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Wave propagation through an assembly of spheres IV. Relations between different multiple scattering theories

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Abstract. The exact determinantal equation satisfied by the coherent wave vector in a statistically defined medium of spherical scatterers, which was obtained by Lloyd in III of this series of papers, is used to show two things.

First, the determinant can be written as an infinite series similar to that obtained by ordinary resummation methods, except that it does not involve elements of the T matrix off the energy shell.

Secondly, the first two terms of the series are specialized to the case of point scatterers which are uncorrelated except for an infinitesimal sphere of exclusion about each of them, and the results found to disagree with those of other calculations; this discrepancy is clarified.

The formalism is generalized to deal with vector waves, and it is shown that, for electric dipole scattering, the simplest approximations to the functions appearing in the determinant lead to the Lorentz–Lorenz law.

1. Introduction

This is the fourth of a series of papers examining the various aspects of wave propagation in a disordered medium. In the first, Ziman (1966, to be referred to as I) described an approximate method for calculating the refractive index of a medium. In the next two, Lloyd (1967 a, b, to be referred to as II and III respectively) derived and examined an exact formalism for the average density of states in general media. In the present paper we apply this exact formalism to the refractive index problem.

The theory of the multiple scattering of waves in a medium consisting of an infinite number of individual scattering centres, distributed according to a given probability distribution, is concerned both with why such a system behaves as if it were a continuum described by a complex refractive index and with how to calculate this refractive index. Such investigations have a long history; the earliest work is due to Rayleigh and a large number of papers appeared at the beginning of this century (for a comprehensive review, see Twersky 1960). However, these early papers used only the simplest of approximations and the modern investigations date from Foldy (1945) and Lax (1951, 1952) who precisely defined the coherent wave as the ensemble averaged multiply scattered wave, and clearly stated the difficulties involved in its calculation.

As well as formulating the problem precisely, these authors introduced the 'hierarchy method' as a means of calculating the complex propagation vector of the coherent wave, and hence the refractive index of the medium. In this method the additional concept of a conditionally averaged wave function is introduced; a hierarchy of equations can then be formed in which a given member expresses the ensemble averaged wave function with n atoms held in fixed positions in terms of the ensemble averaged wave function with $n+1$ atoms held in given positions. Approximations can then be formed by using some assumption, such as the 'quasi-crystalline' approximation of Lax, in order to express one of the higher-order ensemble averages in terms of lower-order ensemble averages. A closed set of equations can thereby be obtained, which in turn may be solved. While, in principle, increasingly more accurate approximations could be obtained in this way, in practice only the lowest-order approximation may be evaluated.

The majority of authors who have been interested in calculating the complex propagation vector of a given medium have used the hierarchy method as a basis for their calculations. An evaluation of the probable errors involved in truncating the hierarchy of equations has been given by Waterman and Truell (1961). In this paper they considered the point scatterer, or long-wavelength limit, of the multiple scattering problem. In this limit the wavelength is assumed to be long with respect to the lengths describing the deviations of the probability distributions from purely random (the wavelength need not necessarily be long compared with the scattering length of an individual scatterer); the true probability distribution is then replaced by a purely random distribution of point scatterers. This is the limit which is implicit in the derivation of the Lorentz–Lorenz formulae, for example. Waterman and Truell obtain for this model the result

$$k^2 = \kappa^2 + 4\pi\frac{N}{V}f(0) + \frac{\{4\pi(N/V)\}^2}{4\kappa^2}\{f^2(0)-f^2(\pi)\} \tag{1.1}$$

where k is the complex wave number in the medium, κ is the wave number of the incident wave in free space (if this were a quantum-mechanical problem, then the energy would be given by $E = \kappa^2$ in atomic units), N is the number of scattering centres in the volume V, and $f(\theta)$ is the scattering amplitude of an individual scattering centre. The complex refractive index of the medium is then given by $n = k/\kappa$. The first two terms of this result give the 'thin slab' approximation (Fermi 1950) and the total expression has previously been obtained by Urick and Ament (1949) who considered the medium as being composed of many thin slabs joined together. The second part of this expression is, however, incorrect. In § 3 of the present paper we shall show that it arises from just this artificial stratification of the medium into thin slabs.

Even when large scatterers are considered, as by Twersky (1962 a, b, c), it is difficult to avoid this stratification when a plane boundary is introduced into the problem. Twersky attempts to obtain self-consistency by introducing the concept of a 'two-space' or 'schizoid' scatterer. However, by taking the point scatterer limit of his results we shall show that this method is only correct to first order also. Electromagnetic multiple scattering has been considered by Mathur and Yeh (1964). These authors also use the method of Twersky and, if we take the limit of their results to point dipole scatterers (their equation (31)), the result is

$$n = \frac{k}{\kappa} = 1 + \frac{2\pi(N/V)\alpha}{1+(4\pi/15)(N/V)\alpha} \tag{1.2}$$

where α is the polarizability of the point scatterer. This is not of the expected Lorentz–Lorenz form. In § 4 of the present paper we shall show that only minor changes in the formalism for calculating the complex propagation vector for a scalar wave are needed to handle the electromagnetic vector wave. In § 5 we shall then show that in the limit of point electric dipole scatterers one obtains the expected Lorentz–Lorenz form.

The hierarchy method has been used by Fikioris and Waterman (1964) to calculate the refractive index of a medium of large spherical scatterers distributed with a purely random probability distribution, apart from a condition that the individual scattering regions should not overlap. Although in this paper a plane wave was considered falling onto a semi-infinite slab of the material, they avoided the pitfalls associated with the introduction of such a boundary and derived the same result as that obtained by Phariseau and Ziman (1963) and also in I. These authors did not introduce a boundary into the problem. In these papers the final equations to be solved in order to find the complex propagation vector for the medium take the form of an infinite determinant which must be zero when evaluated with the correct propagation vector. As such, the final equations are in quite a different form from, say, equation (1.1).

An alternative method of calculating the complex refractive index of a random medium has arisen out of the application of Green function techniques to the determination of the optical potential in nuclear physics (for a review article, see Fetter and Watson 1965). As the scattering potentials suffer recoil in the nucleus, this problem is not strictly comparable with the present one where the scattering potentials are unaffected by the scattered wave; the Green function technique appropriate to the multiple scattering of a single particle wave in a random distribution of potentials was first used by Edwards (1958) when discussing the conductivity problem. In this method, which we shall call the 'resummation method', a point source of waves is considered to be situated in an infinite medium. The scattering series is then written out completely, giving what Lax has called the 'expanded' representation. In this expanded representation the ensemble average may be taken exactly, without becoming involved in a hierarchy of equations. However, in this expanded representation the coherent wave does not exist; the series must be resummed in order to obtain any result at all. After the series has been resummed into a 'Dyson self-energy' form, the complex propagation vector is given by finding the root of the energy denominator in the complex k plane; as such, this differs from finding the 'quasi-particle' energy, which is the root of this energy denominator in the complex energy plane (cf. in this regard, the discussion of the Phariseau and Ziman paper given by Ballentine and Heine (1964)).

Further, more complete resummations or 'renormalizations' of the multiple scattering series have been investigated by Klauder (1961), Edwards (1961, 1962), Beeby and Edwards (1963), Beeby (1964 a, b, c), des Cloizeaux (1965) and Ballentine (1966). However, these authors have not been directly interested in calculating the refractive index of the medium; instead these have all been papers devoted to calculating the quantum-mechanical density of states in the medium. A consequence of this is that they obtain the equation

$$k^2 = \kappa^2 - \frac{N}{V}\langle\mathbf{k}|T|\mathbf{k}\rangle + \dots \tag{1.3}$$

to be solved for the complex propagation vector $\mathbf{k}$. Here $\langle\mathbf{k}|T|\mathbf{k}\rangle$ is the T matrix of a single scattering centre in a momentum representation, the T matrix being evaluated at the energy $E = \kappa^2$. This differs from the first two terms of equation (1.1) in that the unknown complex propagation vector appears in the representation of the T matrix. Such a T matrix is simply related to the scattering amplitude only when the momentum is 'on the energy shell'. Then we have

$$\langle\boldsymbol{\kappa}|T|\boldsymbol{\kappa}'\rangle = -4\pi f(\theta) \tag{1.4}$$

where $\kappa^2 = \kappa'^2 = E$ and θ is the angle between $\boldsymbol{\kappa}$ and $\boldsymbol{\kappa}'$.

The reason why these off-energy-shell terms appear is that the series (1.3) is valid for any arrangement of the scattering potentials. In particular, it is valid even when the scattering potentials overlap one another. The complex propagation vector can only be expressed in terms of the scattering amplitude of the individual scatterers if there is a specific assumption that the scattering potentials do not overlap. In this case the off-energy-shell parts of the T matrix must be cancelled by later terms in the series (1.3).

The assumption of non-overlapping (or 'muffin tin') potentials has been used in density-of-states calculations by Beeby (1964 b, c). Beeby used an assumption in the resummation method which is equivalent to the quasi-crystalline approximation in the hierarchy method. An investigation of the structure of a complete resummation of the scattering series, when the potentials do not overlap, has been given in II and III. Equation (4.7) of the latter of these two papers gives the equation which must be solved in order to calculate the coherent propagation vector. This equation is

$$\det \|\delta_{L,L'} - \frac{N}{V}\sum_{L''} G^{(\mathrm{m})}_{L,L''}(\mathbf{k})S_{L'',L'}\| = 0. \tag{1.5}$$

Here the determinant is over the composite angular momentum subscripts L, where

$$L = (l, m) \quad \text{and} \quad \sum_L \equiv \sum_{l=0}^{\infty}\sum_{m=l}^{+l}.$$

Complete expansions, with each term represented by a diagram, are then given for the medium propagator $G^{(\mathrm{m})}_{L,L'}(\mathbf{k})$ and the renormalized scattering factor $S_{L,L'}$. The first terms of these expansions are

$$S_{L,L'} = T_L\delta_{L,L'} + \dots \tag{1.6}$$

where $T_L = T_l$ is related to the scattering amplitude by

$$f(\theta) = -\sum_{l=0}^{\infty}(2l+1)T_l\mathrm{P}_l(\cos\theta) \tag{1.7}$$

and hence for phase shift scattering may be expressed in the form

$$T_l = -\frac{1}{\kappa}\sin\eta_l \exp(i\eta_l). \tag{1.8}$$

The medium propagator has the expansion

$$G^{(m)}_{L,L'}(k) = \int G_{L,L'}(\mathbf{r})g(r)\exp(-i\mathbf{k}\,.\,\mathbf{r})\,d^3r + \dots . \tag{1.9}$$

When the length k of the vector $\mathbf{k}$ is a complex number, we must understand this expression as being the analytic continuation of the integral evaluated for real k; $g(r)$ is the pair correlation function of the distribution of the scattering centres and

$$G_{L,L'}(\mathbf{r}) = \sum_{L''} C^{L,L',L''} 4\pi i^{l''}\{-i\kappa \mathrm{h}_{l''}^{+}(\kappa r)\} Y_{L''}(\mathbf{r}) \qquad r > 0. \tag{1.10}$$

Here $Y_L(\mathbf{r}) = Y_{l,m}(\theta, \phi)$ is the normalized spherical harmonic of the angular components of the vector $\mathbf{r}$, as defined by Messiah (1964, p. 494); $\mathrm{h}_l^{+}(x) = \mathrm{j}_l(x) + i\mathrm{n}_l(x)$ is the outgoing spherical Bessel function (Messiah does not use this notation for the Bessel function, he uses this symbol for what we shall denote by $i\mathrm{h}_l^{+}(x)$) and

$$C^{L,L',L''} = \int Y_L{}^*(\Omega) Y_{L'}(\Omega) Y_{L''}{}^*(\Omega)\, d\Omega. \tag{1.11}$$

Messiah (1964, p. 1057) gives a relationship between this quantity and the Clebsch–Gordan coefficients. Cruzan (1962) has discussed some of the mathematical properties of this quantity; the relationship between his quite different notation and ours is given in appendix 2.

If only the first two terms of the expansions (1.6) and (1.9) are retained in the determinant (1.5), the result is identical with the determinant obtained by Phariseau and Ziman (1963) and also in I by means of the hierarchy method. If, further, the pair correlation function $g(r)$ is simplified to the pair correlation function used by Fikioris and Waterman (1964), it is equivalent to the homogeneous set of linear equations which these authors obtained. The form of the equation (1.5) is, however, not suitable for making easy comparisons either with the more usual results of the resummation method, in which the off-energy-shell terms have not been removed (equation (1.3)), or with many of the results obtained by the hierarchy method, such as equation (1.1). In § 2 of this paper the determinant (1.5) is expanded to give a series similar to that of the resummation method (1.3), but with all the off-energy-shell terms removed (the assumption of non-overlapping potentials has been used in deriving (1.5)).

In this paper, then, we first expand the determinant so as to obtain the usual multiple scattering series in the resummation method, but with the off-energy-shell terms removed (§ 2). We then compare this result with some of the expansions made by the hierarchy method; in order to make this comparison we shall take the limit of various results to the point scattering case (§ 3). Next we show that the determinant form may be written down just as easily for the multiple scattering of electromagnetic waves as for scalar waves (§ 4), and finally we show that in the point scattering limit this gives the usual Lorentz–Lorenz formulae (§ 5).

2. The expansion of the determinant

The series expansion of the determinant (equation (1.5)) in the form of equation (1.3) with the off-energy-shell elements of the T matrix removed may be obtained by expanding the determinant about the pole in $G^{(m)}_{L,L'}(\mathbf{k})$ which occurs when $k^2 = \kappa^2$. This pole arises from the assumed long-range uniformity of the probability distributions, i.e. it is assumed that the pair correlation function satisfies

$$g(r) \to 1 \quad \text{as} \quad r \to \infty. \tag{2.1}$$

Moreover, an examination of the terms in the series expansion for the medium propagator shows that only the first term, i.e. the term explicitly shown in equation (1.9), has this pole.

Hence to achieve this expansion we must substitute

$$g(r) = 1 + h_2(r) \tag{2.2}$$

into this term.

When this division of the pair correlation function is made, care must be taken with the contribution of the integral from the origin. The non-overlapping condition is

$$h_2(r) = -1 \qquad r < R_{\mathrm{m}} \tag{2.3}$$

and, if this is directly substituted into the first term, the integral is not defined at the origin. The integral involving $g(r)$ is, however, well defined and this allows a consistent procedure to be found. We shall define the principal-valued integral as follows:

$$\fint \{i^l Y_L(\mathbf{r}) \mathrm{h}_l^+(\kappa r) \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}} h_2(r)\} \, d^3r \equiv \lim_{\epsilon \to 0} \left[\int_{|\mathbf{r}|>\epsilon} \{i^l Y_L(\mathbf{r}) \mathrm{h}_l^+(\kappa r) \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}} h_2(r)\} \, d^3r - \frac{4\pi i}{\kappa} Y_L(\mathbf{k}) \frac{(k/\kappa)^l - 1}{k^2 - \kappa^2} \right]. \tag{2.4}$$

This quantity is regular as $k \to \kappa$. The last term is, by definition, the difference between our definition of the principal value of the integral and the value obtained by removing a small sphere from around the origin.

With the above definition for the principal value, the first term in the expansion for the medium propagator (equation (1.9)) may be written as

$$\int G_{L,L'}(\mathbf{r}) g(r) \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}} \, d^3r = (4\pi)^2 \frac{Y_L^*(\mathbf{k}) Y_{L'}(\mathbf{k})}{\kappa^2 - k^2} + \fint G_{L,L'}(\mathbf{r}) \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{r}} h_2(r) \, d^3r. \tag{2.5}$$

The last part of this expression we now combine with all the other terms in the series expansion for the medium propagator to define $G^{\mathrm{R}}_{L,L'}(\mathbf{k})$. Hence the medium propagator may now be expressed in the form

$$G^{(\mathrm{m})}_{L,L'}(\mathbf{k}) = (4\pi)^2 \frac{Y_L^*(\mathbf{k}) Y_{L'}(\mathbf{k})}{\kappa^2 - k^2} + G^{\mathrm{R}}_{L,L'}(\mathbf{k}). \tag{2.6}$$

This expression explicitly exhibits the singularity in the medium propagator; $G^{\mathrm{R}}_{L,L'}(\mathbf{k})$ does not contain a pole when $k^2 = \kappa^2$.

With the medium propagator expressed in this form we may now expand the determinant by writing the equation from which it arises as a homogeneous linear equation, of the form

$$A_L - \frac{Y_L^*(\mathbf{k})}{\kappa^2 - k^2} B - \frac{N}{V} \sum_{L'',L'} G^{\mathrm{R}}_{L,L''}(\mathbf{k}) S_{L'',L'} A_{L'} = 0 \tag{2.7}$$

where

$$B = \frac{N}{V} (4\pi)^2 \sum_{L,L'} Y_L(\mathbf{k}) S_{L,L'} A_{L'}. \tag{2.8}$$

The unknown constants A_L may then be eliminated from these two equations. When this has been done we find that the constant B cancels from both sides of the resulting equation. (This would not have happened if the pole of $\mathscr{G}^{\mathrm{m}}_{L,L'}$ had been picked out in some other way.) The result is

$$k^2 = \kappa^2 - (4\pi)^2 \frac{N}{V} \sum_{L,L',L''} Y_L(\mathbf{k}) S_{L,L'} \left\{ 1 - \frac{N}{V} G^{\mathrm{R}}(k) S \right\}^{-1}_{L',L''} Y_{L''}(\mathbf{k}). \tag{2.9}$$

The matrix inverse in this equation can now be expanded out. If this is done, and the series expressed as a diagrammatic expansion, the result is just the series obtained by the usual resummation methods (slightly further resummed). Now, however, unlike in equation (1.3), the off-energy-shell components of the T matrix do not appear.

3. The second-order term

From equation (2.9) we may expand the complex propagation vector to second order in the scattering amplitude. This gives the result

$$k^2 = \kappa^2 - (4\pi)^2 \frac{N}{V} \sum_L Y_L(\mathbf{k}) T_L Y_L^*(\mathbf{k})$$
$$+ \lim_{\mathbf{k}\to\kappa} \left\{ -\left(4\pi \frac{N}{V}\right)^2 \sum_{L,L} Y_L(\mathbf{k}) T_L \oint G_{L,L'}(r) \mathrm{e}^{-i\mathbf{k}.\mathbf{r}} h_2(r)\, d^3r\, T_{L'} Y_{L'}^*(\mathbf{k}) \right\}. \quad (3.1)$$

Using the expression

$$f(\theta) = -4\pi \sum_L Y_L(\mathbf{k}) T_L Y_L^*(\mathbf{k}') \quad (3.2)$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$, and the first part of this expression is just the thin slab result. The second part is more difficult and cannot be explicitly evaluated without knowing the pair correlation function.

If we now consider the limit to point scatterers of this expression, a limit which implies a knowledge of the correlation function, then the expression (3.1) may be evaluated. By using the generating function for the Legendre polynomials, the result may be expressed in terms of the scattering amplitude; this is

$$k^2 = \kappa^2 + 4\pi \frac{N}{V} f(0)$$
$$+ \frac{\{4\pi(N/V)\}^2}{4\kappa^2} \left[-f^2(0) + f^2(\pi) - \int_0^\pi \frac{1}{\sin\frac{1}{2}\theta} \frac{d}{d\theta} \{f^2(\theta)\}\, d\theta \right]. \quad (3.3)$$

This expression differs from the expression derived by Waterman and Truell (equation (1.1)) both in the signs of the forward and backward scattering terms and in the additional term which is present. It is worth while understanding the cause of this discrepancy, for it has appeared in many papers discussing multiple scattering (Twersky 1962 a, c, Mathur and Yeh 1964, and others). The error arises when a semi-infinite slab of scattering material is considered and the integrals involved in finding the ensemble average are taken in the natural way, i.e. parallel to the boundary of the region. These integrals alter in character when the position of the last scattering centre is within a distance Δ, where Δ is the radius of the scattering centre, of the point where the ensemble averaged wave function is being evaluated. If the integrals are being taken parallel to the plane boundary (which we shall suppose is perpendicular to the z axis), then this means that the region of integration over a slab-like region of width 2Δ must be treated differently from the rest of the integration. If, as is common, the contribution of this region is ignored, this becomes equivalent to an implicit assumption of a correlation function which is not spherically symmetric but instead is given by

$$h_2(x, y, z) = \begin{cases} -1 & |z| < \Delta \\ 0 & |z| > \Delta. \end{cases} \quad (3.4)$$

This corresponds to a distribution that is random except for the exclusion of a thin sheet of scatterers.

The exact expression (3.1) may be evaluated with this pair correlation function. Expressing the result as the integral with $h_2(r) = -1$ everywhere, minus the contribution from taking $h_2(r) = -1$ outside the slab (the first integral then contains the singular contribution), we find that the second-order term is given by

$$\left(4\pi \frac{N}{V}\right)^2 \left[\left\{ \frac{f^2(0)}{\kappa^2 - k^2} \right\} - \left\{ \frac{f^2(0)}{2\kappa(k-\kappa)} + \frac{f^2(\pi)}{2\kappa(k+\kappa)} \right\} \right]. \quad (3.5)$$

Here we have also taken the limit $\Delta \to 0$ for simplicity. In the limit $\mathbf{k} \to \boldsymbol{\kappa}$ this is just the term derived by Waterman and Truell (equation (1.1)).

Twersky (1962 b) has introduced the concept of a 'two-space' scatterer in an attempt to obtain self-consistency. This is not an analytic continuation of the T matrix; the two-space 'phase shift' $T_L{}^s$ is given in terms of the true phase shifts T_L by equating the logarithmic derivative of

$$\mathrm{j}_L(\kappa r) - i\kappa T_L \mathrm{h}_L{}^+(\kappa r) \tag{3.6}$$

to the logarithmic derivative of

$$\mathrm{j}_L(kr) - i\kappa T_L{}^s \mathrm{h}_L{}^+(\kappa r) \tag{3.7}$$

at some radius a which is determined by the available volume. However, Twersky also integrated parallel to the plane boundary and did not treat correctly the slab of thickness 2Δ about the point of evaluation. He obtained the result (equation (8) of paper by Twersky (1962 c), specialized to normal incidence)

$$k^2 - \kappa^2 = 2\pi \frac{N}{V}\left\{\frac{k+\kappa}{\kappa} f^s(0) - \frac{k-\kappa}{\kappa} f^s(\pi)\right\} \tag{3.8}$$

where $f^s(\theta)$ is the scattering amplitude constructed using the two-space phase shifts. We may compare this with the exact result by taking the limit to point scatterers, which gives

$$T_L{}^s = T_L\left(\frac{k}{\kappa}\right)^l \tag{3.9}$$

and then expanding equation (3.8) to second order in the phase shifts. Expressing the result as a series in T_L we find that the second-order term is as follows:

Exact (equation (3.3)):

$$\frac{1}{\kappa^2}\left(4\pi \frac{N}{V}\right)^2 \{3T_0T_1 + 10T_0T_2 + 6T_1{}^2 + 33T_1T_2 + \ldots\}. \tag{3.10}$$

Waterman and Truell (equation (1.1)):

$$\frac{1}{\kappa^2}\left(4\pi \frac{N}{V}\right)^2 \{3T_0T_1 + 0 + 0 + 15T_1T_2 + \ldots\}. \tag{3.11}$$

Twersky (equation (3.8)):

$$\frac{1}{\kappa^2}\left(4\pi \frac{N}{V}\right)^2 \{3T_0T_1 + 5T_0T_2 + 9T_1{}^2 + 30T_1T_2 + \ldots\}. \tag{3.12}$$

We see that only the first terms of all these expressions agree; the errors in the last two expressions occur basically for the reasons we have already discussed.

4. Electromagnetic scattering

Mathur and Yeh (1964) have considered the multiple scattering of electromagnetic waves from spherical scattering centres. However, they used the analogue of the method of Twersky and, as we have indicated, this is not exact. The determinant analogous to equation (1.5) can, however, easily be written down by analogy with the scalar case. We shall write down these equations, and form the analogy, using the language of phase shift scattering rather than the language of Green functions.

The scalar wave satisfies, in free space, the equation

$$p^2\Psi - \kappa^2\Psi = 0 \tag{4.1}$$

where $\mathbf{p} = (1/i)\nabla$ is the momentum operator. The harmonic time-varying solution only is considered. The solutions to this equation may be expanded about a regular point of the field in the form

$$\Psi(\mathbf{r}) = \sum_L A_L 4\pi i^l \mathrm{j}_l(\kappa r) Y_L(\mathbf{r}) \tag{4.2}$$

where the constants in the expansion are given by

$$4\pi i\, A_L \mathrm{j}_l(\kappa r) = \int \Psi(\mathbf{r}) Y_L{}^*(\Omega)\, d\Omega_r. \tag{4.3}$$

The electromagnetic field satisfies, in free space, the equations

$$\left.\begin{aligned} \mathbf{p} \wedge \mathbf{E} - \kappa\mathbf{H} &= 0 \\ \mathbf{p} \wedge \mathbf{H} + \kappa\mathbf{E} &= 0 \end{aligned}\right\}. \tag{4.4}$$

Here we use units such that $C = 1$; κ is then either the frequency or the free-space wave number. The electromagnetic field may be expressed in terms of the electric and magnetic radial Hertz potentials, Π^1 and Π^2 (we shall consistently use the superscripts 1, 2 to denote electric and magnetic respectively; hence $\mathbf{E}^1 \equiv \mathbf{E}$, $\mathbf{E}^2 \equiv \mathbf{H}$, $\epsilon^1 = \epsilon$, $\epsilon^2 = \mu$, etc.) by means of the equations

$$\left.\begin{aligned} \mathbf{E}^1 \equiv \mathbf{E} &= \mathbf{p} \wedge \mathbf{L}\Pi^1 + \kappa\mathbf{L}\Pi^2 \\ \mathbf{E}^2 \equiv \mathbf{H} &= \mathbf{p} \wedge \mathbf{L}\Pi^2 - \kappa\mathbf{L}\Pi^1 \end{aligned}\right\} \tag{4.5}$$

where $\mathbf{L} = \mathbf{r} \wedge \mathbf{p}$ is the angular momentum operator. The solutions to the field equations may be expanded at a regular point in the field in the form

$$\Pi^n = \sum_{\substack{L \\ L\neq 0}} A_L{}^{(n)} 4\pi i^l \mathrm{j}_l(\kappa r) Y_L(\mathbf{r}) \tag{4.6}$$

where

$$l(l+1)4\pi i^l A_L{}^{(n)} \mathrm{j}_l(\kappa r) = \int \mathbf{r}\,.\,\mathbf{E}^{(n)} Y_L{}^*(\Omega)\, d\Omega_r. \tag{4.7}$$

The exciting field in scattering theory always satisfies the free-space field equation. The scattered field resulting from a scattering of the exciting field by a spherical symmetric scattering centre may be expressed, in the scalar case, in the form

$$\Psi_{\mathrm{sc}}(\mathbf{r}) = \sum_L A_L T_L 4\pi i^l \{-i\kappa \mathrm{h}_l{}^+(\kappa r)\} Y_L(\mathbf{r}). \tag{4.8}$$

In the electromagnetic case, the scattered field is similarly given by

$$\Pi_{\mathrm{sc}}{}^n(\mathbf{r}) = \sum_L A_L{}^{(n)} T_L{}^{(n)} 4\pi i^l \{-i\kappa \mathrm{h}_l{}^+(\kappa r)\} Y_L(\mathbf{r}). \tag{4.9}$$

In both these equations the constants T_L need not necessarily be expressible in terms of a (real) phase shift form; however, if the scattering is elastic these constants may be expressed in the form

$$T_L{}^{(n)} = -\frac{1}{\kappa} \sin \eta_l{}^{(n)} \exp\{i\eta_l{}^{(n)}\}. \tag{4.10}$$

If, in the scalar case, the scattering is simple potential scattering from a radially symmetric potential $V(r)$, then the phase shifts may be found from the solutions of the radial equation

$$-\frac{1}{r}\frac{d^2}{dr^2} rR(r) + \left\{V(r) + \frac{l(l+1)}{r^2} - \kappa^2\right\} R(r) = 0. \tag{4.11}$$

Similarly, if the electromagnetic scattering is from spherically symmetric dielectric functions $\epsilon^{(n)}(r)$, then the phase shifts may be found from the solutions of the radial equations

$$-\frac{1}{r}\frac{d}{dr}\frac{1}{\epsilon^n(r)}\frac{d}{dr} r\epsilon^n(r) R^n(r) + \left\{\frac{l(l+1)}{r^2} - \kappa^2 \mu(r)\epsilon(r)\right\} R^n(r) = 0. \tag{4.12}$$

In both cases the phase shifts are given from the asymptotic relation

$$R^{(n)}(r) \sim \mathrm{j}_l(\kappa r) - \tan \eta_l{}^n \mathrm{n}_l(\kappa r). \tag{4.13}$$

In order to calculate the multiple scattering, we must be able to calculate the excitation amplitude at a second scattering centre due to the scattered wave from the first at a distance Δ from it. In the scalar case the excitation amplitude at the second site, $\bar{A}_L$, may be expressed in terms of the excitation amplitude at the first site, and the constants T_L, by means of the relation

$$\bar{A}_L = \sum_{L'} G_{L,L'}(\Delta) A_{L'} T_{L'} \tag{4.14}$$

where $G_{L,L'}(\Delta)$ is given by equation (1.10). Similarly, in the electromagnetic scattering case the excitation amplitudes at the second centre are given by

$$\bar{A}_L{}^{(n)} = \sum_{L',n'} G^{n,n'}_{L,L'}(\Delta) A_{L'}{}^{n')} T_{L'}{}^{(n')}. \tag{4.15}$$

Here the propagators are given by similar equations to the scalar case, namely

$$G^{11}_{L,L'}(\Delta) = G^{22}_{L,L'}(\Delta) = \sum_{L''}{}' \frac{D^{L,L',L''}}{l(l+1)} 4\pi i^{l''}\{-i\kappa \mathrm{h}_{l''}{}^{+}(\kappa\Delta)\} Y_{L''}(\Delta) \tag{4.16}$$

$$G^{12}_{L,L'}(\Delta) = -G^{21}_{L,L'}(\Delta) = \sum_{L''}{}' \frac{E^{L,L',L''}}{l(l+1)} 4\pi i^{l''}\{-i\kappa \mathrm{h}_{l''}{}^{+}(\kappa\Delta)\} Y_{L''}(\Delta) \tag{4.17}$$

where

$$D^{L,L',L''} = \int [\mathbf{L} Y_L(\Omega)]^* . [\mathbf{L} Y_{L'}(\Omega)] Y_{L''}{}^*(\Omega)\, d\Omega \tag{4.18}$$

$$E^{L,L',L''} = \int [\mathbf{L} \wedge \hat{\mathbf{k}} Y_L(\Omega)]^* . [\mathbf{L} Y_{L'}(\Omega)] Y_{L''}{}^*(\Omega)\, d\Omega. \tag{4.19}$$

A derivation of these propagators is given in appendix 1. The coefficients D and E have been discussed by Cruzan (1962) and the relation between the present formalism and Cruzan's notation is given in appendix 2.

It is clear that the expanded representation of the multiple scattering series in the electromagnetic case has exactly the same structure as in the scalar case. The series may then be resummed, just as in the scalar case, to give the determinant for the complex propagation vector as

$$\det\|\delta_{L,L'}\delta^{n,n'} - \frac{N}{V} \sum_{L'',n''} G^{n,n''}_{L,L''}(\mathbf{k}) S^{n'',n'}_{L'',L'}\| = 0. \tag{4.20}$$

The diagrammatic expansions for the renormalized scattering amplitude and the medium propagator are then exactly the same as in the scalar case, but now the meaning of the diagrams is slightly altered to allow for the superscripts n. The first terms of these expansions are then (cf. equations (1.5) and (1.8))

$$S^{n,n'}_{L,L'} = T_L{}^{(n)} \delta_{L,L'} \delta^{n,n'} + \dots \tag{4.21}$$

$$G^{n,n'}_{L,L'}(\mathbf{k}) = \int G^{n,n'}_{L,L'}(\mathbf{r}) g(r) \mathrm{e}^{-i\mathbf{k}.\mathbf{r}}\, d^3 r + \dots . \tag{4.22}$$

5. Electric dipole scattering

If only electric dipole scattering is present, then all the phase shifts in the above formalism are zero with the exception of

$$T_1{}^1 = -\frac{2\alpha\kappa^2}{3}. \tag{5.1}$$

The scattered field, as given by equation (4.9), is then identical with the field radiated by the dipole $\mathbf{p} = \alpha\mathbf{E}$ (Stratton 1941, p. 435), where $\mathbf{E}$ is the incident electric field at the centre of the scatterer. This latter identification may be made by expanding equations (4.5) and (4.6) in a Taylor series about the origin. When this is the only non-zero term, the determinant (4.20) reduces to a three-by-three determinant.

If, further, we use only the first terms in the series expansion (4.21) and (4.22) then the determinant factorizes over the three m coordinates. The correct root in this case (unlike the scalar case) comes from the terms $m = \pm 1$. This gives the equation for the complex propagation vector as

$$\frac{(k/\kappa)^2-1}{(k/\kappa^2)+2} = \frac{(4\pi/3)(N/V)\alpha}{1-4\pi(N/V)\alpha F(k)} \tag{5.2}$$

where

$$F(k) = \tfrac{1}{3}i\kappa^3 \int_0^\infty \{2\mathrm{j}_0(kr)\mathrm{h}_0{}^+(\kappa r)+\mathrm{j}_2(kr)\mathrm{h}_2{}^+(\kappa r)\}h_2(r)r^2\,dr. \tag{5.3}$$

It is easy to see that in the limit of point scatterers, i.e. $h_2(r) = 0$, this reduces to the familiar Lorentz–Lorenz formula.

6. Conclusion

Ordinary resummation methods give an equation for the coherent propagation vector in the form of a series whose terms contain off-energy-shell elements of the T matrix, even when the scatterers do not overlap. We have shown in § 2 that the exact relation (1.4) (which is valid only for non-overlapping scatterers) can be expanded into a series very similar to those derived by resummation; in this new series, of course, the unphysical off-energy-shell elements are not present.

The second-order term of the series has been derived before by the hierarchy method, and, when applied to the special case of point scatterers in a medium which is random except for a small sphere of exclusion about each centre, the results disagree with ours. In § 3 it was shown that in this earlier work the distribution function actually used involved a thin sheet of exclusion parallel to the boundary of the scattering system.

The formalism used here was extended in § 4 to cover the scattering of vector waves. As a check, we applied the results in § 5 to the case of electric dipole scattering; by retaining only the first terms in the scattering functions (4.21) and (4.22) it was possible to evaluate the determinant exactly (and not in one of the series forms considered previously). The result was the Lorentz–Lorenz formula.

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Appendix 1

We shall only calculate $G^{12}_{L,L'}(\mathbf{r})$; the same method may be applied to the other propagators. Let

$$F_l(k) = \frac{2}{\pi}\frac{(k/\kappa)^l}{E-k^2+i\epsilon} \tag{A1}$$

so that

$$4\pi i^l\{-i\kappa \mathrm{h}_l{}^+(\kappa r)\}Y_L(\mathbf{r}) = \int F_l(k)\mathrm{e}^{i\mathbf{k}.\mathbf{r}}Y_L(\mathbf{k})\,d^3k. \tag{A2}$$

From equation (4.9) and (4.7) we have that

$$\begin{aligned} I &= l(l+1)4\pi i^l \mathrm{j}_l(\kappa r)G^{1,2}_{L,L'}(\Delta) \\ &= \int Y_L{}^*(\Omega)\,d\Omega_r \int d^3k\,\kappa F_{l'}(\mathbf{k})\mathbf{r}\,.\,\{(\mathbf{r}+\Delta)\wedge \mathbf{p}\}\mathrm{e}^{i\mathbf{k}.(\mathbf{r}+\Delta)}. \end{aligned} \tag{A3}$$

Allowing the operators to act on the exponential and using the Hermitian property of the angular momentum operator in a momentum representation, we have

$$L_k = i\frac{\partial}{\partial \mathbf{k}} \wedge \mathbf{k} \equiv \mathbf{k} \wedge \tfrac{1}{2}\frac{\partial}{\partial \mathbf{k}}.$$

Then

$$\begin{aligned} I &= \int Y_L{}^*(\Omega)\,d\Omega_r\left(\int d^3k\,\mathrm{e}^{i\mathbf{k}.\mathbf{r}}\left[i\frac{\partial}{\partial \mathbf{k}}\{\mathrm{e}^{i\mathbf{k}.\Delta}\kappa F_l(k)\mathbf{L}Y_{L'}(\mathbf{k})\}\right]\right) \\ &= 4\pi i^l \int d^3k \left\{\frac{\partial}{i\partial \mathbf{k}}\mathrm{j}_l(kr)Y_L{}^*(\mathbf{k})\right\}[\mathbf{L}Y_{L'}(\mathbf{k})]\kappa F_{l'}(k)\mathrm{e}^{i\mathbf{k}.\Delta} \end{aligned}$$

on taking the spatial angular integral and using the Hermitian property of $i(\partial/\partial\mathbf{k})$. Now

$$\frac{1}{i}\frac{\partial}{\partial\mathbf{k}} = \frac{1}{k}\left\{\mathbf{k}\frac{\partial}{i\partial k} + [\mathbf{L}\wedge\hat{\mathbf{k}}]^*\right\}$$

where $\hat{\mathbf{k}}$ is a unit vector in the direction of $\mathbf{k}$. As $\mathbf{k}.\mathbf{L} \equiv 0$ and $[\mathbf{L}\wedge\hat{\mathbf{k}}]^*$ operates only on the angular coordinates of $\mathbf{k}$, the angular integration of the $\mathbf{k}$ variable may be completed. The integration over $k = |\mathbf{k}|$ can now be evaluated by contour integration and, after substituting into equation (A3), we obtain the result quoted in equation (4.17) and (4.19).

Appendix 2

Many of the mathematical properties of the constants derived from the integration over the spherical harmonics have been discussed by Cruzan (1962). The relation between our notation and his notation is as follows. Let

$$a_L = (4\pi)^{1/2}\left\{2(l+1)\frac{(l-m)!}{(l+m)!}\right\}^{1/2} \tag{A4}$$

then

$$4\pi C^{L,L',L''}a_{L''} = a_L a_{L'}\delta^{m',m+m''}a(m,l|m',l'|l'') \tag{A5}$$

$$a_L a_{L''}D^{L,L',L''} = l(l+1)a_{L'}(-1)^m i^{l'-l-l''}\delta^{m',m+m''}a(m',l'|-m,l|l'')a(l',l,l'') \tag{A6}$$

and

$$a_L a_{L''}E^{L,L',L''} = il(l+1)a_{L'}(-1)^{m+1}i^{l'-l-l''}\delta^{m',m}a(m',l'|-m,l|l'',l''-1)b(l',l,l''). \tag{A7}$$

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