# MULTIPLE SCATTERING BY MULTIPLE SPHERES: A NEW PROOF OF THE LLOYD–BERRY FORMULA FOR THE EFFECTIVE WAVENUMBER*

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**Abstract.** We provide the first classical derivation of the Lloyd–Berry formula for the effective wavenumber of an acoustic medium filled with a sparse random array of identical small scatterers. Our approach clarifies the assumptions under which the Lloyd–Berry formula is valid. More precisely, we derive an expression for the effective wavenumber which assumes the validity of Lax's quasi-crystalline approximation but makes no further assumptions about scatterer size, and then we show that the Lloyd–Berry formula is obtained in the limit as the scatterer size tends to zero.

**Key words.** multiple scattering, effective wavenumber, random media, acoustics

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**1. Introduction.** Suppose that we are interested in the scattering of sound by many small scatterers; for example, we might be interested in using ultrasound to determine the quality of certain composites [14], fresh mortar [2], or food products such as mayonnaise [21]. If we knew the shape, size, and location of every scatterer, we could solve the multiple-scattering problem by solving a boundary integral equation, for example. However, usually we do not have this information. Thus, it is common to regard the volume containing the scatterers as a random medium, with certain average (homogenized) properties. Here, we are concerned with finding an *effective wavenumber*, $K$, that can be used for modelling wave propagation through the scattering volume. This is a classical topic, with a large literature: we cite well-known papers by Foldy [7], Lax [16, 17], Waterman and Truell [25], Twersky [23], and Fikioris and Waterman [6], and we refer to the book by Tsang *et al.* [22] for more information.

A typical problem is the following. The region $z < 0$ is filled with a homogeneous compressible fluid of density $\rho$ and sound-speed $c$. The region $z > 0$ contains the same fluid and many scatterers; to fix ideas, suppose that the scatterers are identical spheres. Then, a time-harmonic plane wave with wavenumber $k = \omega/c$ ($\omega$ is the angular frequency) is incident on the scatterers. The scattered field may be computed exactly for any given configuration (ensemble) of $N$ spheres, but the cost increases as $N$ increases. If the computation can be done, it may be repeated for other configurations, and then the average reflected field could be computed (this is the Monte-Carlo approach). Instead of doing this, we shall do some ensemble averaging in order to calculate the average (coherent) field. One result of this is a formula for $K$.

Foldy [7] considered isotropic point scatterers; this is an appropriate model for small sound-soft scatterers. He obtained the formula

$$K^2 = k^2 - 4\pi \mathrm{i} g n_0/k, \tag{1.1}$$

where $n_0$ is the number of spheres per unit volume and $g$ is the scattering coefficient for an isolated scatterer. The formula (1.1) assumes that the scatterers are independent

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and that $n_0$ is small. We are interested in calculating the correction to (1.1) (a term proportional to $n_0^2$), and this will require saying more about the distribution of the scatterers; specifically, we shall use pair correlations. Thus, our goal is a formula of the form

$$K^2 = k^2 + \delta_1 n_0 + \delta_2 n_0^2, \tag{1.2}$$

with computable expressions for $\delta_1$ and $\delta_2$. Moreover, we do not only want to restrict our formula to sound-soft scatterers.

There is some controversy over the proper value for $\delta_2$. In order to state one such formula, we introduce the *far-field pattern* $f$. For scattering by one sphere, we have $u_{\rm in} = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})$ for the incident plane wave, where $\boldsymbol{k} = k\hat{\boldsymbol{k}}$, $\boldsymbol{r} = r\hat{\boldsymbol{r}}$, $k = |\boldsymbol{k}|$ and $r = |\boldsymbol{r}|$; the angle of incidence, $\theta_{\rm in}$, is defined by $\cos\theta_{\rm in} = \hat{\boldsymbol{k}}\cdot\hat{\mathbf{z}}$, where $\hat{\mathbf{z}} = (0,0,1)$ is a unit vector in the $z$-direction. Then the scattered waves satisfy

$$u_{\rm sc} \sim (\mathrm{i}kr)^{-1}\mathrm{e}^{\mathrm{i}kr} f(\Theta) \quad \text{as } kr \to \infty, \tag{1.3}$$

where $\cos\Theta = \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}}$. Then, Twersky [23] has obtained (1.2) with

$$\delta_1 = -(4\pi\mathrm{i}/k)f(0) \quad \text{and} \quad \delta_2 = (4\pi^2/k^4)\sec^2\theta_{\rm in}\left\{[f(\pi - 2\theta_{\rm in})]^2 - [f(0)]^2\right\}. \tag{1.4}$$

This formula involves $\theta_{\rm in}$, so that it gives a different effective wavenumber for different incident fields. The same formulas but with $\theta_{\rm in} = 0$ (normal incidence) were given by Urick and Ament [24] and by Waterman and Truell [25]:

$$\delta_1 = -(4\pi\mathrm{i}/k)f(0) \quad \text{and} \quad \delta_2 = (4\pi^2/k^4)\left\{[f(\pi)]^2 - [f(0)]^2\right\}. \tag{1.5}$$

Other formulas were obtained more recently [13, 27].

In 1967, Lloyd and Berry [19] showed that the formula for $\delta_2$ should be

$$\delta_2 = \frac{4\pi^2}{k^4}\left\{-[f(\pi)]^2 + [f(0)]^2 + \int_0^\pi \frac{1}{\sin(\theta/2)}\frac{\mathrm{d}}{\mathrm{d}\theta}[f(\theta)]^2\,\mathrm{d}\theta\right\}, \tag{1.6}$$

with no dependence on $\theta_{\rm in}$. They used methods and language coming from nuclear physics. Thus, in their approach, which they "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 [but then] the coherent wave does not exist; the series must be resummed in order to obtain any result at all." The main purpose of the present paper is to demonstrate that a proper analysis of the semi-infinite model problem (with arbitrary angle of incidence) leads to the Lloyd–Berry formula. Our analysis does not involve "resumming" series or divergent integrals. It builds on a conventional approach, in the spirit of the paper by Fikioris and Waterman [6].

There are two good reasons for giving a new derivation of the Lloyd–Berry formula. First, our analysis clarifies the assumptions that lead to (1.6). Second, erroneous formulas (such as (1.4) or (1.5)) continue to be used widely, perhaps because they are simpler than (1.6) or perhaps because the original derivation in [19] seems suspect. For some representative applications, see [14, 2, 20] and [21, chapter 4].

The paper begins with a brief summary of some elementary probability theory. The pair-correlation function is introduced, including the notion of "hole correction", which ensures that spheres do not overlap during the averaging process. In §3, we consider isotropic scatterers, and derive the integral equations of Foldy (independent scatterers, no hole correction) and of Lax (hole correction included). Foldy's equation is solved exactly. A method is developed in §3.2 for obtaining an expression for $K$ which does not require an exact solution of the integral equation, merely an assumption that an effective wavenumber can be used at some distance from the "interface" at $z = 0$ between the homogeneous region ($z < 0$) and the region occupied by many small scatterers ($z > 0$). The virtue of this method is that it succeeds when the governing integral equation cannot be solved exactly. Thus, in §3.3, we obtain an expression for $K$ from Lax's integral equation; Foldy's approximation is recovered when the hole correction is removed. The same method is used in §4 but without the restriction to isotropic scatterers. We start with an exact, deterministic theory for acoustic scattering by $N$ spheres; the spheres can be soft, hard, or penetrable. We combine multipole solutions in spherical polar coordinates with an appropriate addition theorem. This method is well known; for some recent applications, see [15, 9, 11]. The exact system of equations is then subjected to ensemble averaging in §4.3; Lax's "quasi-crystalline approximation" [17] is invoked. This leads to a homogeneous infinite system of linear algebraic equations; the existence of a non-trivial solution determines $K$. We solve the system for small $n_0$ and recover the Lloyd–Berry formula.

An analogous theory can be developed in two dimensions, and leads to a result that is reminiscent of the Lloyd–Berry formula [18]. However, the three-dimensional calculations described below are much more complicated, as they involve addition theorems for spherical wavefunctions and properties of spherical harmonics. Nevertheless, the final results are rather simple.

**2. Some probability theory.** In this section, we give a very brief summary of the probability theory needed. For more information, see [7], [16] or chapter 14 of [12].

Suppose we have $N$ scatterers located at the points $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N$; denote the configuration of points by $\Lambda_N = \{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N\}$. Then, the ensemble (or configurational) average of any quantity $F(\boldsymbol{r}|\Lambda_N)$ is defined by

$$\langle F(\boldsymbol{r})\rangle = \int \cdots \int p(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)\, F(\boldsymbol{r}|\Lambda_N)\, \mathrm{d}V_1 \cdots \mathrm{d}V_N, \tag{2.1}$$

where the the integration is over $N$ copies of the volume $B_N$ containing $N$ scatterers. Here, $p(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)\, \mathrm{d}V_1\, \mathrm{d}V_2 \cdots \mathrm{d}V_N$ is the probability of finding the scatterers in a configuration in which the first scatterer is in the volume element $\mathrm{d}V_1$ about $\boldsymbol{r}_1$, the second scatterer is in the volume element $\mathrm{d}V_2$ about $\boldsymbol{r}_2$, and so on, up to $\boldsymbol{r}_N$. The joint probability distribution $p(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ is normalized so that $\langle 1\rangle = 1$. Similarly, the average of $F(\boldsymbol{r}|\Lambda_N)$ over all configurations for which the first scatterer is fixed at $\boldsymbol{r}_1$ is given by

$$\langle F(\boldsymbol{r})\rangle_1 = \int \cdots \int p(\boldsymbol{r}_2, \ldots, \boldsymbol{r}_N|\boldsymbol{r}_1)\, F(\boldsymbol{r}|\Lambda_N)\, \mathrm{d}V_2 \cdots \mathrm{d}V_N, \tag{2.2}$$

where the conditional probability $p(\boldsymbol{r}_2, \ldots, \boldsymbol{r}_N|\boldsymbol{r}_1)$ is defined by $p(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = p(\boldsymbol{r}_1)\, p(\boldsymbol{r}_2, \ldots, \boldsymbol{r}_N|\boldsymbol{r}_1)$. If two scatterers are fixed, say the first and the second, we can define

$$\langle F(\boldsymbol{r})\rangle_{12} = \int \cdots \int p(\boldsymbol{r}_3, \ldots, \boldsymbol{r}_N|\boldsymbol{r}_1, \boldsymbol{r}_2)\, F(\boldsymbol{r}|\Lambda_N)\, \mathrm{d}V_3 \cdots \mathrm{d}V_N, \tag{2.3}$$

where $p(\boldsymbol{r}_2, \ldots, \boldsymbol{r}_N|\boldsymbol{r}_1) = p(\boldsymbol{r}_2|\boldsymbol{r}_1)\, p(\boldsymbol{r}_3, \ldots, \boldsymbol{r}_N|\boldsymbol{r}_1, \boldsymbol{r}_2)$.

As each of the $N$ scatterers is equally likely to occupy $\mathrm{d}V_1$, the density of scatterers at $\boldsymbol{r}_1$ is $Np(\boldsymbol{r}_1) = n_0$, the (constant) number of scatterers per unit volume. Thus

$$p(\boldsymbol{r}) = n_0/N = |B_N|^{-1}, \tag{2.4}$$

where $|B_N|$ is the volume of $B_N$. For spheres of radius $a$, the simplest sensible choice for the pair-correlation function is

$$p(\boldsymbol{r}_2|\boldsymbol{r}_1) = (n_0/N)H(R_{12} - b), \quad \text{where } R_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2| \tag{2.5}$$

and $H$ is the Heaviside unit function: $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x < 0$. The parameter $b$ (the "hole radius") satisfies $b \geq 2a$ so that spheres are not allowed to overlap.

**3. Foldy–Lax theory: isotropic scatterers.** Foldy's theory [7] begins with a simplified deterministic model for scattering by $N$ identical scatterers, each of which is supposed to scatter isotropically. Thus, the total field is assumed to be given by the incident field plus a point source at each scattering center, $\boldsymbol{r}_j$:

$$u(\boldsymbol{r}|\Lambda_N) = u_{\text{in}}(\boldsymbol{r}) + g\sum_{j=1}^{N} u_{\text{ex}}(\boldsymbol{r}_j;\boldsymbol{r}_j|\Lambda_N)\, h_0(k|\boldsymbol{r} - \boldsymbol{r}_j|). \tag{3.1}$$

Here, $h_n(w) \equiv h_n^{(1)}(w)$ is a spherical Hankel function, $g$ is the (assumed known) scattering coefficient, and the exciting field $u_{\text{ex}}$ is given by

$$u_{\text{ex}}(\boldsymbol{r};\boldsymbol{r}_n|\Lambda_N) = u_{\text{in}}(\boldsymbol{r}) + g\sum_{\substack{j=1\\ j\neq n}}^{N} u_{\text{ex}}(\boldsymbol{r}_j;\boldsymbol{r}_j|\Lambda_N)\, h_0(k|\boldsymbol{r} - \boldsymbol{r}_j|); \tag{3.2}$$

the $N$ numbers $u_{\text{ex}}(\boldsymbol{r}_j;\boldsymbol{r}_j|\Lambda_N)$ $(j = 1, 2, \ldots, N)$ required in (3.1) are to be determined by solving the linear system obtained by evaluating (3.2) at $\boldsymbol{r} = \boldsymbol{r}_n$.

If we try to compute the ensemble average of $u$, using (3.1) and (2.1), we obtain

$$\langle u(\boldsymbol{r})\rangle = u_{\text{in}}(\boldsymbol{r}) + gn_0\int_{B_N} \langle u_{\text{ex}}(\boldsymbol{r}_1)\rangle_1\, h_0(k|\boldsymbol{r} - \boldsymbol{r}_1|)\,\mathrm{d}V_1, \tag{3.3}$$

where we have used (2.2), (2.4) and the indistinguishability of the scatterers. For $\langle u_{\text{ex}}(\boldsymbol{r}_1)\rangle_1$, we obtain

$$\langle u_{\text{ex}}(\boldsymbol{r})\rangle_1 = u_{\text{in}}(\boldsymbol{r}) + g(N-1)\int_{B_N} p(\boldsymbol{r}_2|\boldsymbol{r}_1)\,\langle u_{\text{ex}}(\boldsymbol{r}_2)\rangle_{12}\, h_0(k|\boldsymbol{r} - \boldsymbol{r}_2|)\,\mathrm{d}V_2, \tag{3.4}$$

where we have used (2.3) and (3.2). Equations (3.3) and (3.4) are the first two in a hierarchy, involving more and more complicated information on the statistics of the scatterer distribution. In practice, the hierarchy is broken using an additional assumption. At the lowest level, we have Foldy's assumption,

$$\langle u_{\text{ex}}(\boldsymbol{r})\rangle_1 \simeq \langle u(\boldsymbol{r})\rangle, \tag{3.5}$$

at least in the neighborhood of $\boldsymbol{r}_1$. When this is used in (3.3), we obtain

$$\langle u(\boldsymbol{r})\rangle = u_{\text{in}}(\boldsymbol{r}) + gn_0\int_{B_N} \langle u(\boldsymbol{r}_1)\rangle\, h_0(k|\boldsymbol{r} - \boldsymbol{r}_1|)\,\mathrm{d}V_1, \quad \boldsymbol{r} \in B_N. \tag{3.6}$$

We call this *Foldy's integral equation* for $\langle u \rangle$. The integral on the right-hand side is an acoustic volume potential. Hence, an application of $(\nabla^2 + k^2)$ to (3.6) eliminates the incident field and shows that $(\nabla^2 + K^2)\langle u \rangle = 0$ in $B_N$, where $K^2$ is given by Foldy's formula, (1.1).

At the next level, we have Lax's quasi-crystalline assumption (QCA) [17],

$$\langle u_{\text{ex}}(\boldsymbol{r})\rangle_{12} \simeq \langle u_{\text{ex}}(\boldsymbol{r})\rangle_{2}. \tag{3.7}$$

When this is used in (3.4) evaluated at $\boldsymbol{r} = \boldsymbol{r}_1$, we obtain

$$v(\boldsymbol{r}) = u_{\text{in}}(\boldsymbol{r}) + g(N-1)\int_{B_N} p(\boldsymbol{r}_1|\boldsymbol{r})\, v(\boldsymbol{r}_1)\, h_0(k|\boldsymbol{r}-\boldsymbol{r}_1|)\,\mathrm{d}V_1, \quad \boldsymbol{r} \in B_N, \tag{3.8}$$

where $v(\boldsymbol{r}) = \langle u_{\text{ex}}(\boldsymbol{r})\rangle_1$. We call this *Lax's integral equation.*

In what follows, we let $N \to \infty$ so that $B_N \to B_\infty$, a semi-infinite region, $z > 0$.

**3.1. Foldy's integral equation: exact treatment.** Consider a plane wave at oblique incidence, so that

$$u_{\text{in}} = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\alpha z}\exp(\mathrm{i}\boldsymbol{k}_T\cdot\boldsymbol{q}) \tag{3.9}$$

where $\boldsymbol{r} = (x, y, z)$, $\boldsymbol{q} = (x, y, 0)$, $\boldsymbol{k} = \boldsymbol{k}_T + \alpha\hat{\mathbf{z}}$, $\hat{\mathbf{z}} = (0, 0, 1)$, the wavenumber vector $\boldsymbol{k}$ is given in spherical polar coordinates by

$$\boldsymbol{k} = k\hat{\boldsymbol{k}} \quad \text{with} \quad \hat{\boldsymbol{k}} = (\sin\theta_{\text{in}}\,\cos\phi_{\text{in}},\ \sin\theta_{\text{in}}\,\sin\phi_{\text{in}},\ \cos\theta_{\text{in}}), \quad 0 \le \theta_{\text{in}} < \pi/2,$$

$\alpha = k\cos\theta_{\text{in}}$ and $\boldsymbol{k}_T$ is the transverse wavenumber vector, satisfying $\boldsymbol{k}_T\cdot\hat{\mathbf{z}} = 0$.

For a semi-infinite domain $B_\infty$ $(z > 0)$, Foldy's integral equation (3.6) becomes

$$\langle u(x,y,z)\rangle = u_{\text{in}}(x,y,z) + gn_0\int_0^\infty\int_{-\infty}^\infty\int_{-\infty}^\infty \langle u(x+X, y+Y, z_1)\rangle\, h_0(k\varrho_1)\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}z_1,$$

for $0 \le |x| < \infty$, $0 \le |y| < \infty$ and $z > 0$, where $\varrho_1 = \sqrt{X^2 + Y^2 + (z-z_1)^2}$. This equation can be solved exactly. Thus, writing

$$\langle u(x,y,z)\rangle = U(z)\,\exp(\mathrm{i}\boldsymbol{k}_T\cdot\boldsymbol{q}), \quad 0 \le |\boldsymbol{q}| < \infty, \quad z > 0, \tag{3.10}$$

we obtain

$$U(z) = \mathrm{e}^{\mathrm{i}\alpha z} + gn_0\int_0^\infty\int_{-\infty}^\infty\int_{-\infty}^\infty U(z_1)\,h_0(k\varrho_1)\,\exp(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q})\,\mathrm{d}X\,\mathrm{d}Y\,\mathrm{d}z_1 \tag{3.11}$$

for $z > 0$, where $\mathbf{Q} = (X, Y, 0)$.

In Appendix B, it is shown that

$$\int_{-\infty}^\infty\int_{-\infty}^\infty h_0(k\varrho_1)\,\exp(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q})\,\mathrm{d}X\,\mathrm{d}Y = \frac{2\pi}{k\alpha}\,\mathrm{e}^{\mathrm{i}\alpha|z-z_1|}. \tag{3.12}$$

Thus, we see that $U$ solves

$$U(z) = \mathrm{e}^{\mathrm{i}\alpha z} + \frac{2\pi gn_0}{k\alpha}\int_0^\infty U(z_1)\,\mathrm{e}^{\mathrm{i}\alpha|z-z_1|}\,\mathrm{d}z_1, \quad z > 0. \tag{3.13}$$

Now, put $U(z) = U_0\,\mathrm{e}^{\mathrm{i}\lambda z}$, so that (3.13) gives

$$U_0\,\mathrm{e}^{\mathrm{i}\lambda z} - \mathrm{e}^{\mathrm{i}\alpha z} = \frac{2\pi gn_0}{\mathrm{i}k\alpha}U_0\left(\frac{2\alpha\mathrm{e}^{\mathrm{i}\lambda z}}{\lambda^2-\alpha^2} - \frac{\mathrm{e}^{\mathrm{i}\alpha z}}{\lambda-\alpha}\right),$$

where we have assumed that $\operatorname{Im}\lambda > 0$. If we compare the coefficients of $\mathrm{e}^{\mathrm{i}\lambda z}$, we see that $U_0$ cancels, leaving

$$\lambda^2 - \alpha^2 = -4\pi \mathrm{i} g n_0 / k, \tag{3.14}$$

which determines $\lambda$. Then, the coefficients of $\mathrm{e}^{\mathrm{i}\alpha z}$ give $U_0 = 2\alpha/(\lambda + \alpha)$. A similar method can be used to find $\langle u \rangle$ when $B_\infty$ is a slab of finite thickness, $0 < z < h$.

It is natural to define an effective wavenumber vector by

$$\begin{aligned} \mathbf{K} &= K(\sin\vartheta\cos\varphi,\ \sin\vartheta\sin\varphi,\ \cos\vartheta) = K\hat{\mathbf{K}} \\ &= (k\sin\theta_{\text{in}}\cos\phi_{\text{in}},\ k\sin\theta_{\text{in}}\sin\phi_{\text{in}},\ \lambda), \end{aligned} \tag{3.15}$$

whence

$$\lambda = K\cos\vartheta \quad \text{and} \quad K\sin\vartheta = k\sin\theta_{\text{in}}. \tag{3.16}$$

The last equality is recognized as Snell's law, even though $K$ and $\vartheta$ are complex, with $\operatorname{Im} K > 0$. Hence, we see that

$$\lambda^2 - \alpha^2 = K^2 - k^2, \tag{3.17}$$

whence (3.14) reduces to Foldy's formula (1.1).

**3.2. Foldy's integral equation: alternative treatment.** We have seen that Foldy's integral equation can be solved exactly, and that the solution process has two parts: first find $\lambda$ (and hence the effective wavenumber) and then find $U_0$. In fact, $\lambda$ can be found without finding the complete solution; the reason for pursuing this is that we cannot usually find exact solutions. Thus, consider (3.13), and suppose that

$$U(z) = U_0\mathrm{e}^{\mathrm{i}\lambda z} \quad \text{for } z > \ell,$$

where $U_0$, $\lambda$ and $\ell$ are unknown. To proceed, we need say nothing about the solution $U$ in the "boundary layer" $0 < z < \ell$. Now, evaluate the integral equation for $z > \ell$; we find that

$$\begin{aligned} U_0\,\mathrm{e}^{\mathrm{i}\lambda z} - \mathrm{e}^{\mathrm{i}\alpha z} &= \frac{2\pi g n_0}{k\alpha}\,\mathrm{e}^{\mathrm{i}\alpha z}\int_0^\ell U(t)\,\mathrm{e}^{-\mathrm{i}\alpha t}\,\mathrm{d}t + \frac{2\pi g n_0}{k\alpha}\int_\ell^\infty U(t)\,\mathrm{e}^{\mathrm{i}\alpha|z-t|}\,\mathrm{d}t \\ &= \mathcal{A}\,\mathrm{e}^{\mathrm{i}\lambda z} + \mathcal{B}\,\mathrm{e}^{\mathrm{i}\alpha z} \quad \text{for } z > \ell, \end{aligned}$$

where $\mathcal{A} = -4\pi\mathrm{i} g n_0 U_0/[k(\lambda^2 - \alpha^2)]$ and

$$\mathcal{B} = \frac{2\pi g n_0}{k\alpha}\int_0^\ell U(t)\,\mathrm{e}^{-\mathrm{i}\alpha t}\,\mathrm{d}t + \frac{2\pi\mathrm{i} g n_0 U_0}{k\alpha(\lambda - \alpha)}\,\mathrm{e}^{\mathrm{i}(\lambda-\alpha)\ell}.$$

Then, setting $U_0 = \mathcal{A}$ gives (3.14) again, without knowing the solution $U$ everywhere. This basic method will be used again below.

**3.3. Lax's integral equation.** Using (2.5) for $p(\boldsymbol{r}_1|\boldsymbol{r})$ in (3.8) gives

$$v(\boldsymbol{r}) = u_{\text{in}}(\boldsymbol{r}) + g n_0\,\frac{N-1}{N}\int_{B_N^b} v(\boldsymbol{r}_1)\,h_0(kR_1)\,\mathrm{d}\boldsymbol{r}_1, \quad \boldsymbol{r} \in B_N, \tag{3.18}$$

where $B_N^b(\boldsymbol{r}) = \{\boldsymbol{r}_1 \in B_N : R_1 = |\boldsymbol{r} - \boldsymbol{r}_1| > b\}$, which is $B_N$ with a (possibly incomplete) ball excluded.

Let $N \to \infty$ and take an incident plane wave, (3.9), giving

$$v(x,y,z) = \mathrm{e}^{\mathrm{i}\alpha z} \exp(\mathrm{i}\boldsymbol{k}_T \cdot \boldsymbol{q}) + gn_0 \int_{z_1>0,\ \varrho_1>b} v(x+X, y+Y, z_1)\, h_0(k\varrho_1)\, \mathrm{d}X\, \mathrm{d}Y\, \mathrm{d}z_1,$$

for $0 \le |\boldsymbol{q}| < \infty$ and $z > 0$. As in §3.1, we write

$$v(x,y,z) = V(z)\, \exp(\mathrm{i}\boldsymbol{k}_T \cdot \boldsymbol{q}), \quad 0 \le |\boldsymbol{q}| < \infty, \quad z > 0, \tag{3.19}$$

giving

$$V(z) = \mathrm{e}^{\mathrm{i}\alpha z} + gn_0 \int_{z_1>0,\ \varrho_1>b} V(z_1)\, h_0(k\varrho_1)\, \exp(\mathrm{i}\boldsymbol{k}_T \cdot \mathbf{Q})\, \mathrm{d}X\, \mathrm{d}Y\, \mathrm{d}z_1, \tag{3.20}$$

for $0 \le |\boldsymbol{q}| < \infty$ and $z > 0$. Then, using (3.12), we see that $V$ solves

$$V(z) = \mathrm{e}^{\mathrm{i}\alpha z} + gn_0 \int_0^\infty V(z_1)\, \mathcal{L}(z-z_1)\, \mathrm{d}z_1, \quad z > 0, \tag{3.21}$$

where the kernel, $\mathcal{L}(z-z_1)$, is given by

$$\begin{aligned} \mathcal{L}(Z) &= \frac{2\pi}{k\alpha}\mathrm{e}^{\mathrm{i}\alpha|Z|} - \int_0^{c(Z)} \int_0^{2\pi} h_0(k\sqrt{Q^2+Z^2})\mathrm{e}^{\mathrm{i}kQ\sin\theta_{\mathrm{in}}\cos(\Phi-\phi_{\mathrm{in}})} Q\, \mathrm{d}\Phi\, \mathrm{d}Q \\ &= \frac{2\pi}{k\alpha}\, \mathrm{e}^{\mathrm{i}\alpha|Z|} - 2\pi \int_0^{c(Z)} h_0(k\sqrt{Q^2+Z^2})\, J_0(kQ\sin\theta_{\mathrm{in}})\, Q\, \mathrm{d}Q \end{aligned} \tag{3.22}$$

with $c(Z) = \sqrt{b^2 - Z^2}\, H(b - |Z|)$; here, $J_n$ is a Bessel function and we have written the double integral over $X$ and $Y$ in (3.20) as an integral over all $X$ and $Y$ minus an integral through the cross-section of the ball at $z$, if necessary.

We have been unable to solve (3.21) exactly. However, the alternative method described in §3.2 can be used. Thus, let us suppose that

$$V(z) = V_0\, \mathrm{e}^{\mathrm{i}\lambda z} \quad \text{for } z > \ell, \tag{3.23}$$

where $V_0$, $\lambda$ and $\ell$ are unknown. Then, consider (3.21) for $z > \ell + b$, so that the interval $|z - z_1| < b$ is entirely within the range $z_1 > \ell$. Using (3.22), (3.21) gives

$$\begin{aligned} \frac{V_0\, \mathrm{e}^{\mathrm{i}\lambda z} - \mathrm{e}^{\mathrm{i}\alpha z}}{gn_0} &= \frac{2\pi}{k\alpha}\, \mathrm{e}^{\mathrm{i}\alpha z} \int_0^\ell V(t)\, \mathrm{e}^{-\mathrm{i}\alpha t}\, \mathrm{d}t + \frac{2\pi}{k\alpha} \int_\ell^\infty V(t)\, \mathrm{e}^{\mathrm{i}\alpha|z-t|}\, \mathrm{d}t \\ &\quad - 2\pi \int_{z-b}^{z+b} V(t) \int_0^{c(z-t)} h_0(k\sqrt{Q^2+(z-t)^2})\, J_0(kQ\sin\theta_{\mathrm{in}})\, Q\, \mathrm{d}Q\, \mathrm{d}t \end{aligned} \tag{3.24}$$

for $z > \ell + b$. Equation (3.23) can be used in the second and third integrals. The second integral is elementary, and has the value

$$\frac{2\pi\mathrm{i}V_0}{k\alpha} \left\{ \frac{\mathrm{e}^{\mathrm{i}(\lambda-\alpha)\ell}}{\lambda-\alpha}\, \mathrm{e}^{\mathrm{i}\alpha z} - \frac{2\alpha}{\lambda^2-\alpha^2}\, \mathrm{e}^{\mathrm{i}\lambda z} \right\}.$$

Denote the third integral in (3.24) by $I_3$; we have

$$\begin{aligned} I_3 &= -2\pi V_0 \int_{-b}^{b} \mathrm{e}^{\mathrm{i}\lambda(z+\xi)} \int_0^{\sqrt{b^2-\xi^2}} h_0(k\sqrt{Q^2+\xi^2})\, J_0(kQ\sin\theta_{\mathrm{in}})\, Q\, \mathrm{d}Q\, \mathrm{d}\xi \\ &= -2\pi V_0\, \mathrm{e}^{\mathrm{i}\lambda z} \int_0^\pi \int_0^b \mathrm{e}^{\mathrm{i}\lambda r\cos\theta}\, h_0(kr)\, J_0(kr\sin\theta\sin\theta_{\mathrm{in}})\, r^2 \sin\theta\, \mathrm{d}r\, \mathrm{d}\theta \\ &= -V_0\, \mathrm{e}^{\mathrm{i}\lambda z} \int_0^{2\pi} \int_0^\pi \int_0^b \mathrm{e}^{\mathrm{i}r[\lambda\cos\theta + k\sin\theta\sin\theta_{\mathrm{in}}\cos(\phi-\phi_{\mathrm{in}})]}\, h_0(kr)\, r^2 \sin\theta\, \mathrm{d}r\, \mathrm{d}\theta\, \mathrm{d}\phi. \end{aligned}$$

Using (3.16), the exponent simplifies to $\mathbf{K}\cdot\boldsymbol{r}$, whence

$$\begin{aligned}
I_3 &= -V_0\,\mathrm{e}^{\mathrm{i}\lambda z}\int_{r<b} \exp\left(\mathrm{i}\mathbf{K}\cdot\boldsymbol{r}\right) h_0(k|\boldsymbol{r}|)\,\mathrm{d}V(\boldsymbol{r}) \\
&= -2\pi V_0\,\mathrm{e}^{\mathrm{i}\lambda z}\int_0^b\int_0^\pi \frac{\mathrm{e}^{\mathrm{i}kr}}{\mathrm{i}kr}\,\mathrm{e}^{\mathrm{i}Kr\cos\theta}\,r^2\sin\theta\,\mathrm{d}\theta\,\mathrm{d}r \\
&= \frac{2\pi V_0}{kK}\,\mathrm{e}^{\mathrm{i}\lambda z}\int_0^b \mathrm{e}^{\mathrm{i}kr}\left(\mathrm{e}^{\mathrm{i}Kr}-\mathrm{e}^{-\mathrm{i}Kr}\right)\mathrm{d}r = \frac{4\pi\mathrm{i}V_0}{k(K^2-k^2)}\,\mathrm{e}^{\mathrm{i}\lambda z}\{1-\mathcal{N}_0(Kb)\},
\end{aligned}$$

where $\mathcal{N}_0(x) = \mathrm{e}^{\mathrm{i}kb}\{\cos x - \mathrm{i}(kb/x)\sin x\}$. Using these results in (3.24), noting (3.17), we obtain

$$V_0\,\mathrm{e}^{\mathrm{i}\lambda z} - \mathrm{e}^{\mathrm{i}\alpha z} = \mathcal{A}\,\mathrm{e}^{\mathrm{i}\lambda z} + \mathcal{B}\,\mathrm{e}^{\mathrm{i}\alpha z} \quad \text{for } z > \ell + b,$$

where

$$\mathcal{A} = \frac{4\pi\mathrm{i}gn_0V_0}{k(k^2-K^2)}\,\mathcal{N}_0(Kb), \quad \mathcal{B} = \frac{2\pi gn_0}{k\alpha}\int_0^\ell V(t)\,\mathrm{e}^{-\mathrm{i}\alpha t}\,\mathrm{d}t + \frac{2\pi\mathrm{i}gn_0V_0}{k\alpha(\lambda-\alpha)}\,\mathrm{e}^{\mathrm{i}(\lambda-\alpha)\ell}.$$

For a solution, we must have $\mathcal{A} = V_0$, whence

$$K^2 = k^2 - 4\pi\mathrm{i}g(n_0/k)\,\mathcal{N}_0(Kb), \tag{3.25}$$

which is a nonlinear equation for $K$. Notice that this equation does not depend on the angle of incidence, $\theta_{\mathrm{in}}$.

We have $\mathcal{N}_0(Kb) \to 1$ as $Kb \to 0$ so that, in this limit, we recover Foldy's formula for the effective wavenumber, (1.1).

Let us solve (3.25) for small $n_0$. (We could use the dimensionless volume fraction $\frac{4}{3}\pi a^3 n_0$, but it is customary to use $n_0$.) Begin by writing

$$K^2 = k^2 + \delta_1 n_0 + \delta_2 n_0^2 + \cdots, \tag{3.26}$$

where $\delta_1$ and $\delta_2$ are to be found; for $\delta_1$, we expect to obtain the result given by (1.1). It follows that $K = k + \frac{1}{2}\delta_1 n_0/k + O(n_0^2)$ and then

$$\begin{aligned}
\mathcal{N}_0(Kb) &= \mathcal{N}_0(kb) + (Kb-kb)\mathcal{N}_0'(kb) + \cdots \\
&= 1 - \tfrac{1}{2}\mathrm{i}b(n_0/k)\delta_1 d_0(kb) + O(n_0^2),
\end{aligned}$$

where $d_0(x) = 1 - x^{-1}\mathrm{e}^{\mathrm{i}x}\sin x$. When this approximation for $\mathcal{N}_0(Kb)$ is used in (3.25), we obtain

$$K^2 = k^2 - 4\pi\mathrm{i}gn_0/k - 2\pi bg(n_0/k)^2\delta_1 d_0(kb).$$

Comparison of this formula with (3.26) gives $\delta_1 = -4\pi\mathrm{i}g/k$ (as expected) and $\delta_2 = 8\pi^2\mathrm{i}g^2bk^{-3}d_0(kb)$, so that we obtain the approximation

$$K^2 = k^2 - \frac{4\pi\mathrm{i}g}{k}n_0 + \frac{8\mathrm{i}b(\pi gn_0)^2}{k^3}\left(1 - \mathrm{e}^{\mathrm{i}kb}\frac{\sin kb}{kb}\right). \tag{3.27}$$

(Recall that a common choice for the hole radius is $b = 2a$.) As far as we know, the formula (3.27) is new. Note that the second-order term in (3.27) vanishes in the limit $kb \to 0$.

**4. A finite array of identical spheres: exact theory.** Let $O$ be the origin of three-dimensional Cartesian coordinates, so that a typical point has position vector $\boldsymbol{r} = (x, y, z)$ with respect to $O$. Define spherical polar coordinates $(r, \theta, \phi)$ at $O$, so that $\boldsymbol{r} = r\hat{\boldsymbol{r}} = r(\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta)$. We consider $N$ identical spheres, $S_j$, $j = 1, 2, \ldots, N$. The sphere $S_j$ has radius $a$ and center $O_j$ at $\boldsymbol{r} = \boldsymbol{r}_j$. We define spherical polar coordinates $(\rho_j, \theta_j, \phi_j)$ at $O_j$, so that $\boldsymbol{r} = \boldsymbol{\rho}_j + \boldsymbol{r}_j$ with

$$\boldsymbol{\rho}_j = \rho_j\hat{\boldsymbol{\rho}}_j = \rho_j(\sin\theta_j\cos\phi_j,\ \sin\theta_j\sin\phi_j,\ \cos\theta_j).$$

We assume that $\theta_j = 0$ is in the $z$-direction ($\theta = 0$).

Exterior to the spheres the pressure field is $u$, where

$$\nabla^2 u + k^2 u = 0. \tag{4.1}$$

Inside $S_j$, the field is $u_j$, where

$$\nabla^2 u_j + \kappa^2 u_j = 0, \tag{4.2}$$

$\kappa = \omega/\tilde{c}$ and $\tilde{c}$ is the sound speed inside the spheres. The transmission conditions on the spheres are

$$u = u_j, \qquad \frac{1}{\rho}\frac{\partial u}{\partial \rho_j} = \frac{1}{\tilde{\rho}}\frac{\partial u_j}{\partial \rho_j} \quad \text{on} \quad \rho_j = a, \quad j = 1, \ldots, N, \tag{4.3}$$

where $\tilde{\rho}$ is the fluid density inside the spheres.

A plane wave, given by (3.9), is incident on the spheres. The problem is to calculate the scattered field outside the spheres, defined as $u_{\mathrm{sc}} = u - u_{\mathrm{in}}$. We start with just one sphere, in order to fix our notation.

**4.1. Scattering by one sphere.** For the incident plane wave, we have

$$u_{\mathrm{in}}(\boldsymbol{r}) = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) = 4\pi\sum_{n,m} \mathrm{i}^n \hat{\psi}_n^m(\boldsymbol{r})\,\overline{Y_n^m(\hat{\boldsymbol{k}})}, \tag{4.4}$$

where $\hat{\psi}_n^m(\boldsymbol{r}) = j_n(kr)Y_n^m(\hat{\boldsymbol{r}})$, $j_n(w)$ is a spherical Bessel function, $Y_n^m(\hat{\boldsymbol{r}}) = Y_n^m(\theta, \phi)$ is a spherical harmonic (see Appendix A), the overbar denotes complex conjugation and we have used the shorthand notation

$$\sum_{n,m} \equiv \sum_{n=0}^{\infty}\sum_{m=-n}^{n}.$$

With our choice of normalization, the spherical harmonics are orthonormal; see (A.1).

For the scattered and interior fields, we can write

$$u_{\mathrm{sc}}(\boldsymbol{r}) = 4\pi\sum_{n,m} \mathrm{i}^n A_n^m Z_n \psi_n^m(\boldsymbol{r}) \quad \text{and} \quad u_{\mathrm{int}}(\boldsymbol{r}) = 4\pi\sum_{n,m} \mathrm{i}^n B_n^m j_n(\kappa r)\, Y_n^m(\hat{\boldsymbol{r}}),$$

respectively, where $\psi_n^m(\boldsymbol{r}) = h_n(kr)\, Y_n^m(\hat{\boldsymbol{r}})$, the coefficients $A_n^m$ and $B_n^m$ are to be found, and the factor

$$Z_n = \frac{q j_n'(ka) j_n(\kappa a) - j_n(ka) j_n'(\kappa a)}{q h_n'(ka) j_n(\kappa a) - h_n(ka) j_n'(\kappa a)}, \tag{4.5}$$

with $q = \tilde{\rho}\tilde{c}/(\rho c)$, has been introduced for later convenience. Then, the transmission conditions on $r = a$ yield $A_n^m$ and $B_n^m$; in particular, we obtain $A_n^m = -\overline{Y_n^m(\hat{\boldsymbol{k}})}$. Also, the far-field pattern, defined by (1.3), is given by

$$f(\Theta) = 4\pi \sum_{n,m} Z_n A_n^m \, Y_n^m(\hat{\boldsymbol{r}}) = -\sum_{n=0}^{\infty} (2n+1) Z_n P_n(\cos\Theta), \tag{4.6}$$

where $\cos\Theta = \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{k}}$ and we have used (A.3) in order to evaluate the sum over $m$. Note that we recover the sound-soft results in the limit $q \to 0$, whereas the limit $q \to \infty$ gives the sound-hard results.

**4.2. Scattering by $N$ spheres.** A phase factor for each sphere is defined by $I_j = \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}_j)$, and then we can write

$$u_{\text{in}} = I_j \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\rho}_j) = 4\pi I_j \sum_{n,m} \mathrm{i}^n \hat{\psi}_n^m(\boldsymbol{\rho}_j) \, \overline{Y_n^m(\hat{\boldsymbol{k}})}. \tag{4.7}$$

We seek a solution to (4.1) and (4.2) in the form

$$u = u_{\text{in}} + 4\pi \sum_{j=1}^{N} \sum_{n,m} \mathrm{i}^n A_{nj}^m Z_n \psi_n^m(\boldsymbol{\rho}_j), \quad u_j = 4\pi \sum_{n,m} \mathrm{i}^n B_{nj}^m \, j_n(\kappa\rho_j) \, Y_n^m(\hat{\boldsymbol{\rho}}_j),$$

for some set of unknown complex coefficients $A_{nj}^m$ and $B_{nj}^m$.

Now, in order to apply the transmission conditions on each sphere, we shall need an *addition theorem.* Thus, given vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c} = \boldsymbol{a} + \boldsymbol{b}$, we have

$$\psi_n^m(\boldsymbol{c}) = \sum_{\nu,\mu} S_{n\nu}^{m\mu}(\boldsymbol{b}) \, \hat{\psi}_\nu^\mu(\boldsymbol{a}) \quad \text{for } |\boldsymbol{a}| < |\boldsymbol{b}|, \tag{4.8}$$

where the separation matrix $S_{\nu n}^{\mu m}$ is given by

$$S_{\nu n}^{\mu m}(\mathbf{R}) = 4\pi \mathrm{i}^{n-\nu} (-1)^m \sum_q \mathrm{i}^q \psi_q^{\mu-m}(\mathbf{R}) \, \mathcal{G}(n, m; \nu, -\mu; q). \tag{4.9}$$

In this formula, $\mathcal{G}$ is a Gaunt coefficient (defined by (A.5)) and the sum has a finite number of terms; in fact, $q$ runs from $|n-\nu|$ to $(n+\nu)$ in steps of 2, so that

$$(q + n + \nu) \text{ is even.} \tag{4.10}$$

For more information on the addition theorem, see [3, 9, 10] and references therein.

Let $\mathbf{R}_{sj} = \boldsymbol{r}_s - \boldsymbol{r}_j = \boldsymbol{\rho}_j - \boldsymbol{\rho}_s$ be the position vector of $O_s$ with respect to $O_j$. Then, provided that $\rho_s < R_{sj} = |\mathbf{R}_{sj}|$ for all $j$, we can write the field exterior to the sphere $S_s$ as

$$\begin{aligned} u = {} & 4\pi \sum_{n,m} \mathrm{i}^n \left\{ I_s \hat{\psi}_n^m(\boldsymbol{\rho}_s) \, \overline{Y_n^m(\hat{\boldsymbol{k}})} + A_{ns}^m Z_n \psi_n^m(\boldsymbol{\rho}_s) \right\} \\ & + 4\pi \sum_{n,m} \hat{\psi}_n^m(\boldsymbol{\rho}_s) \sum_{\substack{j=1 \\ j \neq s}}^{N} \sum_{\nu,\mu} \mathrm{i}^\nu A_{\nu j}^\mu Z_\nu S_{\nu n}^{\mu m}(\mathbf{R}_{sj}). \end{aligned} \tag{4.11}$$

The geometrical restriction implies that this expression is valid near the surface of $S_s$ and so (4.11) can be used to apply the transmission conditions on $\rho_s = a$. Thus, after using the orthogonality of the functions $Y_n^m(\hat{\boldsymbol{\rho}}_s)$, (A.1), and then eliminating the coefficients $B_{nj}^m$, we obtain

$$A_{ns}^m + \sum_{\substack{j=1\\ j\neq s}}^{N} \sum_{\nu,\mu} \mathrm{i}^{\nu-n} A_{\nu j}^{\mu} Z_\nu S_{\nu n}^{\mu m}(\mathbf{R}_{sj}) = -I_s \overline{Y_n^m(\hat{\boldsymbol{k}})}, \qquad \begin{array}{l} s = 1, 2, \ldots, N, \\ n = 0, 1, 2, \ldots, \\ m = -n, \ldots, n, \end{array} \tag{4.12}$$

an infinite linear system of equations for $A_{nj}^m$. Note that the quantities $q$, $\kappa$ and $a$ only enter the equations through the terms $Z_\nu$.

**4.3. Arrays of spheres: averaged equations.** The above analysis applies to a specific configuration of scatterers. Now we take ensemble averages. Specifically, setting $s = 1$ in (4.12) and then taking the conditional average, using (2.5), we obtain

$$\langle A_{n1}^m \rangle_1 + n_0 \frac{N-1}{N} \sum_{\nu,\mu} \mathrm{i}^{\nu-n} Z_\nu \int_{B_N:\, R_{12}>b} S_{\nu n}^{\mu m}(\mathbf{R}_{12})\, \langle A_{\nu 2}^{\mu} \rangle_{12}\, \mathrm{d}V_2 = -I_1 \overline{Y_n^m(\hat{\boldsymbol{k}})}, \tag{4.13}$$

for $n = 0, 1, 2, \ldots$ and $m = -n, \ldots, n$. Then, we let $N \to \infty$ so that $B_N$ becomes the half-space $z > 0$, and invoke Lax's QCA, (3.7). This implies that $\langle A_{n2}^m \rangle_{12} = \langle A_{n2}^m \rangle_2$. Hence, (4.13) reduces to

$$\langle A_{n1}^m \rangle_1 + n_0 \sum_{\nu,\mu} \mathrm{i}^{\nu-n} Z_\nu \int_{z_2>0,\, R_{12}>b} S_{\nu n}^{\mu m}(\mathbf{R}_{12})\, \langle A_{\nu 2}^{\mu} \rangle_2\, \mathrm{d}V_2 = -I_1 \overline{Y_n^m(\hat{\boldsymbol{k}})}, \tag{4.14}$$

for $n = 0, 1, 2, \ldots$ and $m = -n, \ldots, n$. As $I_1 = \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}_1) = \mathrm{e}^{\mathrm{i}\alpha z_1} \exp(\mathrm{i}\boldsymbol{k}_T \cdot \boldsymbol{q}_1)$ with $\alpha = k \cos\theta_{\mathrm{in}}$ and $\boldsymbol{q}_s = (x_s, y_s, 0)$, we seek a solution to (4.14) in the form

$$\langle A_{ns}^m \rangle_s = \Phi_n^m(z_s) \exp(\mathrm{i}\boldsymbol{k}_T \cdot \boldsymbol{q}_s) \tag{4.15}$$

so that

$$\Phi_n^m(z_1) + n_0 \sum_{\nu,\mu} \mathrm{i}^{\nu-n} Z_\nu \int_{z_2>0,\, R_{12}>b} S_{\nu n}^{\mu m}(\mathbf{R}_{12}) \exp(\mathrm{i}\boldsymbol{k}_T \cdot \boldsymbol{q}_{21})\, \Phi_\nu^\mu(z_2)\, \mathrm{d}V_2 = -\mathrm{e}^{\mathrm{i}\alpha z_1} \overline{Y_n^m(\hat{\boldsymbol{k}})}, \tag{4.16}$$

for $n = 0, 1, 2, \ldots$ and $m = -n, \ldots, n$, where $\boldsymbol{q}_{sj} = \boldsymbol{q}_s - \boldsymbol{q}_j$.

Proceeding as before, suppose that for sufficiently large $z$ (say $z > \ell$) we can write

$$\Phi_n^m(z) = F_n^m \mathrm{e}^{\mathrm{i}\lambda z}. \tag{4.17}$$

Then if $z_1 > \ell + b$, (4.16) becomes

$$F_n^m \mathrm{e}^{\mathrm{i}\lambda z_1} + n_0 \sum_{\nu,\mu} (-\mathrm{i})^{\nu-n} Z_\nu \left\{ \int_0^\ell \Phi_\nu^\mu(z_2) \mathcal{L}_{\nu n}^{\mu m}(z_{21})\, \mathrm{d}z_2 + F_\nu^\mu \mathrm{e}^{\mathrm{i}\lambda z_1} \mathcal{M}_{\nu n}^{\mu m} \right\} = -\mathrm{e}^{\mathrm{i}\alpha z_1} \overline{Y_n^m(\hat{\boldsymbol{k}})}, \tag{4.18}$$

for $n = 0, 1, 2, \ldots$ and $m = -n, \ldots, n$, where $z_{21} = z_2 - z_1$,

$$\mathcal{L}_{\nu n}^{\mu m}(z_{21}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} S_{\nu n}^{\mu m}(\mathbf{R}_{21}) \exp(\mathrm{i}\boldsymbol{k}_T \cdot \boldsymbol{q}_{21})\, \mathrm{d}x_2\, \mathrm{d}y_2,$$

$$\mathcal{M}_{\nu n}^{\mu m} = \int_{z_2>\ell,\, R_{21}>b} S_{\nu n}^{\mu m}(\mathbf{R}_{21}) \exp(\mathrm{i}\boldsymbol{k}_T \cdot \boldsymbol{q}_{21})\, \mathrm{e}^{\mathrm{i}\lambda z_{21}}\, \mathrm{d}V_2$$

and we have used $S_{\nu n}^{\mu m}(-\boldsymbol{r}) = (-1)^{n+\nu} S_{\nu n}^{\mu m}(\boldsymbol{r})$, a relation that follows from (4.9). Indeed, because of (4.9), it is sufficient to consider

$$L_n^m(z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi_n^m(\mathbf{R}) \exp(\mathrm{i}\boldsymbol{k}_T \cdot \mathbf{Q})\,\mathrm{d}X\,\mathrm{d}Y$$

for $z < 0$ and

$$M_n^m = \int_{z_2>\ell,\, R_{21}>b} \psi_n^m(\mathbf{R}_{21})\,\Psi(\mathbf{R}_{21})\,\mathrm{d}V_2,$$

where $\Psi(\mathbf{R}) = \mathrm{e}^{\mathrm{i}\lambda z}\exp(\mathrm{i}\boldsymbol{k}_T \cdot \mathbf{Q}) = \exp(\mathrm{i}\mathbf{K}\cdot\mathbf{R})$ and $\mathbf{K} = K\hat{\mathbf{K}}$ is defined by (3.15).

From (B.5), we have

$$L_n^m(z_{21}) = \frac{2\pi \mathrm{i}^n}{k\alpha} Y_n^m(\hat{\boldsymbol{k}})\,\mathrm{e}^{\mathrm{i}\alpha(z_1-z_2)} \quad \text{for } z_1 > z_2.$$

Hence, $\mathcal{L}_{\nu n}^{\mu m}$ is proportional to $\mathrm{e}^{\mathrm{i}\alpha(z_1-z_2)}$ and so the integral term in (4.18) is proportional to $\mathrm{e}^{\mathrm{i}\alpha z_1}$.

The volume integral $M_n^m$ can be evaluated readily using Green's theorem. We have $\psi_n^m\nabla^2\Psi - \Psi\nabla^2\psi_n^m = (k^2 - K^2)\psi_n^m\Psi$. It follows that

$$M_n^m = \frac{1}{k^2 - K^2}\int_{\partial B}\left[\psi_n^m \frac{\partial\Psi}{\partial n} - \Psi\frac{\partial\psi_n^m}{\partial n}\right]\mathrm{d}S_2,$$

where $\partial B$ consists of two parts, the plane $z_2 = \ell$ and the sphere $R_{12} = b$. Now, on $z_2 = \ell$, $\partial/\partial n = -\partial/\partial z_2$ and so we have

$$-\int_{z_2=\ell}\left[\psi_n^m\frac{\partial\Psi}{\partial z_2} - \Psi\frac{\partial\psi_n^m}{\partial z_2}\right]\mathrm{d}x_2\,\mathrm{d}y_2 = \frac{2\pi}{k\alpha}\mathrm{e}^{\mathrm{i}(\alpha-\lambda)(z_1-\ell)}\,\mathrm{i}^{n-1}(\lambda+\alpha)\,Y_n^m(\hat{\boldsymbol{k}}),$$

using (B.8). Thus, the plane part of $\partial B$ contributes a term to $\mathcal{M}_{\nu n}^{\mu m}$ proportional to $\mathrm{e}^{\mathrm{i}(\alpha-\lambda)z_1}$, which in turn gives a contribution to (4.18) proportional to $\mathrm{e}^{\mathrm{i}\alpha z_1}$.

Next, from (4.4), we have

$$\Psi = \exp(\mathrm{i}\mathbf{K}\cdot\mathbf{R}) = 4\pi\sum_{\nu,\mu}\mathrm{i}^\nu j_\nu(KR)\,\overline{Y_\nu^\mu(\hat{\mathbf{R}})}\,Y_\nu^\mu(\hat{\mathbf{K}}).$$

Then, the contribution from the sphere $R_{12} = b$ is

$$\begin{aligned}
&-\int_\Omega\left[\psi_n^m\frac{\partial\Psi}{\partial R} - \Psi\frac{\partial\psi_n^m}{\partial R}\right]_{R=b} b^2\,\mathrm{d}\Omega\\
&\quad = 4\pi b^2\sum_{\nu,\mu}\mathrm{i}^\nu Y_\nu^\mu(\hat{\mathbf{K}})\{kj_\nu(Kb)\,h_n'(kb) - Kj_\nu'(Kb)\,h_n(kb)\}\int_\Omega Y_n^m\overline{Y_\nu^\mu}\,\mathrm{d}\Omega\\
&\quad = 4\pi b^2\mathrm{i}^n Y_n^m(\hat{\mathbf{K}})\{kj_n(Kb)\,h_n'(kb) - Kj_n'(Kb)\,h_n(kb)\},
\end{aligned}$$

which is independent of $z_1$; here, $\Omega$ is the unit sphere and we have used (A.1).

Collecting up our results, we find that (4.18) can be written as

$$\mathcal{A}_n^m\,\mathrm{e}^{\mathrm{i}\lambda z_1} + \mathcal{B}_n^m\,\mathrm{e}^{\mathrm{i}\alpha z_1} = -\mathrm{e}^{\mathrm{i}\alpha z_1}\,\overline{Y_n^m(\hat{\boldsymbol{k}})}, \tag{4.19}$$

for $n = 0, 1, 2, \ldots$, $m = -n, \ldots, n$ and $z_1 > \ell + b$, where

$$\mathcal{A}_n^m = F_n^m + \frac{(4\pi)^2 \mathrm{i} n_0 (-1)^m}{k(k^2 - K^2)} \sum_{\nu,\mu} Z_\nu F_\nu^\mu \sum_q Y_q^{\mu-m}(\hat{\mathbf{K}})\, \mathcal{N}_q(Kb)\, \mathcal{G}(n, m; \nu, -\mu; q), \tag{4.20}$$

$$\mathcal{N}_n(x) = \mathrm{i}kb\{x\, j_n'(x)\, h_n(kb) - kb\, j_n(x)\, h_n'(kb)\} \tag{4.21}$$

and we have used (4.10) to remove a factor of $(-1)^{q+n+\nu}$. In particular, we note that $\mathcal{N}_0$ appeared in §3.3 during our analysis of Lax's integral equation.

From (4.19), we immediately obtain $\mathcal{A}_n^m = 0$ for $n = 0, 1, 2, \ldots$, $m = -n, \ldots, n$. These equations yield an infinite homogeneous system of linear algebraic equations for $F_n^m$. The existence of a non-trivial solution to this system determines $K$.

It is worth noting that even though the solution of the system $\mathcal{A}_n^m = 0$ can depend on $\theta_{\mathrm{in}}$ via $\hat{\mathbf{K}}$ (see (3.15)), the effective wavenumber itself, $K$, should not depend on $\theta_{\mathrm{in}}$.

**4.4. Approximate determination of $K$ for small $n_0$.** The only approximation made in the derivation of the system $\mathcal{A}_n^m = 0$ is the QCA, which is expected to be valid for small values of the scatterer concentration ($n_0 a^3 \ll 1$). We now assume (as in §3.3) that $n_0 b/k^2$ is also small and write $K^2 = k^2 + \delta_1 n_0 + \delta_2 n_0^2 + \ldots$. Then

$$\mathcal{N}_n(Kb) = 1 - \tfrac{1}{2}\mathrm{i}b(n_0/k)\delta_1 d_n(kb) + O(n_0^2), \tag{4.22}$$

where

$$d_n(x) = x j_n'(x)[x h_n'(x) + h_n(x)] + [x^2 - n(n+1)] j_n(x)\, h_n(x), \tag{4.23}$$

and so

$$\frac{\mathcal{N}_n(Kb)}{k^2 - K^2} = -\frac{1}{\delta_1 n_0} + \frac{\mathrm{i}b d_n(kb)}{2k} + \frac{\delta_2}{\delta_1^2} + O(n_0). \tag{4.24}$$

If (4.24) is substituted in $\mathcal{A}_n^m = 0$, with $\mathcal{A}_n^m$ defined by (4.20), and $O(n_0^2)$ terms neglected, we obtain

$$F_n^m = \frac{(4\pi)^2 \mathrm{i}}{k\delta_1}(-1)^m \left(1 - \frac{n_0\delta_2}{\delta_1}\right) \sum_{\nu,\mu} Z_\nu F_\nu^\mu W_{n\nu}^{m\mu} + \frac{(4\pi)^2 b n_0}{2k^2}(-1)^m \sum_{\nu,\mu} Z_\nu F_\nu^\mu X_{n\nu}^{m\mu}, \tag{4.25}$$

where

$$W_{n\nu}^{m\mu} = \sum_q Y_q^{\mu-m}(\hat{\mathbf{K}})\, \mathcal{G}(n, m; \nu, -\mu; q), \tag{4.26}$$

$$X_{n\nu}^{m\mu} = \sum_q Y_q^{\mu-m}(\hat{\mathbf{K}})\, \mathcal{G}(n, m; \nu, -\mu; q)\, d_q(kb). \tag{4.27}$$

The Gaunt coefficients appear in the linearisation formula for spherical harmonics, (A.4). Replacing $\mu$ by $-\mu$ and $\hat{\boldsymbol{r}}$ by $\hat{\mathbf{K}}$ in the complex conjugate of (A.4), we obtain

$$W_{n\nu}^{m\mu} = Y_n^{-m}(\hat{\mathbf{K}})\, Y_\nu^\mu(\hat{\mathbf{K}}).$$

So, at leading order, (4.25) gives

$$F_n^m = \frac{(4\pi)^2 \mathrm{i}}{k\delta_1} \overline{Y_n^m(\hat{\mathbf{K}})} \sum_{\nu,\mu} Z_\nu F_\nu^\mu Y_\nu^\mu(\hat{\mathbf{K}}),$$

for $n = 0, 1, 2, \dots$ and $m = -n, \dots, n$. Put $F_n^m = \overline{Y_n^m(\hat{\mathbf{K}})}\,\widetilde{F}_n^m$, whence

$$\widetilde{F}_n^m = \frac{(4\pi)^2 \mathrm{i}}{k\delta_1} \sum_{\nu,\mu} Z_\nu \widetilde{F}_\nu^\mu Y_\nu^\mu(\hat{\mathbf{K}})\,\overline{Y_\nu^\mu(\hat{\mathbf{K}})},$$

for $n = 0, 1, 2, \dots$ and $m = -n, \dots, n$. But the right-hand side of this equation does not depend on $n$ or $m$, so that $\widetilde{F}_n^m = \widetilde{F}$, say. Hence

$$\delta_1 = \frac{(4\pi)^2 \mathrm{i}}{k} \sum_{\nu=0}^{\infty} Z_\nu \sum_{\mu=-\nu}^{\nu} Y_\nu^\mu(\hat{\mathbf{K}})\,\overline{Y_\nu^\mu(\hat{\mathbf{K}})}. \tag{4.28}$$

The sum over $\mu$ can be evaluated using Legendre's addition theorem, (A.3). Putting $\hat{\boldsymbol{r}}_1 = \hat{\boldsymbol{r}}_2 = \hat{\mathbf{K}}$ in (A.3), and noting that $P_n(1) = 1$, we obtain

$$\delta_1 = \frac{4\pi \mathrm{i}}{k} \sum_{\nu=0}^{\infty} (2\nu + 1) Z_\nu = -\frac{4\pi \mathrm{i}}{k} f(0), \tag{4.29}$$

where $f$ is the far-field pattern, given by (4.6).

Returning to (4.25), we now put

$$F_n^m = \overline{Y_n^m(\hat{\mathbf{K}})}\,\widetilde{F} + n_0 G_n^m,$$

and then the $O(n_0)$ terms give

$$G_n^m = \overline{Y_n^m(\hat{\mathbf{K}})}\,V + \frac{(4\pi)^2 b}{2k^2} (-1)^m \widetilde{F} \sum_{\nu,\mu} Z_\nu \overline{Y_\nu^\mu(\hat{\mathbf{K}})}\,X_{n\nu}^{m\mu}, \tag{4.30}$$

where

$$V = \frac{(4\pi)^2 \mathrm{i}}{k\delta_1} \sum_{\nu,\mu} Z_\nu G_\nu^\mu Y_\nu^\mu(\hat{\mathbf{K}}) - \frac{\delta_2}{\delta_1} \widetilde{F}. \tag{4.31}$$

Note that $V$ does not depend on $n$ or $m$. Substituting for $G_\nu^\mu$ from (4.30) in (4.31), making use of (4.28), gives a formula for $\delta_2$:

$$\delta_2 = \frac{(4\pi)^4 \mathrm{i} b}{2k^3} \sum_{n,m} \sum_{\nu,\mu} (-1)^m Z_n Z_\nu Y_n^m(\hat{\mathbf{K}})\,\overline{Y_\nu^\mu(\hat{\mathbf{K}})}\,X_{n\nu}^{m\mu}. \tag{4.32}$$

So far we have not made any assumptions about the size of $ka$ or $kb$ (though clearly $kb \geq 2ka$). Now we will assume that $kb$ is small. In the limit $x \to 0$, we have $d_n(x) \sim \mathrm{i}n/x$. Using this approximation simplifies $X_{n\nu}^{m\mu}$, defined by (4.27). Hence,

$$\delta_2 \sim -\frac{1}{2}(4\pi/k)^4 \sum_{n=0}^{\infty} \sum_{\nu=0}^{\infty} Z_n Z_\nu\, K_{n\nu}(\hat{\mathbf{K}}) \quad \text{as } kb \to 0, \tag{4.33}$$

where

$$K_{n\nu}(\hat{\mathbf{K}}) = \sum_{m=-n}^{n} \sum_{\mu=-\nu}^{\nu} (-1)^m Y_n^m(\hat{\mathbf{K}})\,\overline{Y_\nu^\mu(\hat{\mathbf{K}})} \sum_q q\, Y_q^{\mu-m}(\hat{\mathbf{K}})\,\mathcal{G}(n, m; \nu, -\mu; q). \tag{4.34}$$

From (A.5) and $\int_0^{2\pi} \mathrm{e}^{\mathrm{i}m\phi}\,\mathrm{d}\phi = 2\pi\delta_{0m}$, we have

$$Y_q^{\mu-m}(\hat{\mathbf{K}})\,\mathcal{G}(n,m;\nu,-\mu;q) = (-1)^m \sum_M Y_q^M(\hat{\mathbf{K}}) \int_\Omega \overline{Y_n^m} Y_\nu^\mu \overline{Y_q^M}\,\mathrm{d}\Omega$$
$$= (-1)^m \frac{2q+1}{4\pi} \int_\Omega \overline{Y_n^m}(\hat{\boldsymbol{r}})\, Y_\nu^\mu(\hat{\boldsymbol{r}})\, P_q(\hat{\boldsymbol{r}}\cdot\hat{\mathbf{K}})\,\mathrm{d}\Omega(\hat{\boldsymbol{r}}),$$

using (A.3). Hence, using (A.3) two more times, we obtain

$$K_{n\nu}(\hat{\mathbf{K}}) = \frac{(2n+1)(2\nu+1)}{(4\pi)^3} \sum_q q(2q+1) \int_\Omega P_n(\hat{\boldsymbol{r}}\cdot\hat{\mathbf{K}})\, P_\nu(\hat{\boldsymbol{r}}\cdot\hat{\mathbf{K}})\, P_q(\hat{\boldsymbol{r}}\cdot\hat{\mathbf{K}})\,\mathrm{d}\Omega(\hat{\boldsymbol{r}})$$
$$= \frac{\sqrt{(2n+1)(2\nu+1)}}{(4\pi)^{3/2}} \sum_q q\sqrt{2q+1}\,\mathcal{G}(n,0;\nu,0;q),$$

where we have used $Y_n^0 = \sqrt{(2n+1)/(4\pi)}\,P_n$ and (A.5). When this formula for $K_{n\nu}$ is substituted in (4.33), we obtain complete agreement with the formula of Lloyd and Berry [19]; see Appendix C.

In conclusion, we note that if we were to replace (2.5) with the (clearly unreasonable)

$$p(\boldsymbol{r}_2|\boldsymbol{r}_1) = (n_0/N)H(|z_2 - z_1| - a),$$

a similar analysis to that given above yields Twersky's erroneous expression for $\delta_2$, as given in (1.4). We omit the details of this calculation, but see [19] for a related discussion and [18] for analogous calculations in two dimensions.

**Appendix A. Spherical harmonics.** We define spherical harmonics $Y_n^m$ by

$$Y_n^m(\hat{\boldsymbol{r}}) = Y_n^m(\theta,\phi) = (-1)^m \sqrt{\frac{2n+1}{4\pi}} \sqrt{\frac{(n-m)!}{(n+m)!}} P_n^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi},$$

where $P_n^m$ is an associated Legendre function. We have orthonormality,

$$\text{(A.1)} \qquad \int_\Omega Y_n^m\, \overline{Y_\nu^\mu}\,\mathrm{d}\Omega = \delta_{n\nu}\delta_{m\mu},$$

where $\Omega$ is the unit sphere. Also, $Y_n^{-m} = (-1)^m \overline{Y_n^m}$.

For $0 \le m \le n$, we have the expansion

$$\text{(A.2)} \qquad \frac{P_n^m(t)}{(1-t^2)^{m/2}} = \frac{1}{2^n\,n!}\frac{\mathrm{d}^{m+n}}{\mathrm{d}t^{m+n}}(t^2-1)^n = \sum_{l=0}^{[(n-m)/2]} B_l^{n,m} t^{n-m-2l},$$

where $[n]$ denotes the integer part of $n$. The coefficients $B_l^{n,m}$ are known explicitly, but we shall not need them.

We shall make use of Legendre's addition theorem, namely,

$$\text{(A.3)} \qquad P_n(\hat{\boldsymbol{r}}_1\cdot\hat{\boldsymbol{r}}_2) = \frac{4\pi}{2n+1} \sum_{m=-n}^{n} Y_n^m(\hat{\boldsymbol{r}}_1)\, \overline{Y_n^m(\hat{\boldsymbol{r}}_2)},$$

where $P_n(t)$ is a Legendre polynomial.

The linearisation formula for spherical harmonics is

$$Y_n^m(\hat{\boldsymbol{r}})\,Y_\nu^\mu(\hat{\boldsymbol{r}}) = \sum_q Y_q^{m+\mu}(\hat{\boldsymbol{r}})\,\mathcal{G}(n,m;\nu,\mu;q), \tag{A.4}$$

where $\mathcal{G}$ is a Gaunt coefficient. Note that $\mathcal{G}$ is real. Making use of (A.1), we obtain

$$\mathcal{G}(n,m;\nu,-\mu;q) = (-1)^m \int_\Omega \overline{Y_n^m}\,Y_\nu^\mu\,\overline{Y_q^{\mu-m}}\,\mathrm{d}\Omega. \tag{A.5}$$

**Appendix B. Some integrals.** Consider the integral

$$L(z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} h_0(kR)\,\exp\left(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q}\right)\mathrm{d}X\,\mathrm{d}Y,$$

where $R = |\mathbf{R}|$, $\mathbf{R} = (X,Y,z)$ and $\mathbf{Q} = (X,Y,0)$. Put $\mathbf{Q} = Q(\cos\Phi,\ \sin\Phi,\ 0)$ so that $\boldsymbol{k}_T\cdot\mathbf{Q} = kQ\sin\theta_{\mathrm{in}}\,\cos\left(\Phi-\phi_{\mathrm{in}}\right)$. Hence, as $\mathrm{d}X\,\mathrm{d}Y = Q\,\mathrm{d}Q\,\mathrm{d}\Phi$, we can integrate over $\Phi$, giving

$$L(z) = 2\pi\int_0^\infty h_0(k\sqrt{Q^2+z^2})\,J_0(kQ\sin\theta_{\mathrm{in}})\,Q\,\mathrm{d}Q.$$

We have

$$Qh_0(k\sqrt{Q^2+z^2}) = \frac{Q\,\mathrm{e}^{\mathrm{i}k\sqrt{Q^2+z^2}}}{\mathrm{i}k\sqrt{Q^2+z^2}} = \frac{1}{(\mathrm{i}k)^2}\frac{\mathrm{d}}{\mathrm{d}Q}\mathrm{e}^{\mathrm{i}k\sqrt{Q^2+z^2}},$$

so that an integration by parts (using $J_0' = -J_1$) gives

$$L(z) = 2\pi k^{-2}\{\mathrm{e}^{\mathrm{i}k|z|} - \hat{L}(z)\}, \tag{B.1}$$

where

$$\hat{L}(z) = k\sin\theta_{\mathrm{in}}\int_0^\infty J_1(kQ\sin\theta_{\mathrm{in}})\,\mathrm{e}^{\mathrm{i}k\sqrt{Q^2+z^2}}\,\mathrm{d}Q.$$

Now, from [8, eqn. 6.637(1)] (with $\nu = 1$ therein), we have

$$\int_0^\infty \frac{\mathrm{e}^{-a\sqrt{x^2+\beta^2}}}{\sqrt{x^2+\beta^2}}\,J_1(\gamma x)\,\mathrm{d}x = I_{1/2}(X_-)\,K_{1/2}(X_+), \tag{B.2}$$

where $X_\pm = \frac{1}{2}\beta\{\sqrt{a^2+\gamma^2}\pm a\}$, $\operatorname{Re} a > 0$, $\operatorname{Re}\beta > 0$ and $\operatorname{Re}\gamma > 0$. From [1, 10.2.13 and 10.2.17], the modified Bessel functions are given by

$$I_{1/2}(w) = \{2/(\pi w)\}^{1/2}\sinh w \quad \text{and} \quad K_{1/2}(w) = \{\pi/(2w)\}^{1/2}\,\mathrm{e}^{-w}$$

so that

$$I_{1/2}(X_-)\,K_{1/2}(X_+) = (\beta\gamma)^{-1}\left\{\mathrm{e}^{-a\beta} - \mathrm{e}^{-\beta\sqrt{a^2+\gamma^2}}\right\}.$$

Then, differentiating (B.2) with respect to $a$ gives

$$\gamma\int_0^\infty J_1(\gamma x)\,\mathrm{e}^{-a\sqrt{x^2+\beta^2}}\,\mathrm{d}x = \mathrm{e}^{-a\beta} - \frac{a}{\sqrt{a^2+\gamma^2}}\mathrm{e}^{-\beta\sqrt{a^2+\gamma^2}}. \tag{B.3}$$

The calculations leading to (B.3) are certainly valid for $\operatorname{Re} a > 0$, $\operatorname{Re}\beta > 0$ and $\operatorname{Re}\gamma > 0$. We want to use it for $\beta = z$; as the left-hand side of (B.3) is an even function of $\beta$, we can replace $\beta$ by $|\beta|$ on the right-hand side. We also want to substitute $a = -\mathrm{i}k$ and $\gamma = k\sin\theta_{\rm in}$, so that $\sqrt{a^2+\gamma^2} = \pm\mathrm{i}k\cos\theta_{\rm in}$. To determine the sign, we note that (from [8, eqns. 6.671(1) and 6.671(2)])

$$\gamma\int_0^\infty J_1(\gamma x)\,\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}x = 1 - \frac{k}{\sqrt{k^2-\gamma^2}} \quad \text{for } k > \gamma,$$

implying that we should take $\sqrt{a^2+\gamma^2} = -\mathrm{i}k\cos\theta_{\rm in}$. (Alternatively, we note that the right-hand side of (B.3) is an analytic function of $a$ in a cut plane; we can take the cut between $a = \mathrm{i}\gamma$ and $a = -\mathrm{i}\gamma$ ($\gamma$ real and positive), and we choose the branch so that the right-hand side of (B.3) is real when $a$ is real and positive. This leads to $\sqrt{a^2+\gamma^2} = -\mathrm{i}\sqrt{k^2-\gamma^2}$ when $a = -\mathrm{i}k$ with $k > \gamma > 0$.) Hence,

$$\hat{L}(z) = \mathrm{e}^{\mathrm{i}k|z|} - \mathrm{e}^{\mathrm{i}k|z|\cos\theta_{\rm in}}\sec\theta_{\rm in}$$

and so (B.1) gives

$$L(z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} h_0(kR)\,\exp\left(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q}\right)\mathrm{d}X\,\mathrm{d}Y = \frac{2\pi}{k^2\cos\theta_{\rm in}}\,\mathrm{e}^{\mathrm{i}k|z|\cos\theta_{\rm in}}. \tag{B.4}$$

This formula generalizes. Thus, let

$$L_n^m(z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_n^m(\mathbf{R})\,\exp\left(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q}\right)\mathrm{d}X\,\mathrm{d}Y,$$

with $\psi_n^m(\boldsymbol{r}) = h_n(kr)Y_n^m(\hat{\boldsymbol{r}})$. Then,

$$L_n^m(z) = \frac{2\pi\,\mathrm{i}^n}{k^2\cos\theta_{\rm in}}\,Y_n^m(\hat{\boldsymbol{k}})\,\mathrm{e}^{-\mathrm{i}kz\cos\theta_{\rm in}} \quad \text{for } z < 0, \tag{B.5}$$

with a similar formula for $z > 0$ (which we shall not need). When both $m = 0$ and $\theta_{\rm in} = 0$, (B.5) reduces to a result obtained in [24].

To prove (B.5), begin by assuming that $0 \le m \le n$. Let

$$\Omega_n^m(\boldsymbol{r}) = h_n(kr)\,P_n^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi}. \tag{B.6}$$

($\psi_n^m(\boldsymbol{r})$ is a normalized form of $\Omega_n^m(\boldsymbol{r})$.) Then, we have [5, 26, 4]

$$\Omega_n^m(\boldsymbol{r}) = \mathcal{Y}_n^m h_0(kr),$$

where the Erdélyi operator $\mathcal{Y}_n^m$ is defined by

$$\mathcal{Y}_n^m = (\mathcal{D}_{xy})^m\sum_{l=0}^{[(n-m)/2]}(-1)^l B_l^{n,m}(\mathcal{D}_z)^{n-m-2l}, \quad \mathcal{D}_{xy} = -\frac{1}{k}\left(\frac{\partial}{\partial x} + \mathrm{i}\frac{\partial}{\partial y}\right)$$

and $\mathcal{D}_z = -k^{-1}\partial/\partial z$; the coefficients $B_l^{n,m}$ appear in the expansion (A.2). Hence,

$$O_n^m(z) \equiv \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Omega_n^m(\mathbf{R})\,\exp\left(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q}\right)\mathrm{d}X\,\mathrm{d}Y = \sum_l(-1)^l B_l^{n,m}(\mathcal{D}_z)^{n-m-2l}\mathcal{I}_m(z),$$

where the sum is from $l = 0$ to the integer part of $(n - m)/2$, and

$$\begin{aligned}\mathcal{I}_m(z) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q})\,(\mathcal{D}_{XY})^m h_0(kR)\,\mathrm{d}X\,\mathrm{d}Y \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} h_0(kR)\,(-\mathcal{D}_{XY})^m \exp(\mathrm{i}\boldsymbol{k}_T\cdot\mathbf{Q})\,\mathrm{d}X\,\mathrm{d}Y = \mathrm{i}^m \sin^m\theta_{\mathrm{in}}\,\mathrm{e}^{\mathrm{i}m\phi_{\mathrm{in}}}L(z).\end{aligned}$$

Hence, substituting for $L(z)$ from (B.4), and carrying out the differentiations with respect to $z$, we obtain

$$O_n^m(z) = \frac{2\pi\,\mathrm{i}^n}{k^2\cos\theta_{\mathrm{in}}}\,P_n^m(\cos\theta_{\mathrm{in}})\,\mathrm{e}^{\mathrm{i}m\phi_{\mathrm{in}}}\,\mathrm{e}^{-\mathrm{i}kz\cos\theta_{\mathrm{in}}} \tag{B.7}$$

for $z < 0$. The result (B.5) follows after multiplication by the appropriate normalisation constant. It can be shown that the same result is also true for $-n \le m \le 0$.

Next, we consider an integral required in §4.3. We have

$$\begin{aligned}&-\int_{z_2=\ell}\left[\Omega_n^m\frac{\partial\Psi}{\partial z_2} - \Psi\frac{\partial\Omega_n^m}{\partial z_2}\right]\mathrm{d}x_2\,\mathrm{d}y_2 \\ &\qquad = \mathrm{e}^{\mathrm{i}\lambda(\ell - z_1)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp(\mathrm{i}\boldsymbol{k}_T\cdot\boldsymbol{q}_{21})\left[-\mathrm{i}\lambda\Omega_n^m + \frac{\partial\Omega_n^m}{\partial z_2}\right]_{z_2=\ell}\mathrm{d}x_2\,\mathrm{d}y_2,\end{aligned}$$

where $\Psi = \exp(\mathrm{i}\mathbf{K}\cdot\mathbf{R}_{21})$. Using

$$\mathcal{D}_z\Omega_n^m = (2n+1)^{-1}\{(n-m+1)\Omega_{n+1}^m - (n+m)\Omega_{n-1}^m\}$$

and (B.7) thrice gives the integral's value as

$$\frac{2\pi}{k\alpha}\mathrm{e}^{\mathrm{i}(\alpha-\lambda)(z_1-\ell)}\,\mathrm{i}^{n-1}(\lambda+\alpha)\,P_n^m(\cos\theta_{\mathrm{in}})\,\mathrm{e}^{\mathrm{i}m\phi_{\mathrm{in}}}, \tag{B.8}$$

where we have also used $(2n+1)tP_n^m(t) = (n-m+1)P_{n+1}^m(t) + (n+m)P_{n-1}^m(t)$.

**Appendix C. The Lloyd–Berry formula.** Recall the formula (1.6). From (4.6) and $Y_n^0(\hat{\boldsymbol{r}}) = \sqrt{(2n+1)/(4\pi)}P_n(\cos\theta)$, we obtain

$$f(\theta) = -\sqrt{4\pi}\sum_{n=0}^{\infty}\sqrt{2n+1}\,Z_n Y_n^0.$$

Then, the linearisation formula (A.4) gives

$$[f(\theta)]^2 = \sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\sum_q T(n,\nu;q)\,P_q(\cos\theta), \tag{C.1}$$

where

$$T(n,\nu;q) = \sqrt{4\pi(2n+1)(2\nu+1)(2q+1)}\,Z_n Z_\nu\,\mathcal{G}(n,0;\nu,0;q).$$

Hence,

$$-[f(\pi)]^2 + [f(0)]^2 = \sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\sum_q T(n,\nu;q)\,\{1-(-1)^q\}. \tag{C.2}$$

For the integral term in (1.6), we use (C.1) and

$$\int_0^\pi \frac{1}{\sin(\theta/2)} \frac{\mathrm{d}}{\mathrm{d}\theta} P_q(\cos\theta)\,\mathrm{d}\theta = -\int_{-1}^1 \sqrt{\frac{2}{1-x}}\, P_q'(x)\,\mathrm{d}x = (-1)^q - 1 - 2q. \tag{C.3}$$

(The last equality was obtained as follows. From [8, eqn. 7.225(1)], we have

$$\begin{aligned}\frac{2}{2n+1}\frac{1}{\sqrt{1+x}}\{T_n(x)+T_{n+1}(x)\} &= \int_{-1}^x \frac{1}{\sqrt{x-t}}\, P_n(t)\,\mathrm{d}t \\ &= 2(-1)^n\sqrt{1+x} + 2\int_{-1}^x \sqrt{x-t}\, P_n'(t)\,\mathrm{d}t,\end{aligned}$$

after an integration by parts, where $T_n(\cos\theta) = \cos n\theta$ is a Chebyshev polynomial and we have used $P_n(-1) = (-1)^n$. Now, differentiate this formula with respect to $x$ and then let $x \to 1$, using $T_n(1) = 1$ and $T_n'(1) = n^2$.) Substituting (C.1), (C.2) and (C.3) in (1.6) gives

$$\delta_2 = -\frac{8\pi^2}{k^4} \sum_{n=0}^\infty \sum_{\nu=0}^\infty \sum_q q\, T(n,\nu;q), \tag{C.4}$$

which is the same as (4.33).

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