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Multiple scattering of scalar waves by point scatterers in one dimension. I

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We discuss the problem of scalar wave multiple scattering in one dimension on a target of n identical fixed scatterers with delta-function potentials. We consider in detail a statistical ensemble of configurations of scatterers whose positions are uniformly distributed throughout the scattering region. We succeed in analytically performing a configurational average (over all scatterer positions) for the wave function for the problem of a transmitted wave with constant amplitude. We discuss the relationship between this problem and the standard problem of an incident wave with constant amplitude. From the simple closed form for the average of the wave function, the optical potential for the system is obtained. We then present the large and small incident particle wavelength limits [with respect to the length (L) of the scattering region] for both the average of the wave function and the optical potential. We also examine the question as to where the optical potential can be approximated by the form it takes in the limit of infinite n. (The question of where in parameter space this occurs and how well the transmitted and reflected waves can be predicted with this form is discussed in the following paper.) Furthermore, we consider the large incident particle wave number limit for the average wave function and the optical potential for a general distribution of the scatterer positions in the limit of both n and L approaching infinity but with n/L remaining fixed. Lastly, knowing the simple closed form for the average of the wave function, we prove that the effective field approximation becomes exact in the limit of infinite n with all other parameters held fixed.

[NUCLEAR REACTIONS Multiple scattering, randomly distributed point scatterers, one dimension; configurational average wave function, optical potential; low and high energy limits.]

Methods for describing the multiple scattering of waves have been under continuous investigation since the turn of the century.[1] In the following preliminary remarks, we shall briefly discuss several aspects of the problem as introduced by Foldy.[2] The problem of multiple scattering for pointlike scatters is discussed, and it is shown that, for s-wave scattering, a set of n inhomogeneous equations for the scattering amplitudes can be derived. The solution of these equations can then be used to determine the wave function at any point inside or outside the scattering region. Then in order to calculate the optical potential (or equivalently the index of refraction), the configurational average of the wave function must be found. To expedite the calculation of the optical potential, energy flux, and other properties, the effective field approximation is implemented. This means replacing the average external field by the average of the wave function at that point. (The external field is defined as the incident wave minus the scattered wave emerging at that point.) Using the effective field approximation circumvents the need to calculate the average wave function and leads to a simple expression for the optical potential. This approximation is expected to hold in the limit of large n.

The problem of finding the configurational average for the exact solution remained. In order to avoid this difficulty, Lax[3] discussed the hierarchy method. This meant relating the average of the wave function over m scatterers with that over $m-1$ and then truncating the appropriate series at some value of m by equating the two averages; he termed the first step the quasi-crystalline approximation. Waterman and others[4] extended this concept using a modified effective field approximation and presented an expression for the index of refraction in terms of the forward scattering amplitude for several different examples.

Several other approaches which include a discussion of strong multiple scattering (for nonoverlapping potentials) are briefly discussed below. In Ref. 5, the potential is written as a sum of separable potentials, and a system of n inhomogeneous equations are found. From the solution of these equations, the scatterer amplitudes for the system can be calculated. In Ref. 6, a similar use of Green's function techniques and separable potentials also yields a set of n algebraic equations. The solution of these equations allows the complex propagation vector in the scattering region to be determined. In each of the aforementioned papers, the potentials are expanded in terms of spherical harmonics and the above calculations carried through. The effective field approximation and the assumption of closely packed scatterers are used in Ref. 6. Another approximation, different from the effective field approximation, along with the assumption of closely packed scatterers, is used by Lenk[7] to calculate different partial wave contributions.

Only a few people have dealt directly with the problem we consider. A series of papers by Bazer[8] and Bazer and Karal[9] are concerned with the one-dimensional problem of an incident wave with constant amplitude. In these articles, sufficient conditions for the validity of the effective field approximation are presented. Fikioris[10] calculates three examples for specific values of the parameters and comments on the validity of the effective field approximation. Recently, Olsen and others[11] have considered the validity of certain approximations to multiple scattering in a random medium with discrete scatterers. Thus far no one has yet considered the conditions on n, Γ (the scattering strength per scatterer), k (the incident particle wave number), and L (the length of the scattering region), where the effective field approximation is valid and where the optical potential simplifies and is still a useful approximation in predicting the outcome of the scattering.

The reason for approaching the problem of multiple scattering in one dimension is mainly because of its simplicity in comparison with the three-dimensional problem. It is, however, of considerable interest because it is a prototype of a number of problems in multiple scattering theory. The wave function can be represented as the sum of an incident wave plus scattered waves from all the scatterers. The amplitude of the scattered wave from each scatterer is obtained by solving a system of n inhomogeneous algebraic equations in which the scatterer positions appear as parameters in the coefficients. Physical measurements can measure an average state and, in this case, an ensemble average of the wave function is required. These measurements can be made in both one and three dimensions, so that the ideas from this approach can be directly tested.

Some examples of the three-dimensional problem include: multiple scattering of sound waves by bubbles in a liquid; scattering of electrons in liquid metals and other substances such as amorphous materials; scattering of neutrons or other elementary particles by aggregates of nuclei; and ultrasonic scattering, to name a few. In one dimension, some problems are as follows: scattering from planes, each with a different index of refraction than the scattering medium in the case of normal incidence; the transverse motion of an infinite homogeneous string with pointlike masses located at random along a fixed length; or the passing of a current through a transmission line with lumped impedances randomly located in series along a fixed length. In fact, any problem with a discontinuity in the first derivative which is proportional to the wave function at the discontinuity is described by this theory.

The objective of our papers is to determine the conditions under which a simplified form of the optical potential might be used to describe a multiple scattering experiment. Only the one-dimensional problem is considered in this and the following paper. In this paper an exact expression is calculated for the average wave function given certain boundary conditions. This expression is a finite sum which can be expanded as a convergent power series in k. The first form is suitable for numerical calculations when k is large, while the second is necessary for small k. The calculational difficulties make it necessary to examine these limiting forms of the solution. These limiting forms actually contain all orders of multiple scattering and are not like the normal Born-type approximations. We therefore present large and small kL limits for the wave function and for the optical potential from which scattering effects can be at least roughly calculated. We show that the optical potential may indeed by replaced by a simplified form for all kL for most purposes. In paper II, we extend the analysis numerically to cover the entire range of kL and subsequently discuss where a simplified form of the potential can be used. These results are then compared with those given by a Monte Carlo analysis of the problem, so that one can see whether the same conclusions are applicable to the physical case.

The outline of this paper is as follows. In Sec. I, we define the one-dimensional problem and compare it with a similar three-dimensional problem. In Sec. II, we find a simple closed form solution for the configurational average of the wave function for the one-dimensional problem of a transmitted wave of constant amplitude. This is done for a system of n independent and uniformly distributed scatterers. In Sec. III, we present the large and small kL limits of this solution and also an alternate form for the above mentioned solution. In Sec. IV, we discuss the optical potential in the limits of small kL, large kL, and infinite n. In Sec. V, we present results for the average wave function and the optical potential which are valid for large kL, and a general density distribution for the position of the scatterers as n and L approach infinity but with n/L fixed. In Sec. VI, we consider the relationship of this problem to the standard case where the incident wave has constant amplitude. In the conclusion, we summarize the main results. In the Appendix, we prove that the effective field approximation becomes exact in the limit of n approaching infinity with all other parameters held fixed.

I. THE ONE-DIMENSIONAL PROBLEM

We consider the one-dimensional problem of n identical pointlike scatterers with delta-function

potentials. The scatterers are constrained to lie in the interval 0 to L which we define as the scattering region. The Schrödinger wave equation for this n-scatterer system is

$$-\frac{\hbar^2}{2m}\psi_n''(x)+\frac{\hbar^2}{2m}\sum_{i=1}^{n}\Gamma_i\,\delta(x-x_i)\psi_n(x)=E\psi_n(x)\,. \tag{1}$$

$\psi_n(x)\equiv\psi(x;x_1,x_2\ldots x_n)$, and the prime denotes differentiation with respect to x. The x_i are the positions of the scatterers and $0<x_i<L$. The Γ_i are the interaction strengths associated with each potential; we take all Γ_i to be equal to Γ. If we choose units of $\hbar^2/2m=1$ and consider the nonrelativistic case where $E=\hbar^2k^2/2m$, then Eq. (1) becomes

$$\psi_n''(x)+k^2\psi_n(x)=\Gamma\sum_{i=1}^{n}\delta(x-x_i)\psi_n(x)\,. \tag{2}$$

This is known as the reduced wave equation. The system has a harmonic time dependence so that $\psi_n(x,t)=\psi_n(x)e^{-i\omega t}$, where ω is defined as a function of k by an appropriate dispersion relation.

In order to solve Eq. (2), we need to specify the boundary conditions for the wave function. One approach is to consider a wave incident from the right with a normalized amplitude of unity. An alternate approach (though of less physical interest) is to take the wave to be incident from the right, but to have a transmitted wave with an amplitude normalized to unity. These two cases will be dubbed the "physical" and "alternate" cases. Actually, both are physically realizable, but the first is much easier to establish experimentally. We discuss only the physical case in the remainder of this section.

Equation (2) can be converted to the Lippmann-Schwinger integral equation

$$\psi_n(x)=\psi_0(x)+\sum_{i=1}^{n}\int_{-\infty}^{\infty}G(x,x')U(x',x_i)\psi_n(x')dx'\,, \tag{3}$$

where $\psi_0(x)$ is a solution to the free-space wave equation, $G(x,x')$ is an appropriate Green's function, and $U(x',x_i)=\Gamma\delta(x'-x_i)$. $U(x',x_i)$ is referred to as the reduced potential since we are dealing with units $\hbar^2/2m=1$. For the physical case, $G(x,x')=e^{ik|x-x'|}/2ik$ for all x, x' and $\psi_0(x)=e^{-ikx}$ so that

$$\psi_n(x)=e^{-ikx}+\frac{\Gamma}{2ik}\sum_{i=1}^{n}e^{ik|x-x_i|}\psi_n(x_i)\,. \tag{4}$$

At $x=x_j$ and with $\psi_j\equiv\psi(x_j)$, this becomes

$$\psi_j=e^{-ikx_j}+\frac{\Gamma}{2ik}\sum_{i=1}^{n}e^{ik|x_j-x_i|}\psi_i\,. \tag{5}$$

Equation (16) is a system of n inhomogeneous algebraic equations in the ψ_i. Apart from the incident wave e^{-ikx}, there will also be a reflected wave re^{ikx} $(x>L)$ and a transmitted wave te^{-ikx} $(x<0)$. In particular, r and t are complex constants and functions of the scatterer positions.

In the three-dimensional case, for s-wave scattering, a set of equations similar to Eq. (5) occurs, but in a slightly different form. From Ref. 2, we find that the resulting wave function can be written as

$$\psi(\vec{\mathbf{r}})=\psi_0(\vec{\mathbf{r}})+\sum_{j=1}^{n}A_jG(\vec{\mathbf{r}},\vec{\mathbf{r}}_j)\,, \tag{6}$$

where $\psi^j(\vec{\mathbf{r}})=\psi(\vec{\mathbf{r}})-A_jG(\vec{\mathbf{r}},\vec{\mathbf{r}}_j)$ and the arguments for the positions of the scatterers have been suppressed. Also, A_j is defined as $g\psi^j$, with $\psi^j\equiv\psi^j(\vec{\mathbf{r}}_j)$. Upon substituting $\vec{\mathbf{r}}=\vec{\mathbf{r}}_j$ in Eq. (6), we obtain the following system of n inhomogeneous algebraic equations for the external fields ψ^j:

$$\psi^j=\psi_0(\vec{\mathbf{r}}_j)+g\sum_{l}{}'\psi^lG(\vec{\mathbf{r}}_l,\vec{\mathbf{r}}_j)\,, \tag{7}$$

where the prime indicates that the sum does not contain the term with $l=j$. Solving for the external fields and substituting into Eq. (6) yields the desired solution for $\psi(\vec{\mathbf{r}})$. In most cases there is no simple reduced solution for $\psi(\vec{\mathbf{r}})$ and so, to find the average value of $\psi(\vec{\mathbf{r}})$, a large number of random distributions of scatterer positions must be considered and, each time, Eq. (7) must be solved. For large values of n, this is very time consuming, even with present computer techniques and computer speeds. Returning to one dimension, we obtain a result similar to Eq. (7), except that there is no singularity in the scattered wave at the scatterer's position. We can rewrite Eq. (5) by taking the $i=j$ term in the sum on the right to the left-hand side and defining $\psi^j=(1-\Gamma/2ik)\psi(x_j)$ and $g_1\psi^j=\Gamma\psi(x_j)$; we obtain in either the physical or unphysical cases,

$$\psi^j=\psi_0(x_j)+g_1\sum_{l}{}'\psi^lG(x_l,x_j)\,, \tag{8}$$

where $g_1=\Gamma(1-\Gamma/2ik)^{-1}$. This result is identical in form to that in Eq. (7). Because there is no singularity in the one-dimensional problem, it is easier to express the results in terms of Γ as in Eq. (5) or later as in Eq. (11).

II. THE AVERAGE WAVE FUNCTION

Returning to the one-dimensional problem, the next step toward calculating an optical potential is to determine the average of the wave function. Unfortunately, the determinant associated with the inhomogeneous equations in Eq. (5) is dependent on the position of the scatterers, and performing the integrals analytically is not possible. We therefore turn to the alternate case, on which

we focus our attention for the remainder of this paper.

In the alternate case, the transmitted wave has constant amplitude and is taken to be e^{-ikx} for $x \leq 0$. The Green's function is

$$G(x, x') = \theta(x - x') \frac{\sin k(x - x')}{k} . \tag{9}$$

For any particular random distribution of scatterer positions, we relabel the scatterers so that $x_i \leq x_{i+1}$ for all i between 1 and n. Evaluating Eq. (3) at $x = x_j$ with $G(x_j, x_i)$ taken from Eq. (9), we obtain

$$\psi_j = e^{-ikx_j} + \frac{\Gamma}{k} \sum_{i=1}^{n} \theta(x_j - x_i) \sin k(x_j - x_i)\psi_i . \tag{10}$$

The determinant of the coefficients of ψ_i in Eq. (10) is triangular in form with unit elements on the diagonal, and is accordingly unity. Thus there is no denominator term for $\psi_n(x)$ in the alternate case, and the resulting average wave function will be different from that in the physical case. Solving for the ψ_i and using Eq. (3), we obtain

$$\psi_n(x) = e^{-ikx} + \frac{\Gamma}{k} \sum_{i=1}^{n} \theta(x - x_i) \sin k(x - x_i)\psi_{i-1}(x_i) . \tag{11}$$

The quantity $\psi_{i-1}(x_i)$ is the wave function for $i - 1$ scatterers at the point x_i, where we take $\psi_0(x_1)$ to be e^{-ikx_1}. For $x > L$, there are two other waves: an incident wave ae^{-ikx} and a reflected wave be^{ikx}. Both a and b are complex constants depending on the positions of the scatterers.

The alternate and physical wave functions can be related. In fact, we can obtain the solution to Eq. (4) by calculating the coefficient of e^{-ikx} at $x = L$ in Eq. (11) and then dividing Eq. (11) by this term [which is just the determinant of the coefficients of ψ_i in Eq. (5)].

In order to calculate the optical potential, the average of the wave function must be calculated. We present the details of this calculation for an independent (uncorrelated) uniform distribution of the scatterer positions. In this case, the probability distribution becomes

$$p(x_1, x_2, \ldots, x_n) = p(x_1)p(x_2)\ldots p(x_n) , \tag{12}$$

where $p(x_i) = 1/L$ is the probability distribution of the position of an individual scatterer. The average wave function is then

$$\langle \psi_n(x) \rangle_n = \int_0^L \ldots \int_0^L \int_0^L \frac{\psi_n(x)}{L^n} dx_1 dx_2 \ldots dx_n . \tag{13}$$

The subscript n outside the angular brackets implies that an average over all n scatterer positions has been performed.

We evaluate Eq. (13) by examining the terms of pth order in (Γ/k) in Eq. (11). Using $\psi_0(x) = e^{-ikx}$ in Eq. (11), we can recursively calculate $\psi_n(x)$. In this way, we find that the pth order part of $\psi_n(x)$ for $x > x_p$ is

$$\phi_p(x) = \sin k(x - x_p) \sin k(x_p - x_{p-1}) \ldots \sin k(x_2 - x_1) e^{-ikx_1} . \tag{14}$$

There are $\binom{n}{p}$ terms of this type in Eq. (11), where $\binom{n}{p}$ is the standard combinatoric notation for $n!/(n-p)!p!$. Since the scatterer positions have been ordered so that $x_i \leq x_{i+1}$, we must include a factor $p!$ to count the number of different orderings possible. Thus, the average value of $\psi_n(x)$ is obtained by summing over all orders of Γ/k. It is

$$\langle \psi_n(x) \rangle_n = \sum_{p=0}^{n} \binom{n}{p} p! \left(\frac{\Gamma}{k}\right)^p I_p(x) , \tag{15}$$

where we have defined $I_0(x) = e^{-ikx}$ and for $p > 0$

$$I_p(x) = \left(\frac{1}{L}\right)^p \int_0^x \int_0^{x_p} \cdots \int_0^{x_2} \phi_p(x) dx_1 \ldots dx_{p-1} dx_p . \tag{16}$$

Using Leibniz's rule for differentiating an integral with limits dependent on the variable with which differentiation occurs, from Eq. (16) we obtain (for $p > 0$)

$$I_p''(x) = -k^2 I_p(x) + \frac{k}{L} I_{p-1}(x) . \tag{17}$$

In evaluating $I_p(x)$, the following type of integral appears:

$$J_q = \int_0^{x_q} x_{q-1}^s e^{-ikx_{q-1}} \sin k(x_q - x_{q-1}) dx_{q-1} \tag{18}$$

with $0 \leq s \leq q - 2$, $2 \leq q \leq p + 1$, and $1 \leq p \leq n$, and $x_{n+1} = x$. Writing $\sin k(x_q - x_{q-1})$ in terms of exponentials and integrating by parts s times, we find

$$J_q = \frac{i}{2} s! \left[\frac{x_q^{s+1}}{(s+1)!} e^{-ikx_q} + \frac{e^{-ikx_q}}{2ik} \sum_{r=0}^{s} \left(\frac{1}{2ik}\right)^r \frac{x_q^{s-r}}{(s-r)!} - \frac{e^{ikx_q}}{(2ik)^{s+1}} \right] . \tag{19}$$

The structure of the terms in Eq. (19) allows us to decide on the final form for $I_p(x)$, except for the number of contributions to terms in $e^{\pm ikx}$. We therefore take the general form of $I_p(x)$ to be

$$I_p(x) = \left(\frac{ix}{2L}\right)^p \left[e^{-ikx} \sum_{l=0}^{p} \frac{(2ikx)^{-l}}{(p-l)!} A_{l,p} - \sum_{l=1}^{p} (-1)^{p-l} e^{ikx} \frac{(2ikx)^{-l}}{(p-l)!} B_{l,p} \right] . \tag{20}$$

Substitution into Eq. (17) yields, for $p \geq 1$,

$$A_{l,p}=\binom{p+l-1}{l} \text{ and } B_{l,p}=\binom{p+l-1}{l-1}.$$

The $p=1$ solution can be directly calculated, and it determines the initial conditions $A_{0,p}=1$ and $B_{1,p}=1$ as well as the overall sign. Inserting these results into Eq. (20), using Eq. (16), and rearranging the coefficients, gives the average of the wave function as

$$\langle\psi_n(x)\rangle_n = e^{-ikx} + \sum_{p=1}^{n}\binom{n}{p}\left(\frac{i\Gamma x}{2kL}\right)^p e^{-ikx} + \sum_{p=1}^{n}\binom{n}{p}\left(\frac{i\Gamma x}{2kL}\right)^p \sum_{l=1}^{p}\frac{(p+l-1)!\,(2ikx)^{-l}}{(p-l)!\,(l-1)!}\left[\frac{p}{l}e^{-ikx}-(-1)^{p-l}e^{ikx}\right]. \quad (21)$$

Without Eq. (21), we would have to generate an ensemble of configurations for the positions of the scatterers and calculate the average numerically. In the physical case (where no such simple reduced form exists for the average) the situation is even worse, for Eq. (5) must be solved to find the ψ_i first. The process of inverting Eq. (5) is very time consuming as n gets larger, so that Eq. (21) saves a tremendous amount of computational time. Unfortunately, for calculational purposes Eq. (21) is not very suitable for small kL when transcribed to a computer because of large cancellations in the sums. For this reason an alternate form is derived for small kL [see the discussion of $\langle\psi_n(x)\rangle_n$ toward the end of the next section].

Lastly, we comment that the integrals in Eq. (16) can be performed analytically if $p(x)=1/L$ is replaced by a normalized polynomial, sinusoidal, or exponential distribution. Whether or not the combinations can be simply arranged and what sums can be explicitly performed are questions in need of further study. In Sec. V, we are able to make some statements about the large k behavior of the average wave function and optical potential for a general distribution.

III. THE SMALL AND LARGE kL LIMITS

A. The large kL limit

The amount of labor required in calculating $\langle\psi_n(x)\rangle_n$ can be reduced further in the limits of large and small kL. For kL large enough, the first two terms in Eq. (21) can be assumed to dominate. In this instance,

$$\langle\psi_n(x)\rangle_n \simeq \left(1+\frac{i\Gamma x}{2kL}\right)^n e^{-ikx}. \quad (22)$$

If we retain the $l=1$ term in the sum over l in Eq. (21), and use the fact that $\sum_{p=0}^{n} p^m\binom{n}{p}y^p$ can be expressed in terms of the binomial expansion of $(1+y)^n$, we can find the next order in $1/k$ contribution. Employing this technique, we find, for $n\geq 2$,

$$\sum_{p=1}^{n}\binom{n}{p}\left(\frac{i\Gamma x}{2kL}\right)^p \frac{p}{2ikx}\left[pe^{-ikx}-(-1)^{p-1}e^{ikx}\right] = \frac{n\Gamma}{4k^2L}\left[e^{-ikx}\left(1+\frac{i\Gamma x}{2kL}\right)^{n-2}\left(1+\frac{in\Gamma x}{2kL}\right) - e^{ikx}\left(1-\frac{i\Gamma x}{2kL}\right)^{n-1}\right]. \quad (23)$$

This term must then be added to $[1+(i\Gamma x/2kL)]^n e^{-ikx}$ to obtain $\langle\psi_n(x)\rangle_n$ to first order in $1/k$. An important question to answer here is: "When can the result of Eq. (23) be neglected with respect to $[1+(i\Gamma x/2kL)]^n e^{-ikx}$?" An examination of the ratio of Eq. (23) to Eq. (22) is required to find where this ratio is far less than unity for any fixed set of parameters. In general, as the density of scatterers increases or kL decreases, it becomes necessary to include more terms in the summation over l in Eq. (21).

B. The small kL limit

It is worthwhile examining $\langle\psi_n(x)\rangle_n$ in the limit $kL\ll 1$. In this case, where we approximate $\sin k(x-x_i)$ by $k(x-x_i)$ and e^{-ikx_1} by $1-ikx_1$ (for $p>1$), $\phi_p(x)$ reduces to

$$\phi_p(x)=k^p(x-x_p)(1-ikx_1)\prod_{l=1}^{p-1}(x_l-x_{l-1}). \quad (24)$$

The solution for $I_p(x)$ is now

$$I_p(x)=\left(\frac{k}{L}\right)^p x^{2p}\left(1-\frac{ikx}{2p+1}\right). \quad (25)$$

Using this result, we find

$$\langle\psi_n(x)\rangle_n = \sum_{p=0}^{n}\binom{n}{p}\frac{p!}{(2p)!}\left(\frac{\Gamma x^2}{L}\right)^p\left(1-\frac{ikx}{2p+1}\right) = (-1)^n\frac{n!}{(2n)!}\left[H_{2n}(\alpha x)-\frac{ik}{\alpha}\frac{H_{2n+1}(\alpha x)}{2(2n+1)}\right], \quad (26)$$

where $\alpha=i(n\Gamma/L)^{1/2}$ if $\Gamma>0$, and $\alpha=(n|\Gamma|/L)^{1/2}$ if $\Gamma<0$. The functions $H_{2n}(\alpha x)$ and $H_{2n+1}(\alpha x)$ are Hermite polynomials of order $2n$ and $2n+1$, respectively, with the indicated argument. Regardless of how Eq. (26) is written, in the limit of large n, we obtain

$$\langle\psi_n(x)\rangle_n \simeq \cos(\alpha x) - \frac{ik}{\alpha}\sin(\alpha x). \tag{27}$$

Whether or not a specific n is large is determined by the size of the last term in the sum in Eq. (26). Using Stirling's approximation for $n!$ and $(2n)!$, n is seen to be large if $\Gamma x^2/nL \ll 1$. The above results are valid for $kL \ll 1$ only. Further terms in ikx should be kept as kL increases.

C. An alternate form for $\langle\psi_n(x)\rangle_n$

The above approach may be utilized to rewrite $\langle\psi_n(x)\rangle_n$ in quite a different way from that presented in Eq. (21). By expanding the exponential and sine functions in Eq. (14), Eq. (26) can be extended for any kL to read

$$\langle\psi_n(x)\rangle_n = \sum_{p=0}^{n} \binom{n}{p} p! \left(\frac{\Gamma x^2}{L}\right)^p \sum_{l=0}^{\infty} \frac{f_l(p)}{(2p+l)!}(-ikx)^l. \tag{28}$$

The constants $f_l(p)$ are determined from the recursion relation for I_p, repeated here for convenience,

$$I_p'' = -k^2 I_p + \frac{k}{L} I_{p-1}. \tag{29}$$

The function I_p now is

$$I_p = \left(\frac{k}{L}\right)^p \sum_{l=0}^{\infty} f_l(p) x^{2p} \frac{(-ikx)^l}{(2p+l)!}. \tag{30}$$

This yields the recursion relation for $f_l(p)$,

$$f_l(p) = f_{l-2}(p) + f_l(p-1), \tag{31}$$

whose solution gives

$$f_l(p) = \binom{p + [l/2]}{[l/2]}. \tag{32}$$

The initial terms $f_l(0) = 1$, $f_0(p) = 1$, and $f_1(p) = 1$ for all l and for $p \geq 1$ are obtained from Eq. (26). $[l/2]$ is defined as $l/2$ for l even and $(l-1)/2$ for l odd.

The choice of Eq. (21) over Eq. (28) would appear preferable. In the former, there are only a finite number of terms to consider. However, as can be seen from Eq. (26) or Eq. (28), in the limit of small kL there are $2p$ terms in k^{-1} for each order in (Γ/k) from Eq. (21) which must exactly cancel. This presents calculational difficulties with Eq. (21) and evidently small kL calculations are much easier to handle in Eq. (28). This will be discussed further in paper II.

We have not yet discussed the possibility of including either a nonuniform distribution for the positions of the scatterers or correlation effects. For n identical scatterers, the application of the recursion relation approach may yield fairly simple results once the form of the general solution is ascertained. Similarly, with the appropriate changes in Γ it may be possible to repeat the above procedures with n different scatterers; however, the actual calculation of such a quantity may be laborious. Further investigation along these lines should be carried out if a closer approximation to physical situations is desired.

IV. THE OPTICAL POTENTIAL

The reduced wave equation in a medium with a potential $V(x)$ is

$$\bar{\psi}''(x) + k^2\bar{\psi}(x) = V(x)\bar{\psi}(x), \tag{33}$$

where $\bar{\psi}(x)$ is the wave function of the projectile. Equation (33) defines the optical potential $V_n(x) \equiv V(x)$ if we identify $\bar{\psi}(x)$ with $\langle\psi_n(x)\rangle_n$. For example, integrating Eq. (2) over all the scatterer positions, we obtain

$$\langle\psi_n(x)\rangle_n'' + k^2\langle\psi_n(x)\rangle = \rho\Gamma\langle\psi_n(x; x)\rangle_{n-1}, \tag{34}$$

where

$$\langle\psi_n(x; x)\rangle_{n-1} \equiv \langle\psi_n(x; x_1, \ldots, x_{j-1}, x, x_{j+1}, \ldots, x_n)\rangle_{n-1}. \tag{35}$$

We can make this identification (independent of j) since, with $x_j = x$ in Eq. (11), we find

$$\langle\psi_n(x; x)\rangle_{n-1} = \langle\psi_{n-1}(x)\rangle_{n-1}, \tag{36}$$

where we have relabeled $x_{j+1}, x_{j+2}, \ldots, x_n$ as x_j, $x_{j+1}, \ldots, x_{n-1}$. Upon using the effective field approximation

$$\langle\psi_n(x)\rangle_n \simeq \langle\psi_{n-1}(x)\rangle_{n-1}, \tag{37}$$

Eq. (34) becomes

$$\langle\psi_n(x)\rangle_n'' + k^2\langle\psi_n(x)\rangle_n = V_n(x)\langle\psi_n(x)\rangle_n, \tag{38}$$

with $V_n(x) = \rho\Gamma$ and $\rho = n/L$.

We define the quantity $V_\infty \equiv \rho\Gamma$, as this is the limiting form of the potential as n approaches infinity. That is, $\lim_{n\to\infty} V_n(x)/V_\infty = 1$.

This is true for any fixed set of values for the parameters L, k, and Γ. In general, Γ may be complex, but we consider only real Γ in this paper paper. We also find that $\lim_{\Gamma\to 0} V_n(x)/V_\infty = 1$. Thus in these two limits, the optical potential is local-density dependent. We have defined a local-density dependent potential as one which depends on k and Γ and locally on the density, but has no boundary dependence (no L dependence in this case) The arguments in the preceding paragraph hold true for any distribution of the scatterer positions. Although we have only considered $p(x_i) = 1/L$, it is possible that other distributions (such as Gaussian) might lead to a potential which, in some less restrictive region of parameter space, would be local-density dependent.

The optical potential can be written in a very succinct form by using the recursion relation in

Eq. (20) and the definition of $\langle\psi_n(x)\rangle_n$ from Eq. (15). We find

$$V_n(x) = \rho\Gamma \frac{\langle\psi_{n-1}(x)\rangle_{n-1}}{\langle\psi_n(x)\rangle_n} . \tag{39}$$

We return briefly to a discussion of units. Having set $\hbar^2/2m = 1$ implies that each of ρ, Γ, and k has the dimension $[L^{-1}]$, L being units of length, and $V_n(x)$ has the dimension $[L^{-2}]$. The wave function and optical potential are each a function of three dimensionless quantities n, $\Gamma x/kL$, and kx. This leads to important scaling properties, a further discussion of which is postponed until paper II.

In the Appendix we prove that $\lim_{n\to\infty}\delta'' = 0$, where

$$\delta'' \equiv \left| 1 - \frac{\langle\psi_{n-1}(x)\rangle_{n-1}}{\langle\psi_n(x)\rangle_n} \right| . \tag{40}$$

That is, $\lim_{n\to\infty} V_n(x)/V_\infty = 1$, and in this limit the effective field approximation is exact. We can see why this is true by the following qualitative arguments. As the number of particles gets large, it is not unreasonable to assume that taking out one particle should not significantly affect the average of the wave function. The main difference between $\langle\psi_{n-1}(x)\rangle_{n-1}$ and $\langle\psi_n(x)\rangle_n$ is the fact that the pth term in the former contains $\binom{n-1}{p}$ rather than $\binom{n}{p}$. Another difference is that there are only n-1 terms in $\langle\psi_{n-1}(x)\rangle_{n-1}$ as compared to n terms in $\langle\psi_n(x)\rangle_n$. If the terms where $\binom{n-1}{p}$ and $\binom{n}{p}$ differ significantly can be ignored, so that only the first p_0 terms in each need be retained, then the potential will be approximately $\rho\Gamma(1 + p_0/n)$. As n increases, we would expect the differences to go to zero, that is, $p_0/n \to 0$, even if p_0 has some mild n dependence. Another problem is to ensure that $\langle\psi_n(x)\rangle_n$ is nowhere zero, for in that case, $V_n(x)$ would be undefined. One physical argument suggesting that this is true for any values of the parameters is the fact that there is always a transmitted wave. In one dimension each scatterer affects the wave function directly, but no one scatterer can cause complete reflection, and therefore, no zero can occur.

Having determined a simple limiting form for V_∞, we are in the position to ask: "When can the optical potential be approximated by V_∞?" We choose to answer this question by finding values of $R \equiv n|\Gamma|/k$ where $\delta < \epsilon$ for some small positive value of ϵ, where

$$\delta \equiv \left| 1 - \mathrm{Re}\left(\frac{V_n(x)}{V_\infty}\right) \right| . \tag{41}$$

In paper II we present bounds for R as a function of kL below which $\delta < \epsilon$ for $\epsilon = 1/n$ and $\epsilon = 0.1$. The real part of the potential (estimated here by V_∞) can then be supplemented by an approximation to the imaginary part and the transmitted and reflected waves calculated. These details are discussed thoroughly in paper II.

As an example of the determination of R such that Eq. (41) is satisfied, we consider the large kL limit. Using Eq. (22) and taking $n|\Gamma|/k^2L \ll 1$, we find

$$V_n(x) = \frac{\rho\Gamma}{1 + (i\Gamma x/2kL)} . \tag{42}$$

The real part of $V_n(x)$ is

$$\rho\Gamma\left(1 + \frac{\Gamma^2x^2}{4k^2L^2}\right)^{-1}$$

and the imaginary part is

$$-\rho\Gamma\left(\frac{\Gamma x}{2kL}\right)\left(1 + \frac{\Gamma^2x^2}{4k^2L^2}\right)^{-1} .$$

Equation (41) then implies for $R \equiv n|\Gamma|/k$ and $R < 2n[\sqrt{\epsilon}/(1-\epsilon)^{1/2}]$ that $\delta < \epsilon$. If we choose $\epsilon = 1/n$, then the magnitude of the ratio of imaginary to real parts of the potential is $1/\sqrt{n}$. In calculating the transmitted and reflected waves, we would then use $\mathrm{Re}V_n(x) = \rho\Gamma$ and $\mathrm{Im}V_n(x) = -\rho\Gamma^2x/2kL$.

An alternative to using δ would be to use

$$\hat{\delta} \equiv \left| 1 - \frac{V_n(x)}{V_\infty} \right| . \tag{43}$$

In the example just discussed, $\delta < 1/n$ is equivalent to $\hat{\delta} < 1/\sqrt{n}$. Using $\hat{\delta}$ then is a much more restrictive condition on R, one which is not really necessary since we supplement $\mathrm{Re}\,V_n(x)$ with an imaginary part. In the limit of small kL, $V_n(x)$ is essentially real, and $\delta < \epsilon$ will be equivalent to $\hat{\delta} < \epsilon$.

Bazer[8] has shown for any distribution of the scatterer positions that the effective field approximation becomes exact as n approaches infinity. For the physical case he shows that $\lim_{n\to\infty}\delta' = 0$, where

$$\delta' \equiv \left| \langle\psi_n(x)\rangle_n - \langle\psi_{n-1}(x)\rangle_{n-1} \right| . \tag{44}$$

Of course $\lim_{n\to\infty}\delta' = 0$ implies that $\lim_{n\to\infty} V_n(x) = \rho\Gamma$. Bazer and Karal[9] have shown that as n gets large, δ' varies as R^2/n, which is the same behavior exhibited by δ. (In their notation $\Gamma/k = iz/Z$ and $R = 2i\zeta$.) They also show how to calculate these higher order in $1/n$ corrections. However, in the lowest order correction, they must assume n satisfies the appropriate sufficient conditions. These give rather large values of n for moderate values of R. In paper II, we have shown the region of validity in R for $\delta < \epsilon$ for several n over the entire range of kL. In the alternate case, the limits of R are both necessary and sufficient and a function of kL. They are much less restrictive conditions than those of Bazer.[8]

V. THE GENERAL LARGE k SOLUTION

Some very interesting results can be determined for a general density in the limit of large n and large L such that $\rho_0 = n/L$ is fixed. Retaining the statistical independence of the position of the scatterers, we can define the general density $\rho(x)$ in terms of the single particle distribution $p(x)$ as follows:

$$\rho(x) = np(x) = \rho_0 f(x) . \tag{45}$$

This set of equalities defines $f(x)$ which, because $p(x)$ is normalized to unity, has the following property

$$\frac{1}{L}\int_0^x f(x)dx = 1 . \tag{46}$$

Also, for convenience, we define

$$g(x) = \int_0^x \rho(x)dx . \tag{47}$$

We can reexpress the large kL limit for $\langle\psi_n(x)\rangle_n$ in terms of ρ_0, $g(x)$, and n. To find $\langle\psi_n(x)\rangle_n$, we need to replace Eq. (14) with the general form of $\phi_p(x)$,

$$\phi_p(x) = f(x_p)\sin k(x - x_p) f(x_{p-1})\sin k(x_p - x_{p-1}) \ldots f(x_1)\sin k(x_2 - x_1)e^{-ikx_1} . \tag{48}$$

Using Eq. (48), we find

$$I_p(x) = \int_0^x f(x_p) I_{p-1}(x_p)\sin k(x - x_p)dx_p . \tag{49}$$

This relation is useful in a step by step determination of $I_p(x)$, starting with $I_0(x) = e^{-ikx}$. Expanding the sine function, ignoring terms proportional to k^{-m} for m greater than one, and for cases when $f(0) = 0$, we find

$$I_p(x) = e^{-ikx}\left(\frac{i}{2n}\right)^p\left[g^p(x)/p! - \frac{i}{2k}\left(\rho_0 f(x)g^{p-1}(x)/(p-1)! + \rho_0^2\int_0^x f(x_p)g^{p-2}(x_p)dx_p/(p-2)!\right.\right.$$
$$\left.\left. + \cdots \rho_0^p\int_0^x f(x_p)\int_0^{x_p} f(x_{p-1}) \cdots \int_0^{x_2} f^2(x_1)dx_1dx_2 \ldots dx_p\right)\right] . \tag{50}$$

Even in the case of the uniform distribution, we saw that it was difficult to ascertain exactly what relation exists for $\rho(x)$ such that the second term in Eq. (50) can be ignored; we can only demand that the second term be far less than unity. Nevertheless, for sufficiently large k, the average of the wave function becomes

$$\langle\psi_n(x)\rangle_n \simeq \left[1 + \frac{i\Gamma g(x)}{2kn}\right]^n e^{-ikx} . \tag{51}$$

In the limit of infinite n, we find that

$$\lim_{n\to\infty}\langle\psi_n(x)\rangle_n = \exp[-ikx + i\Gamma g(x)/2k] . \tag{52}$$

So that flux is at least conserved, Eq. (52) should be divided by $1 - \rho(x)\Gamma/4k^2$. Actually, if we had kept all terms to order $\rho(x)\Gamma/k^2$, we would have found a reflected wave and a total flux less than unity. This latter fact is because of the statistical nature of the problem.

Using Eq. (33), the optical potential in this limit becomes

$$\lim_{n\to\infty} V_n(x) = \rho(x)\Gamma\left(1 - \frac{\rho(x)\Gamma}{4k^2} + \frac{\rho'(x)}{2\rho(x)k}\right) . \tag{53}$$

The above form for the potential may be suspect, as the last two terms in the parentheses may already be negligible. For example, in the case of a uniform distribution, and also a polynomial distribution, one necessary condition in neglecting terms of order $1/k$ in Eq. (50) is $\rho(x)\Gamma/k^2 \ll 1$. Avoiding any ambiguity, we assume that both $\rho(x)\Gamma \ll k^2$ and $\rho'(x) \ll \rho(x)k$. These two conditions are just those required for the application of the WKB method or equivalently the Eikonal approximation in one dimension. The limiting potential will be called $V_\infty(x)$ and is $\rho(x)\Gamma$ under the above assumptions.[12] The two conditions can now be put in the familiar forms $V_\infty(x) \ll k^2$ and $[1/V_\infty(x)][dV_\infty(x)/dx] \ll k$. The average wave function can then be rewritten as

$$\lim_{n\to\infty}\langle\psi_n(x)\rangle_n = \exp\left\{-i\int_0^x [k^2 - \rho(x)\Gamma]^{1/2}dx\right\} . \tag{54}$$

Under the above conditions, the potential and average wave function satisfy the criteria of a local-density dependent function; that is, there is no dependence on the length of the scattering region for a fixed density ρ_0 in the large k and infinite n limits.

VI. THE ALTERNATE VERSUS THE PHYSICAL CASE

Although it is instructive to have a solution to the reduced wave equation in a form which allows an analysis of limits to be made without the neces-

sity of numerical analysis (or inverting the set of n equations for each random distribution and then averaging), the solution is unconventional in that the resulting optical potential represents that which produces a transmitted wave of the same amplitude each time. How can we relate this result to the conventional one, where the incident wave always has the same amplitude? Since the essential difference lies in the normalization factor relating the two wave functions for a specific single configuration, if this factor is independent of the scatterer positions, then the results for $\langle\psi_n(x)\rangle_n$ and the optical potential $V_n(x)$ will be similar. There are three conditions when this may be true. First, if k is very small then the determinant of the matrix in Eq. (5) is $1-n\Gamma/2ik$, which is independent of the scatterer positions. Second, in the intermediate region of Γ/k and kL it is possible that the effects of the determinant may average out since $V_n(x)$ is a ratio of functions [see Eq. (40)]. Third, for large kL the functions e^{ikx_i} are rapidly oscillating functions and so the renormalization factor may not affect the results for $V_n(x)$ significantly. These estimates are not unreasonable, as it has been shown that in the physical and alternate cases the optical potential approaches the same limit. A more detailed comparison between the resulting optical potential in both instances will be presented in paper II, where we find that in the regions we are concerned with the above qualitative estimates are verified.

CONCLUSIONS

In summary, we have obtained a tractable solution to a one-dimensional problem of scalar wave multiple scattering for n identical pointlike scatterers with δ-function potentials and whose positions are uniformly distributed throughout the scattering region. We have calculated a simple reduced form for the average of the wave function in the case of a transmitted wave with constant amplitude and shown that as n approaches infinity the effective field approximation becomes exact. As a consequence of this, we find $\lim_{n\to\infty} V_n(x)/\rho\Gamma = 1$. In this paper, we also briefly discuss where the optical potential can be replaced by $\rho\Gamma$ to within a given accuracy. In paper II, we extend this discussion to answer the more general question as to where a simple form of the optical potential can be used to predict the outcome of the scattering. Further, we have presented results for the large k limit as n and L approach infinity with n/L fixed, in the case of a general probability distribution for the position of the scatterers. The average of the wave function is shown to be local-density dependent and equivalent to that obtained in the WKB approximation, with the corresponding potential being the density times the scattering strength of an individual scatterer.

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APPENDIX

In Sec. IV, we gave a qualitative outline as to why $V_\infty = \rho\Gamma$. Here, we show that if the wave function has no zeros then $V_\infty = \rho\Gamma$. The proof is broken into three parts. First, we show that the infinite sum over l in Eq. (28) is bounded for any value of p. Second, we show that there exists a $p = p_0(n)$ such that the sum over p for $p \geq p_0(n)$ is bounded and goes to zero as n approaches infinity. Third, we show that the remaining sum over p implies that $V_\infty = \rho\Gamma$. Following this, we discuss why there are no zeros in the small and large kL limits.

The expression for the average of the wave function can be written as

$$\langle\psi_n(x)\rangle_n = \sum_{p=0}^{n} \binom{n}{p} \left(\frac{\Gamma x^2}{L}\right)^p \frac{p!}{(2p)!} h_p(kx), \tag{A1}$$

where

$$h_p(kx) = \sum_{l=0}^{\infty} \frac{l!\,(2p)!}{(2p+l)!} \binom{p+[l/2]}{[l/2]} (-ikx)^l/l! \,. \tag{A2}$$

As the coefficient of $(-ikx)^l/l!$ is less than or equal to unity for any l or p, then $|h_p(kx)|$ converges to $M(kx)$, where $M(kx)$ is less than e^{kx} for any p greater than zero. The next two steps involve breaking the sum over p in Eq. (A1) into two parts. We shall show that the sum over p from p_0 to n is bounded by some function which goes to zero as n approaches infinity.

First, we examine the behavior of $|y|$, where

$$y \equiv M(kx)\binom{n}{p}\left(\frac{\Gamma x^2}{L}\right)^p \frac{p!}{(2p)!} \,. \tag{A3}$$

If we replace $\binom{n}{p}$ by 2^n and use Stirling's approximation, then for large p and n we find that $|y|$ is bounded above by

$$\hat{y}(p) \equiv 2^{n-1} M(kx)\left(\frac{|\Gamma|L}{4p}\right)^p \,. \tag{A4}$$

Defining $r = p/n$, $\hat{y}(p)$ becomes

$$\frac{M(kx)}{2}\left(\frac{2^{1/r}|\Gamma|L}{4rn}\right)^{rn} \,. \tag{A5}$$

For fixed $r = r_0$, there exists an $n(r_0)$ such that for

$n > n(r_0)$

$$\frac{2^{1/r_0}|\Gamma|L}{4r_0 n} < \epsilon,$$

where ϵ is an arbitrary small positive real number. Then, $n(r_0)$ is determined by replacing the inequality by an equality and solving for n. The sum over $\hat{y}(p)$ from p_0 to n is bounded by the infinite geometric series $\sum_{p=p_0}^{\infty} \epsilon^p = \epsilon^{p_0}/(1-\epsilon)$. This is less than $2\epsilon^{p_0} = 2\exp(-r_0 n|ln\epsilon|)$ and so the sum over $\hat{y}(p)$ goes to zero exponentially for fixed r_0 and any $\epsilon < \frac{1}{2}$ as n approaches infinity. The same conclusions can be drawn if $\binom{n}{p}$ is replaced by $\binom{n-1}{p}$ in y. Thus we need only consider the sum from 0 to p_0 in the arguments to follow.

The final step is to show, using only the remaining terms in p, that $V_\infty = \rho\Gamma$. Each term in the sum over p in the numerator of Eq. (39) differs by that in the denominator by p/n times the pth term in the denominator. However, since we divide by the denominator, the maximum difference these terms contribute to the potential is just $\rho\Gamma p/n$. Summing over all p from 0 to p_0 implies that $[V_n(x)/V_\infty - 1]$ is of order $p_0/n = r_0$. Therefore, in the limit of r_0 going to zero or n approaching infinity, we find that $V_n(x)/V_\infty$ goes to unity.

In the small and large kL limits we can show that $\langle\psi_n(x)\rangle_n$ has no zeros for physical values of the parameters. From Eq. (26), which expresses $\langle\psi_n(x)\rangle_n$ in terms of Hermite polynomials of order $2n$ and $2n+1$ since the roots of different order Hermite polynomials are distinct, when the real part is zero the imaginary part cannot be zero. In the large kL limit, examination of Eq. (23) once again reveals that there can be no zeros. In the qualitative arguments presented above, Γ could be complex and we might expect no zeros to occur for k and x real, although this has not been shown here.

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