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Multiple Scattering in Closely Packed Systems of Arbitrary Non-Overlapping Shapes

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Abstract

It has long been known that the multiple scattering of waves from a system of obstacles of finite extent can be described completely with a knowledge of the on-shell amplitudes of the individual scatterers, provided that the minimally enclosing spheres concentric with the scattering centers do not overlap. In this paper, it is shown that on-shell amplitudes alone suffice for a wider class of scattering configurations, in which the individual scatterers do not overlap, but their geometries do not satisfy the above condition. These extended geometries require a careful treatment of certain partial wave sums. An example is also discussed in which a pair of non-overlapping scatterers requires more than the on-shell amplitudes for a solution.

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1. INTRODUCTION

The multiple-scattering theory of waves is a very old subject. Dating back at least to the time of Rayleigh [1], it has since seen application in most branches of physics, including electron energies in solids [2-4] and liquids [5], hadron-nucleus scattering [6-11], and a variety of phenomena involving electromagnetic or acoustic waves [12-14].

The general theory is simplified greatly under certain conditions where the scatterers are *non-overlapping*, i.e., the scatterers are of finite extent and the free wave equation is satisfied in the intervening regions. For example, if the scatterers are spherical (circular) in three (two) dimensions, one can show that the only ingredients to multiple scattering are the free Green's function and the asymptotic scattering amplitudes for the individual obstacle (i.e., for quantum-mechanical scattering, only *on-shell* amplitudes are required), provided that the spheres (circles) are non-overlapping. This simplification is the cornerstone for "muffin-tin" [2] calculations of electron energy bands in solids [3,4], as well as the electronic theory of liquid metals [5], for various theories of hadron-nucleus scattering [8-11], and for classical multiple-scattering problems [14]. Indeed, one's intuitive picture of multiple scattering often relies upon the non-overlap/on-shell theorem.

If the scatterers are not spherical (circular), the non-overlap theorem justifying the use of on-shell amplitudes still holds, provided that the scatterers can be enclosed by spheres (circles) concentric with the individual scattering center, which do not overlap. This condition has been relaxed somewhat by Williams and Morgan [15], but there are still many geometries where even their more relaxed conditions of the non-overlap theorem cannot be met, even though the scatterers are *physically* separated by regions in which free waves propagate. To date, such examples have neither been shown to allow the use of the non-overlap theorem, nor that additional information is essential to a calculation.

While the general theory of multiple scattering accounts even for the possibility of physically overlapping scatterers, it requires a knowledge of more than the free amplitudes, i.e., off-shell information. A practical calculation which includes such effects can be quite complicated [16] (see, however, Ref. [9]), and is model dependent, because one must supply details of the scatterers not described by asymptotic phase shifts. Since there are in fact examples in band structure theory [15] as well as classical scattering problems (e.g., electromagnetic scattering from a closely packed array of cubical conductors) wherein the usual spherical non-overlap condition is violated, it is of practical importance to know whether the non-overlap/on-shell theorem can be extended, or whether off-shell information is required to solve the multiple-scattering problem.

The purpose of this paper is to show that one can, in fact, solve the multiple-scattering problem, using only on-shell amplitudes, for a wider class of geometries involving physically non-overlapping scatterers. Following a brief overview of the multiple-scattering formalism in Section 2, the on-shell theorem for the standard and extended geometries is developed in Section 3. These new geometries require a careful treatment of partial wave summations. Not only can there be extra sums to perform, but the *order* of summation can be important, as discussed in Section 4. For geometric configurations of physically non-overlapping scatterers which fail even the less restrictive requirements for the on-shell theorem, nothing is rigorously proven in this paper, but an example and some speculations are given in Section 5 which suggest that off-shell information is, in fact, required for such geometries. The results are summarized in the context of other approaches in Section 6.

2. OVERVIEW OF THE FORMALISM

This section contains a brief outline of the multiple-scattering formalism employed in the subsequent discussion. Since almost all of the references cited so far (particularly the books and review articles) contain extensive discussions of such formalisms, only the salient features will be presented here, with particular regard to notation needed to prove the on-shell theorem. The development henceforth is oriented toward three-dimensional problems, but a similar approach applies in two dimensions.

For most of the applications in which the extended geometries apply, it suffices to consider a system of N *fixed* scatterers located at positions $\vec{r}_i$. (No attempt to examine the effects of target recoil is made in this paper.) The problem is to find the scattering amplitude $F(\vec{k}',\vec{k})$, $|\vec{k}'| = |\vec{k}| = k$, which can be written as

$$F(\vec{k}',\vec{k}) = \sum_{i=1}^{N} e^{-i\vec{k}'\cdot\vec{r}_i}\, F^{(i)}(\vec{k}',\vec{k}) \ , \tag{2.1}$$

where the $F^{(i)}$ satisfy the multiple-scattering equations

$$F^{(i)}(\vec{k}',\vec{k}) = f^{(i)}\ (\vec{k}',\vec{k})\ e^{i\vec{k}\cdot\vec{r}_i} + \sum_{j\neq i} \int \frac{d^3t}{(2\pi)^3}\, f^{(i)}\ (\vec{k}',\vec{t}) \times$$
$$\times \frac{e^{i\vec{t}(\vec{r}_i-\vec{r}_j)}}{t^2-k^2-i\epsilon}\, F^{(j)}(\vec{t},\vec{k}) \ . \tag{2.2}$$

The $f^{(i)}$ describe scattering from obstacle (i) in the absence of other scatterers. For quantum mechanical potential scattering, a convenient form is

$$f^{(i)}(\vec{k}',\vec{k}) = -\frac{1}{4\pi} \int d^3r\ e^{i\vec{k}'\cdot\vec{r}}\ V(\vec{r})\psi^{(+)}_{\vec{k}}(\vec{r}) \ , \tag{2.3}$$

where $V(\vec{r})$ is the potential and $\psi_{\vec{k}}^{(+)}$ is the solution to the wave equation with outgoing wave boundary conditions. However, it is more useful to have a prescription which avoids reference to a potential altogether [14]:

$$f^{(i)}(\vec{k}',\vec{k}) = -\frac{1}{4\pi}\left\{e^{-i\vec{k}'\cdot\vec{r}}, \psi_{\vec{k}}^{(+)}(\vec{r})\right\}_{\sigma_i} , \tag{2.4}$$

where

$$\left\{A(\vec{r}),B(\vec{r})\right\}_{\sigma} \equiv \oint_{\sigma} dS\left[A\frac{\partial B}{\partial n} - B\frac{\partial A}{\partial n}\right] \tag{2.5}$$

denotes an integral over the surface σ of the scatterer involving normal derivatives. The half-off-shell extension of Eq. (2.4) which is consistent with quantum potential scattering [17] is:

$$f^{(i)}(\vec{t},\vec{k}) = \frac{1}{4\pi}(t^2-k^2)\int_{\Omega_i} d^3r\, e^{-i\vec{t}\cdot\vec{r}}\, \psi_{\vec{k}}^{(+)}(\vec{r}) - \frac{1}{4\pi}\left\{e^{-i\vec{t}\cdot\vec{r}}, \psi_{\vec{k}}^{(+)}(\vec{r})\right\}_{\sigma_i} , \tag{2.6}$$

where the first integral covers the volume Ω_i of the scatterer. Note that for rigid scatterers (singular potentials) the first term vanishes. Extrapolating in the second variable, one has

$$f^{(i)}(\vec{k},\vec{t}) = \frac{1}{4\pi}(t^2-k^2)\int_{\Omega_i} d^3r\, \psi_{\vec{k}}^{(-)*}(\vec{r})\, e^{i\vec{t}\cdot\vec{r}} - \frac{1}{4\pi}\left\{\psi_{\vec{k}}^{(-)*}(\vec{r}), e^{i\vec{t}\cdot\vec{r}}\right\}_{\sigma_i} , \tag{2.7}$$

where $\psi_k^{(-)}$ is obtained with incoming wave boundary conditions.

In a similar fashion, the amplitudes $F^{(i)}$ are defined by

$$F^{(i)}(\vec{t},\vec{k}) = \frac{1}{4\pi}(t^2-k^2)\int_{\Omega_i} d^3r\, e^{-i\vec{t}\cdot\vec{r}}\, \Psi_{\vec{k}}^{(+)}(\vec{r}) - \frac{1}{4\pi}\left\{e^{-i\vec{t}\cdot\vec{r}}, \Psi_{\vec{k}}^{(+)}(\vec{r})\right\}_{\sigma_i} , \tag{2.8}$$

which employs the exact multiple-scattering solution $\Psi_{\vec{k}}^{(+)}$.

The above definitions are used below for determining certain analytic properties of the half-off-shell amplitudes. In addition, their partial-wave decompositions will be needed. For spherically symmetric scatterers,

$$f^{(i)}(\vec{t},\vec{k}) = 4\pi\sum_{\ell m} f_{\ell}^{(i)}(t,k)Y_{\ell m}^{*}(\hat{t})Y_{\ell m}(\hat{k}) , \tag{2.9}$$

while for non-symmetric scatterers,

$$f^{(i)}(\vec{k},\vec{t}) = 4\pi \sum_{\ell m} \sum_{\ell' m'} f^{(i)}_{\ell m \ell' m'}(k,t) Y^*_{\ell m}(\hat{k}) Y_{\ell' m'}(\hat{t}) \ . \tag{2.10}$$

The partial wave amplitudes can be obtained directly from Eqs. (2.6) and (2.3). For example, for t=k (on-shell), only the surface term contributes, giving

$$f_{\ell m \ell' m'}(k,k) = -\int d\hat{k} Y_{\ell m}(\hat{k}) \left\{ \psi^{(-)}_{\vec{k}}(\vec{r}),\ i^{\ell'} j_{\ell'}(kr) Y^*_{\ell' m'}(\hat{r}) \right\} \ . \tag{2.11}$$

Analogous forms hold for the $F^{(i)}$. What one would like, therefore, is a solution to the multiple-scattering problem which depends only upon $f^{(i)}_{\ell}(k,k)$, or $f^{(i)}_{\ell m \ell' m'}(k,k)$, which are directly related to asymptotic phase shifts. To clarify the terminology: "on-shell amplitudes" shall be taken as those of the form (2.11), and "on-shell theorem" implies a proof that a multiple-scattering problem can be solved using only such amplitudes. In particular, it is also possible to construct other sorts of amplitudes where $|\vec{t}|=k$, but they are not related to phase shifts (see also the discussions in Sections 3 and 5): these will be regarded as "off shell".

3. ON-SHELL THEOREMS

The key element of Eq. (2.2) is the rescattering integral:

$$I_{ij} \equiv \int \frac{d^3t}{(2\pi)^3} f^{(i)}(\vec{k},\vec{t}) \frac{e^{i\vec{t}\cdot(\vec{r}_i-\vec{r}_j)}}{t^2-k^2-i\varepsilon} F^{(j)}(\vec{t},\vec{k}) \ . \tag{3.1}$$

As it stands, all (off-shell) values of $\vec{t}$ contribute. For the on-shell theorem to apply, one must be able to show that the integral is given entirely by the pole at t=k, in such a way that the residue corresponds to the product of asymptotic scattering amplitudes and a Green's function.

By using Eqs. (2.7) and (2.8), and by interchanging orders of integration, one arrives at the following integral:

$$J^{ij} \equiv \int \frac{d^3t}{(2\pi)^3} e^{i\vec{t}\cdot(\vec{s}_i-\vec{r}_i)} \frac{e^{i\vec{t}\cdot(\vec{r}_i-\vec{r}_j)}}{t^2-k^2-i\varepsilon} e^{-i\vec{t}\cdot(\vec{s}_j-\vec{r}_j)} \ . \tag{3.2}$$

The vectors $\vec{s}_i,\vec{s}_j$ represent points within scatterers (i),(j), respectively, and are to be integrated last. It is assumed at this point the amplitudes involve uniformly convergent integrals over wave functions, and that the $\vec{t}$ integral is also uniformly convergent if $\varepsilon\to 0^+$ at the last step of the calculation. The interchange of the $\vec{s}$ integrals with the partial wave sums is more delicate and is discussed in Section 4.

The partial wave version of J^{ij} is

$$J^{ij}_{\ell m\ell' m'} = 4\pi \sum_{\ell''} \begin{bmatrix} \ell & \ell' & \ell'' \\ m & m' & m'' \end{bmatrix} (-)^{m'} \; i^{\ell} Y^*_{\ell m}(\hat{\rho}_i)\, i^{-\ell'} Y_{\ell' m'}(\hat{\rho}_j)\, i^{\ell''} Y^*_{\ell'' m''}(\hat{r}_{ij})$$

$$\times \int_0^\infty \frac{t^2 dt}{(2\pi)^3} \frac{j_\ell(t\rho_i) j_{\ell'}(t\rho_j) j_{\ell''}(tr_{ij})}{t^2-k^2-i\varepsilon} , \qquad (3.3)$$

where

$$\begin{bmatrix} \ell & \ell' & \ell'' \\ m & m' & m'' \end{bmatrix} \equiv \left[\frac{(2\ell+1)2\ell'+1)(2\ell''+1)}{4\pi}\right]^{1/2} \begin{pmatrix} \ell & \ell' & \ell'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & \ell' & \ell'' \\ m & m' & m'' \end{pmatrix}$$

and

$$\vec{\rho}_i \equiv (\vec{s}_i - \vec{r}_i),\ \vec{r}_{ij} \equiv (\vec{r}_i - \vec{r}_j) . \qquad (3.4)$$

The next step is to evaluate the integral in Eq. (3.3). The remainder of this section deals with four distinct classes of scatterer geometry in which the integral has the desired form.

Class I (Standard Geometry)

Suppose $|\vec{\rho}_i| < a_i$ and $|\vec{\rho}_j| < a_j$, that is, scatterers (i) and (j) can be enclosed by spheres of radii a_i and a_j, centered at $\vec{r}_i$ and $\vec{r}_j$, respectively. If these spheres do not overlap, then $r_{ij} > a_i+a_j$, as illustrated in Fig. 1(I). The 3-j symbol [18] and the Bessel function properties [19] imply an even integrand. The classic procedure is to extend the integration limits to $\pm\infty$ and write $j_{\ell''} = \frac{1}{2}\left[h^{(1)}_{\ell''}+h^{(2)}_{\ell''}\right]$. As Im(t) $\to +\infty(-\infty)$, the integrand involving $h^{(1)}_{\ell''}$ $(h^{(2)}_{\ell''})$ is exponentially small, allowing one to close the contour in the appropriate half-plane to obtain

$$J^{ij}_{\ell m\ell' m'} = \left\{i^{\ell} j_\ell\left(k\rho_i\right) Y^*_{\ell m}\left(\hat{\rho}_i\right)\right\} \; G\left(\vec{r}_{ij}\right)_{\ell m\ell' m'} \left\{i^{-\ell'} j_{\ell'}\left(\rho_j\right) Y_{\ell' m'}\left(\hat{\rho}_j\right)\right\} . \quad (3.5)$$

The inter-scatterer Green's function is

$$G\left(\vec{r}_{ij}\right)_{\ell m\ell' m'} \equiv \frac{ik}{4\pi} \sum_{\ell''} \begin{bmatrix} \ell & \ell' & \ell'' \\ m & m' & m'' \end{bmatrix} (-)^{m'} i^{\ell''} h^{(1)}_{\ell''}\left(kr_{ij}\right) Y^*_{\ell'' m''}\left(\hat{r}_{ij}\right) \; . \quad (3.6)$$

The quantities in braces which contribute to the remaining integrals over $\vec{s}_i$ and $\vec{s}_j$ are precisely those which generate the *on-shell* partial wave contributions to $F^{(i)}$ and $F^{(j)}$, respectively, as in Eq. (2.11). The multiple scattering problem then reduces to a matrix equation, the details of which are discussed in Section 4. Provided one can truncate the partial wave series, the solution can be obtained using standard techniques. Note that Eq. (3.5) applies whether or not the scatterers have spherical symmetry: they only need to be enclosable in non-overlapping spheres centered at the sites $\vec{r}_i$.

Class II (Williams-Morgan Extension)

Williams and Morgan [15] were able to extend the allowed geometries for the on-shell theorem beyond Class I. A key ingredient in their approach, as well as for Classes III and IV below, is the partial wave addition theorem. It is convenient to introduce a translation matrix

$$O(\vec{b})_{\ell m\ell' m'} \equiv 4\pi \sum_{\ell''} \begin{bmatrix} \ell & \ell' & \ell'' \\ -m & m' & m'' \end{bmatrix} (-)^{m} \; i^{\ell''} j_{\ell''}(kb) Y_{\ell'' m''}(\hat{b}) \; , \quad (3.7)$$

which is unitary:

$$O^{-1}(\vec{b}) = O(-\vec{b}) = O^{\dagger}(\vec{b}) \; . \quad (3.8)$$

For Bessel functions, the coordinate origin can be shifted via

$$i^{\ell} j_\ell(k|\vec{a}+\vec{b}|) Y_{\ell m}(\widehat{a+b}) = \sum_{\ell' m'} O(\vec{b})_{\ell m\ell' m'} \; i^{\ell'} j_{\ell'}(ka) Y_{\ell' m'}(\hat{a}) \; , \quad (3.9)$$

while for Hankel functions,

$$i^{\ell} h_{\ell}^{(1)}(k|\vec{a}+\vec{b}|)Y_{\ell}(\widehat{a+b}) = \sum_{\ell' m'} O(\vec{b})_{\ell m \ell' m'}\; i^{\ell'} h_{\ell'}^{(1)}(ka) Y_{\ell' m'}(\hat{a}),\ a>b. \quad (3.10)$$

The inequality (a>b) is crucial for the convergence of the ℓ' sum, as discussed in Section 4.

Williams and Morgan considered the geometries

$$\text{A:}\quad |\vec{s}_i-\vec{r}_i| < |\vec{s}_j-\vec{r}_i| \text{ and } |\vec{s}_j-\vec{r}_j| < r_{ij},\ \forall\, \vec{s}_i\in\Omega_i,\ \vec{s}_j\in\Omega_j \quad (3.11)$$

or

$$\text{B:}\quad |\vec{s}_j-\vec{r}_j| < |\vec{s}_i-\vec{r}_j| \text{ and } |\vec{s}_i-\vec{r}_i| < r_{ij}\ \ \forall\, \vec{s}_i\in\Omega_i,\ \vec{s}_j\in\Omega_j\,. \quad (3.12)$$

Without loss of generality, one can consider the first case, an example of which is shown in Fig. 1(II). The integral (3.2) can be written as

$$J^{ij} = \int \frac{d^3t}{(2\pi)^3}\, e^{i\vec{t}\cdot(\vec{s}_i-\vec{r}_i)}\, \frac{e^{i\vec{t}\cdot(\vec{r}_i-\vec{s}_j)}}{t^2-k^2-i\varepsilon}\quad . \quad (3.13)$$

The two exponentials in Eq. (3.13) are first partial-wave decomposed. Because of the first inequality in (3.11), the contour integral over t yields a Bessel function involving $(\vec{s}_i-\vec{r}_i)$, and a Hankel function involving $(\vec{r}_i-\vec{s}_j)$. Because of the second inequality, the Hankel function can be shifted to argument $\vec{r}_{ij}$ via the addition theorem (3.10), whereupon one obtains, again, exactly Eq. (3.5), as in Class I. The only difference between these two classes turns out to be the treatment of the partial wave sums, as discussed in the next section.

Class III (Mutually Convex Shapes)

Consider an adjacent pair of rectangular solids in the array of Fig. 1(III). Their geometry does not qualify for either Class I or Class II, though the scatterers are physically *non*-overlapping. However, it is still possible to obtain a set of equations involving only on-shell amplitudes *by shifting the scattering centers.*

Clearly, each scatterer in an isolated *pair* of rectangular solids can be enclosed by a large sphere, centered at some new $\vec{r}_i{}' = \vec{r}_i+\Delta_i$, such that the two spheres do not overlap. This new geometry qualifies for Case I: the problem can be solved using *on-shell* amplitudes with centers $\vec{r}_i{}'$. These amplitudes can in turn be obtained from on-shell amplitudes centered at $\vec{r}_i$ inside the scatterer via the phase relation [cf. Eqs. (2.1) and (2.2)]:

$$f^{(i)\prime}(\vec{k}',\vec{k}) = e^{i(\vec{k}-\vec{k}')\cdot\vec{\Delta}_i}\, f^{(i)}(\vec{k}',\vec{k}) \quad . \tag{3.14}$$

While this scheme yields an on-shell theorem for *two* such mutually convex scatterers, what happens when there are others nearby? The key to the answer, as will be shown, is that the multiple-scattering equations can be cast in a form where *only the geometry of pairs need be considered.* The following development therefore follows in spirit the simple example discussed above.

The exponential integral (3.2) can be written in the form

$$J^{ij} = \int \frac{d^3t}{(2\pi)^3}\, e^{i\vec{t}\cdot(\vec{s}_i-\vec{r}_i{}')}\, \frac{e^{i\vec{t}\cdot(\vec{r}_i{}'-\vec{r}_j{}')}}{t^2-k^2-i\varepsilon}\, e^{-i\vec{t}\cdot(\vec{s}_j-\vec{r}_j{}')} , \tag{3.15}$$

where $\vec{r}_i{}' = \vec{r}_i+\vec{\Delta}_{ij}$, $\vec{r}_j{}' = \vec{r}_j+\vec{\Delta}_{ji}$, and $\vec{\Delta}_{ij}$ is the shift of the i^{th} scattering center due to the proximity of scatterer (j). If the scatterers are mutually convex, in the sense discussed above, the relevant shift vectors can be found such that $r_{ij}{}' > a_i{}' + a_j{}'$, where $\vec{r}_{ij}{}' = \vec{r}_i{}'-\vec{r}_j{}'$ and $a_i{}', a_j{}'$ are the radii of the large enclosing spheres. The partial wave version of J^{ij} then becomes, analogously to Eq. (3.5),

$$J^{ij}_{\ell m \ell' m'} = \left\{ i^{\ell} j_{\ell}\left(k\rho_i{}'\right) Y^{*}_{\ell m}\left(\hat{\rho}_i{}'\right)\right\} G\left(\vec{r}_{ij}{}'\right)_{\ell m \ell' m'} \left\{ i^{-\ell'} j_{\ell'}\left(k\rho_j{}'\right) Y_{\ell' m'}\left(\hat{\rho}_j{}'\right)\right\} , \tag{3.16}$$

with $\vec{\rho}_i{}' \equiv \vec{s}_i-\vec{r}_i{}'$. The variables $\vec{\rho}_i{}', \vec{\rho}_j{}'$ which occur in the braces can be shifted back to the values $\vec{\rho}_i, \vec{\rho}_j$ by means of the addition theorem, with the result:

$$J^{ij}_{\ell m\ell'm'} = \sum_{\lambda\mu}\sum_{\lambda'\mu'} \left\{ i^{\lambda} j_{\lambda}(k\rho_i) Y^{*}_{\lambda\mu}(\hat{\rho}_i) \right\} O^{\dagger}(\vec{\Delta}_{ij})_{\lambda\mu\ell m}$$

$$\times\ G(\vec{r}_{ij}{}')_{\ell m\ell'm'}\ \ O(\vec{\Delta}_{ji})_{\ell'm'\lambda'\mu'} \left\{ i^{-\lambda'} j_{\lambda'}(k\rho_j) Y_{\lambda'\mu'}(\hat{\rho}_j) \right\} . \quad (3.17)$$

At this point it is worth mentioning that the necessary inequalities of the Hankel function are satisfied such that one can write, schematically,

$$O^{\dagger}(\vec{\Delta}_{ij}) G(\vec{r}_{ij}{}') O(\vec{\Delta}_{ji}) = G(\vec{r}_{ij}) \ . \quad (3.18)$$

Eq. (3.18) can be demonstrated explicitly by manipulating Eqs. (3.6), (3.7) and various angular momentum identities [18]. Formally, at least, Eq. (3.17) is then equivalent to Eq. (3.5): one has the same ingredients of on-shell amplitudes with propagation between them. Whether or how one should perform the multiplication in Eq. (3.18), however, involves questions of partial wave convergence reserved for Section 4. Nevertheless, apart from such questions, it appears from Eq. (3.17) that on-shell amplitudes alone suffice for *systems* of mutually convex scatterers. Among other things, Class III includes all crystal lattice structures in which an electron potential is confined inside a Wigner-Seitz unit cell [20,21]. In particular, Williams and Morgan [15] found that, in contrast to other periodic forms, the diamond and zinc blende structures do not qualify for Class I or II: under the conditions for Class III, one can now in principle describe these lattices with a KKR band structure approach [3] as well.

Class IV (Enclosing Scatterers)

A fourth set of geometries qualifying for the on-shell theorem can be obtained by combining the scattering center shift idea of Class III with the Williams-Morgan inequalities (3.11) and (3.12) of Class II. That is, for each pair of scatterers, the scattering centers are shifted to points

$\vec{r}_i', \vec{r}_j'$, such that either of the inequalities (3.11) or (3.12) (modified by the substitution $\vec{r}_i \to \vec{r}_i'$, $\vec{r}_j \to \vec{r}_j'$) is satisfied. One follows a procedure analogous to that following Eq. (3.13), and obtains precisely Eq. (3.17) of Class III.

An example of such a geometry is shown in Fig. 1(IV). For a pair consisting of a sphere and a partially enclosing shell, one must be able to enclose the shell inside a larger sphere which does not contain the center of the spherical scatterer. That is, the shell can extend at most over a hemispherical solid angle.

All of the results of this section were obtained by manipulating Eq. (3.2) as a contour integral. Particularly for scatterers of finite extent, the point is not so much whether one can obtain the pole at $t=k$, but rather whether the result has the form where the braces in Eq. (3.5) contain Bessel functions, with a Hankel function in between. One can always find a combination of coordinates such that the contour can be closed in the upper or lower half-plane and the pole taken at $t=k$, but the price is one of introducing Hankel functions into the integrals (2.6) and (2.8) [16]. The amplitudes thus generated in the latter case are "on-shell" in the sense that $t=k$, but involve different solutions of the wave equation, are not connected to phase shifts, and require additional information about the scatterer.

4. PARTIAL-WAVE CONVERGENCE

The results of the previous section form the foundation for solving the multiple-scattering problem with on-shell amplitudes. This section provides the procedure necessary for obtaining a solution. In particular, each of the four geometric classes described above carry specific restrictions as to the number *and the order* of partial wave sums necessary for a convergent result.

It is useful to consider first the partial wave convergence properties of the amplitudes $f^{(i)}$. Throughout this section, rigid scatterers (singular potentials) will be used, with the expectation that they have, if anything, more slowly converging partial wave expansions than any non-rigid scatterer. For spherical scatterers of radius a, the on-shell amplitude for large ℓ has the behavior

$$f_\ell \xrightarrow[\ell\to\infty]{} \left[\frac{(ka)^\ell}{(2\ell+1)!!}\right]^2 . \tag{4.1}$$

For non-spherical scatterers, the precise behavior depends upon the geometry. A convenient formalism for scattering from arbitrary shapes has been given by Waterman [22], who expresses the partial wave amplitude as the solution to the equation

$$Qf = -P , \tag{4.2}$$

where (with notation differing slightly from his),

$$\begin{bmatrix} Q \\ P \end{bmatrix}_{\ell m \ell' m'} \equiv \oint_\sigma dS \, \frac{\partial}{\partial n}\left[i^{-\ell} Y^*_{\ell m}(\hat r) \; j_\ell(kr)\right] i^{\ell'} Y_{\ell' m'}(\hat r) \begin{bmatrix} h^{(1)}_\ell(kr) \\ j_\ell(kr) \end{bmatrix} . \tag{4.3}$$

Waterman also argues that, if Eq. (4.2) has a solution, it must have the large ℓ form

$$f_{\ell m \ell' m'} \xrightarrow[\ell,\ell'\to\infty]{} C_{\ell m \ell' m'} \frac{(ka)^\ell}{(2\ell+1)!!} \frac{(ka)^{\ell'}}{(2\ell'+1)!!} , \tag{4.4}$$

where *a* now represents the maximum radial extent of the scatterer. The coefficient $C_{\ell m \ell' m'}$ depends upon the shape. It is certainly controlled by the multipole moment, of the surface, and one would expect it to decrease when $|\ell-\ell'|$ is substantially greater than the dominant moments. The *rate* of decrease could be as slow as a small power of $|\ell-\ell'|^{-1}$, depending upon the degree of smoothness of the surface as a function of angle. This idea is borne out in two-dimensional numerical calculations [23], in which

Eq. (4.2) *converges more rapidly for a square* (whose dominant moment is $m=4$, *in spite of sharp corners*) than for a highly eccentric ellipse. In any event, further discussion of the convergence properties of the single *scatterer amplitude is beyond the scope of this paper. It is sufficient* for the remainder of this section to assume that the amplitude has a convergent partial wave expansion of the form (4.4), with $C_{\ell m \ell' m'}$ taken to be constant. It is also inferred from (4.4) that f is sufficiently well behaved to be invertible.

The convergence properties of the multiple-scattering equations must now be addressed. Each of the four classes of the previous section is considered in turn.

Class I. Equation (3.5), along with Eqs. (2.2) and (2.10), implies that the multiple-scattering problem can be expressed in terms of algebraic equations. Suppressing partial wave indices, one has the matrix form

$$\sum_j \left[\delta_{ij} - f^{(i)} G(\vec{r}_{ij})\right] F^{(j)} = f^{(i)} 0(\vec{r}_i) \ , \qquad (4.5)$$

which has the formal solution

$$F^{(i)} = \sum_j \left[1 - fG\right]^{-1 ij} f^{(j)} 0 \ . \qquad (4.6)$$

The Green's function G is defined to be zero if $i=j$. While this is the standard form of the equations found in the literature, it is more useful to write them as

$$\sum_j \left[f^{(i)} f^{ij} - f^{(i)} G(\vec{r}_{ij}) f^{(j)}\right] f^{(j)-1} F^{(j)} = f^{(i)} 0(\vec{r}_i) \ , \qquad (4.7)$$

with the solution

$$F^{(i)} = f^{(i)} \sum_j \left[f - fGf\right]^{-1 ij} f^{(j)} 0 \ . \qquad (4.8)$$

Thus, for all four classes of geometries, the remaining question of convergence concerns the double scattering amplitude fGf, with possible shift operators sandwiched inside.

The double scattering amplitude fGf has the same large ℓ behavior in its *outer* indices as the single scattering amplitude, based upon the discussion following Eq. (4.4), and is assumed to be convergent if f is convergent. The real issue is the convergence of the intermediate sums. Returning to Eq. (3.5), the task is to evaluate

$$\sum_{\ell m}\sum_{\ell' m'} J^{ij}_{\ell m \ell' m'} = \sum_{\ell m}\sum_{\ell' m'}\left\{i^{\ell} j_\ell(k\rho_i) Y^*_{\ell m}(\hat{\rho}_i)\right\} G(\vec{r}_{ij})_{\ell m \ell' m'} \times \left\{i^{-\ell'} j_{\ell'}(k\rho_j) Y_{\ell' m'}(\hat{\rho}_j)\right\} . \quad (4.9)$$

The analysis of Eq. (4.9) is only useful if the integrals of Eqs. (2.6) and (2.7) can be interchanged with the sums. This question is discussed below. Note also that the volume integrals in (2.6) and (2.7) vanish on shell, so that the variables $\vec{s}_i$ and $\vec{s}_j$ can be considered to lie on the scatterer surfaces.

Performing the sum over ($\ell' m'$) first yields, using the addition theorem (3.10),

$$\sum_{\ell' m'} G(\vec{r}_{ij})_{\ell m \ell' m'}\left\{i^{-\ell'} j_{\ell'}(k\rho_j) Y_{\ell' m'}(\hat{\rho}_j)\right\} = \frac{ik}{(4\pi)^2}\, i^{-\ell} h^{(1)}_\ell(k|\vec{s}_j-\vec{r}_i|) Y_{\ell m}(s_j \hat{-} r_j) \ , \quad (4.10)$$

provided $r_{ij} > \rho_j$. The remaining sum over (ℓm) is therefore

$$\frac{ik}{(4\pi)^2}\sum_{\ell m} j_\ell(k\rho_i) Y^*_{\ell m}(\hat{\rho}_i)\ h^{(1)}_\ell(k|\vec{s}_j-\vec{r}_i|) Y_{\ell m}(s_j \hat{-} r_i) = \frac{1}{(4\pi)^2}\cdot\frac{e^{ik|\vec{s}_i-\vec{s}_j|}}{4\pi|\vec{s}_i-\vec{s}_j|} . \quad (4.11)$$

That is, the free Green's function between the surfaces of scatterers (i) and (j) is reproduced [as expected by cancelling the factors $\vec{r}_i$ and $\vec{r}_j$ in Eq. (3.2)], *provided also* that $|\vec{s}_j-\vec{r}_i| > \rho_i$. These two inequalities constitute condition A, Eq. (3.11) in the Williams-Morgan approach.

Performing the sums in the opposite order yields the same result *provided* condition B, Eq. (3.12), is satisfied. Since the geometry of Class I satisfies *both* conditions, *the sums can be done in either order.*

Furthermore, for non-overlapping scatterers, $|\vec{s}_i-\vec{s}_j|$ can never vanish, in which case the partial wave sums are uniformly convergent. The surface integrals involve the scattering waves $\psi_{\vec{k}}^{(\pm)}$, and are, in general, convergent. Under those conditions, the sums and integrals can therefore be interchanged. In practical terms, this means that the products $[f^{(i)}G(\vec{r}_{ij})f^{(j)}]$ of Eq. (4.7), forming the matrix to be inverted in Eq. (4.8), can be evaluated by summing the partial waves of the *amplitudes* in any order.

For the remaining three classes of geometries, the multiple partial wave sums, if they converge at all, also converge uniformly to Eq. (4.11), in which case the sums and integrals are again interchangeable. Thus, in subsequent discussion, for the question of convergence of products involving *amplitudes*, such as in Eq. (4.8), it suffices to examine the convergence of products involving *integrands*, such as in Eq. (4.9).

Class II. The Williams-Morgan geometries involve the same sums given by Eq. (4.9), as in Class I. However, the *order* of summation is now important. If only *one* of the conditions A or B is satisfied, then the order of summation must be commensurate with it. *Reversing the order in such cases gives a divergent series.* For example, referring to Fig. 1(II), if scatterer (i) is a sphere and scatterer (j) an adjacent cube, then the product in Eq. (4.8) must be partitioned as $f^{(i)}[G(\vec{r}_{ij})f^{(1)}]$, with the product in brackets evaluated first.

Class III. Equation (3.17) implies that the matrix equation to be solved, analogous to (4.7), is

$$\sum_j \left[f^{(i)}\delta^{ij} - f^{(i)}O^\dagger(\vec{\Delta}_{ij})G(\vec{r}_{ij}{}')O(\vec{\Delta}_{ji})f^{(i)}\right]f^{(j)-1}F^{(j)} = f^{(i)}O(\vec{r}_i), \quad (4.12)$$

with a solution

$$F^{(i)} = f^{(i)}\sum_j \left[f - fO^\dagger GO\,f\right]^{-1\,ij}f^{(j)}O \ . \quad (4.13)$$

To investigate the convergence question, one must consider the sums of the quantities in Eq. (3.17):

$$\sum_{\ell m}\sum_{\ell' m'} J^{ij}_{\ell m\ell' m'} = \sum_{\ell m}\sum_{\ell' m'}\sum_{\lambda\mu}\sum_{\lambda'\mu'}\left\{i^\lambda j_\lambda(k\rho_i)Y^*_{\lambda\mu}(\hat{\rho}_i)\right\}O^\dagger(\vec{\Delta}_{ij})_{\lambda\mu\ell m}$$
$$\times\, G(\vec{r}_{ij}{}')_{\ell m\ell' m'}O(\vec{\Delta}_{ji})_{\ell' m'\lambda'\mu'}\left\{i^{-\lambda'}j_{\lambda'}(k\rho_j)Y_{\lambda'\mu'}(\hat{\rho}_j)\right\}. \quad (4.14)$$

As noted above, the shift operators can be combined with G, in which case precisely Eq. (4.9) of Classes I and II is obtained. The relevant inequalities can always be satisfied, so there is no trouble with this step. However, the subsequent sums over $(\lambda\mu),(\lambda'\mu')$ will then, in general, diverge, since there is no reason for r_{ij} to be greater than a_i or a_j within Class III. On the other hand, if the $(\lambda\mu),(\lambda'\mu')$ sums are performed *first*, one gets the analog of Eq. (3.16):

$$\sum_{\ell m}\sum_{\ell' m'} J^{ij}_{\ell m\ell' m'} = \sum_{\ell m}\sum_{\ell' m'}\left\{i^\ell j_\ell(k\rho_i{}')Y^*_{\ell m}(\hat{\rho}_i{}')\right\}G(\vec{r}_{ij}{}')_{\ell m\ell' m'}$$
$$\times\left\{i^{-\ell'}j_{\ell'}(k\rho_j{}')Y_{\ell' m'}(\hat{\rho}_j{}')\right\} . \quad (4.15)$$

By construction, the vectors $\vec{\rho}_i{}'$, $\vec{\rho}_j{}'$, $\vec{r}_{ij}{}'$ satisfy both the inequalities (3.11) and (3.16), so the remaining sums over $(\ell m),(\ell' m')$ can then be done *in either order*, with the result given by Eq. (4.11). Thus, in Eqs. (4.12) and (4.13), the matrix products must be partitioned as $[f^{(i)}O^\dagger][G(\vec{r}_{ij}{}')][O\,f^{(j)}]$: the bracketed quantities can be combined in either order, provided their contents are evaluated first.

Class IV. In this case, the starting point is again Eq. (4.12). As in Class III, the $(\lambda\mu),(\lambda'\mu')$ sums must be done first. Then, as in Class II, the remaining sums over $(\ell m),(\ell' m')$ must be done *in the order commensurate with inequality* (3.11) or (3.12). For example, referring to Fig. 1(IV), if scatterer (i) is a sphere and scatterer (j) a shell, the products in Eq. (4.2) have a *hierarchy* of partitions: $\{f^{(i)}0^{+}\}\{G(\vec{r}_{ij})[0\, f^{(j)}]\}$, with the inner brackets evaluated first.

The fact that the order of partial wave summation can control the convergence of the result may be disturbing to some. It is, in fact, a classic case of the theorem of Riemann, which states that a conditionally convergent series can be re-arranged to give any finite or infinite result [24]! This concern can be addressed in several ways.

The order of summation in this case is completly analogous to the process of *analytic continuation* discussed in textbooks, in which multiple Taylor series are used to extend a function outside the circle of convergence dictated by the nearest singular point [24]. Such multiple series are conditionally convergent: obviously, they could be re-arranged back to the single series which diverged in the first place, but only *one* ordering yields the analytic continuation. In the multiple scattering problem, one must analytically continue the wave function *inside* the sphere centered at the scattering site. Physically, one is disassembling the wave and reassembling it with a new and more convenient source point, via Huygens' principle. Finally, for Class III at least, the required procedure is *exactly* that described in Section 3 for a pair of scatterers; questions of convergence were never at issue, because the problem was manipulated to have a Class I geometry.

The problem of partial wave convergence for arbitrary non-overlapping geometries was noticed by Ziesche [25], who concluded (correctly) that one cannot simply apply the standard on-shell equations, i.e., Eq. (4.5), to such systems and expect to get meaningful results, because the resulting series diverges. On the other hand, Faulkner [26] observed (correctly) that the scattered wave outside the obstacle but inside the *concentric* sphere is not an outgoing wave, but rather a non-singular (j_ℓ) function, and concluded that more than on-shell information can be required, in agreement with the discussions at the end of Section 3. The use of shifted centers is the resolution to both of these observations: the sums can be rendered convergent, and the scattered wave can always be obtained just outside any convex surface by calculating an outgoing wave *from a shifted source* using on-shell amplitudes.

The price to be paid for the on-shell theorem with extended geometries is the presence of extra partial wave sums. Furthermore, they can involve many terms. For large shifts $\vec{\Delta}$, the upper limit is of order $(k\Delta)$. The necessary $|\vec{\Delta}|$ for Class III, for example, is proportional to L^2/d, where d is the separation of the surfaces and L the common length. On the other hand, the sums need only be evaluated once. By contrast, the number of partial waves required for the *outer* indices of the matrix [f - fGF] in Eq. (4.8) (i.e., the dimensionality of the inversion or diagonalization problem) depends instead on the geometry of the individual scatterers, or at worst, the extended geometry of the combined (ij) pair, *but not the shift vectors*.

It should also be noted that for the non-standard Classes II-IV, Eq. (4.8) *must* be used in place of Eq. (4.6), which is the standard form found in the literature. This is because, for certain (i) and (j), evaluating the product $f^{(i)}G(\vec{r}_{ij})$ amounts to summing the partial waves in the wrong order. The partial wave index which should have been summed first becomes a label in a truncated matrix equation whose accuracy cannot be improved by adding more partial waves, since the implied series ultimately diverges. On the other hand, the reason that Eq. (4.8) avoids this problem is that the source of divergent series is the Green's function: by sandwiching G *between* the amplitudes and performing the properly ordered sums, the delicate portion of the calculation is completed *before* matrix inversion or diagonalization.

5. BREAKDOWN OF THE ON-SHELL THEOREM: AN EXAMPLE

While the purpose of this paper has been to expand the number of geometric configurations in which the on-shell theorem can be utilized, there still remain many cases of physically non-overlapping scatterers which fail to satisfy even the more relaxed criteria. For example, one such class of configurations involves scatterers with nesting surfaces, as with two sawtooth patterns. The obvious question is whether a more sophisticated on-shell proof is yet to be found for such cases, or whether off-shell information is *essential* for a solution to the multiple scattering equations.

Ideally, one would like some sort of *off-shell* theorem, which specifies the precise conditions under which more than on-shell amplitudes are needed. Unfortunately, no such theorem is available to date. However, some light can be shed on the matter by considering the example illustrated in Fig. 2, in which a symmetric sphere is enclosed by a penetrable spherical shell. The full scatterers are physically non-overlapping, at least in the sense that the free wave equation is satisfied in the region between them, but they clearly fall outside all four classes described above for the on-shell theorem. The distinctive feature of this problem is that it can be solved directly, without reference to multiple-scattering theory.

In the absence of the spherical scatterer, the radial wave inside the shell must be $\xi_\ell j_\ell(kr)$ for any given ℓ, while outside it is $\left[j_\ell(kr) + ikf_\ell^{(\text{shell})}\ h_\ell^{(1)}(kr)\right]$, where $f_\ell^{(\text{shell})}$ is the usual partial wave amplitude. If the sphere is present, then the solution in the inner free region must be proportional to $\left[j_\ell(kr) + ikf_\ell^{(\text{sphere})}\ h_\ell^{(1)}(kr)\right]$. Now suppose that one has solved a problem in which the interior solution is purely $ih_\ell^{(1)}(kr)$, and that matching boundary conditions yields an exterior solution of the form $\zeta_\ell\left[j_\ell(kr) + ikg_\ell^{(\text{shell})}\ h_\ell^{(1)}(kr)\right]$. Then, by superposition, the exterior wave with both scatterers present must be

$$\psi_\ell^{(\text{ext})}(r) = j_\ell(kr) + ikF_\ell\ h_\ell^{(1)}(kr)\ , \tag{5.1}$$

where the complete amplitude is

$$F_\ell = \left[f_\ell^{(\text{shell})} + k\zeta_\ell\xi_\ell f_\ell^{(\text{sphere})}\ g_\ell^{(\text{shell})}\right]\Big/\left[1 + k\zeta_\ell\xi_\ell f_\ell{}^{(\text{sphere})}\right]\ . \tag{5.2}$$

The solution thus depends not only upon upon the usual amplitudes f_ℓ, but also upon two additional quantities $(\zeta_\ell\xi_\ell)$ and $g_\ell^{(\text{shell})}$. Indeed, they are related to quantities introduced by Sun and Su in their multiple-scattering treatment of overlapping spheres [16]. They depend upon the boundary matter to the specific wave solutions *inside* the shell: they cannot be determined from $f_\ell^{(\text{shell})}$, and their effects will not in general cancel.

For this particular case, on-shell amplitudes alone are not sufficient to solve the scattering problem. The geometry differs from the four classes discussed above in two respects. First, it is topologically distinct, because one scatterer is completely enclosed inside another. However, one can sidestep this difference in an approximate way by placing a gap in the outer shell and examining the long wavelength limit, for which the results should be similar to Eq. (5.2). The second difference is that the spherical shell surrounds the *singularity* associated with the outgoing wave from the inner sphere. Normally, the outgoing wave from a neighboring scatterer can be expanded as a combination of plane waves, *except* near the singular point. This is the reason why the free amplitudes, which describe *plane wave* scattering, can be used. One can reinterpret the hemispherical shell case of Class IV as the limiting geometry in which the leading edge of the shell faces plane waves, as opposed to singular waves.

Note that the extra information required for this example (and indeed, all that could *ever* be required for configurations of physically non-overlapping scatterers) is "on shell", at least in the sense that only the asymptotic wave number k is involved. Nevertheless, additional knowledge of the wave solution inside the scatterer is needed to determine the near-field properties outside the scatterer. That is to say, the extra information is on the energy (frequency) shell, but "off the geometric shell" of allowed scattering configurations involving *asymptotic* sources and detectors.

6. SUMMARY

It has been shown that the multiple-scattering problem can be solved, using only (asymptotic) on-shell amplitudes of the constituent scatterers, for a larger variety (Classes III and IV) of non-overlapping geometries than had been demonstrated to date. In general, there is a price to pay in terms of the partial wave series. For the new geometries of higher complexity, the *ordering* of the summations becomes important for achieving convergence, and the most complicated classes (III and IV) can require *additional* sums due to the shift operations employed in proving the theorem.

Thus, one is generally left with a problem that is technically more complicated than those for which the non-overlap condition (Class I) applies. Nevertheless, for situations in which little is known about the scatterers except the on-shell information, a non-overlap theorem is desirable, even at extra cost.

For problems where details of the scatterer are known, there are other alternatives. If appropriate off-shell information is provided, the multiple-scattering problem can be solved directly without shifting the scattering centers, or, for that matter, without worrying whether the various geometries non-overlap conditions are satisfied at all. Two different examples of such an approach are those of Refs. [9,16]. For problems in Classes I through IV, one knows in advance that the off-shell effects must eventually cancel, but there can be an advantage of the latter approach in terms of the number of partial waves required. The inclusion of off-shell effects tends to weaken the near-field singularity of the Green's function between the scatterers. Mathematically, this is because the roles of Hankel and Bessel functions are interchanged in, say, Eq. (3.5): additional amplitudes must be provided, but wave propagation between scatterers is described by a non-singular function (see, for example, Refs. [27,28]), and this greatly improves the partial wave convergence.

The use of partial waves in this paper is certainly partial to spherical geometry, and one can always use other coordinate systems. For example, two-dimensional scattering from elliptic cylinders is an obvious element of "Class I" for elliptic coordinates [14]. Of course, the elliptic on-shell amplitudes could in turn be obtained in terms of circular partial wave amplitudes; the resulting equations will then have the *form* of Eq. (4.12).

The actual choice of method, of course, depends upon the particular multiple-scattering problem at hand. One purpose of this paper has been to enlarge the number of available options.

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FIGURE CAPTIONS

1. Examples of non-overlapping geometries corresponding to the four classes defined in the text.
2. A sphere inside a spherical shell, which violates the on-shell theorem.

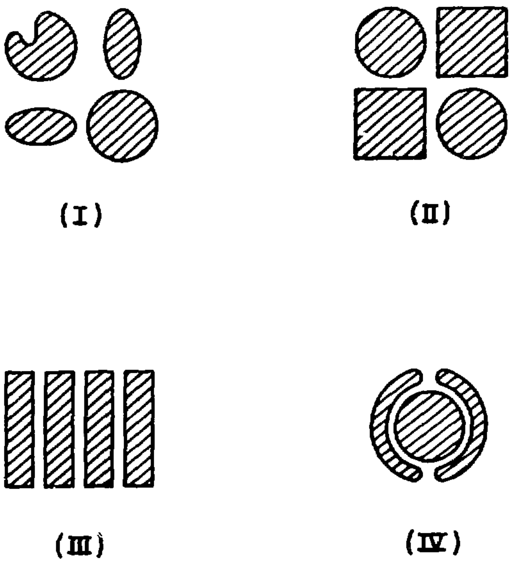

Fig. 1

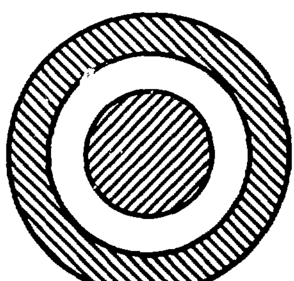

Fig. 2