbf{r})=\exp[ik\mathbf{n}_0\cdot\mathbf{r}+i\delta(\mathbf{n}_0,\mathbf{r})]$$
$$+i\int|\mathbf{r}-\mathbf{r}'|^2\nabla'\cdot\frac{\nabla'S}{|\mathbf{r}-\mathbf{r}'|^2}\psi(\mathbf{r}')F(\mathbf{r},\mathbf{r}')d^3r',$$

where δ now represents the WKB phase shift along a classical trajectory which is incident from infinity along $\mathbf{n}_0$. Again we observe the WKB character of the formulation, with the corrections depending on the rate of change of wave number along the trajectory and the curvature of the trajectory. And again we emphasize that the formulation is not asymptotic. It remains exact even if κ changes discontinuously; surface integrals then appear corresponding to the reflections generated by such a discontinuity.

In the high-energy limit for potentials which are slowly varying, which is also the limit considered by Schiff,[2] δ is different from zero only in the classically accessible scattering region which forms a small cone about the forward direction. Hence the large-angle scattering is determined by the second term and to first approximation is given by the asymptotic behavior of this term with $\psi(\mathbf{r}')$ replaced by

$$\exp[ik\mathbf{n}_0\cdot\mathbf{r}'+i\delta(\mathbf{n}_0,\mathbf{r}')].$$

It is easily seen that the result resembles Schiff's, but here we follow the particle in along its actual classical trajectory and out along its actual classical trajectory (in each case with the correct propagation contant) rather than along straight-line approximations to these trajectories. On the other hand, the forward scattering seems to be most easily computed from the expression, exact if ψ is exact,

$$f(\mathbf{n}_0,\mathbf{n})=\frac{1}{4\pi}\int\exp(-ik\mathbf{n}\cdot\mathbf{r})U(\mathbf{r})\psi(\mathbf{r})d^3r.$$

We expect that in this high-energy limit, the first term in the integral equation for ψ is an adequate representation, as far as the small-angle scattering is concerned, to the actual field in the neighborhood of the scattering potential.[2] Hence, again we are led to an expression which is closely related to Schiff's. These remarks are rather sketchy but we hope to present a more detailed analysis in the near future.

We add one final remark. The discussion in the present note has been limited to scalar fields. It seems clear that the extension to fields with other tensor character should be straightforward. Each component of such a field propagates with the same propagator and it is expected, therefore, that an appropriate Green's function can be constructed without much difficulty.

[6] We assume high enough energies or weak enough potentials that the question of multiple paths and caustics can be ignored. See references 1 and 3 for a discussion of the complication associated with multiple rays.