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Quadratic quantities in acoustics: Scattering cross-section and radiation force

P.A. Martin

Department of Applied Mathematics and Statistics, Colorado School of Mines, Golden, CO 80401-1887, USA

HIGHLIGHTS

- Exact computation of scattering cross-section.
- Exact computation of radiation force.
- All computations done in the near field.

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ABSTRACT

Time-harmonic acoustic waves interact with a scatterer: this interaction is calculated using linear, first-order theory. However, there are quadratic, second-order quantities that are of interest. These include the scattering cross-section and the steady radiation force; these quantities can be expressed as integrals of products of first-order quantities over a sphere. These integrals are evaluated exactly. The results are infinite series of products of the coefficients in the spherical multipole expansions of the incident and scattered fields; they do not depend on the radius of the spherical integration surface. For a specific scattering problem, the coefficients can be connected by an appropriate T-matrix. In most previous work, the spherical surface is moved to infinity so that far-field quantities can be introduced: it is shown that this process is not straightforward and it may introduce spurious difficulties.

1. Introduction

In the context of time-harmonic acoustics, a given incident wave interacts with one or more scatterers surrounded by a lossless inviscid compressible fluid. This process is usually characterised by introducing three "cross-sections" related by

$$\sigma_{\mathrm{sc}} + \sigma_{\mathrm{ab}} = \sigma_{\mathrm{ex}}. \tag{1}$$

The scattering cross-section σ_{sc} gives a measure of how much energy is radiated away by the scatterers whereas the absorption cross-section σ_{ab} gives how much energy is absorbed by the scatterers. Hence the extinction cross-section σ_{ex} describes how much energy has been extracted from the incident wave by the scattering process. (Precise definitions will be given later.) When the scatterers are lossless (for example, sound-soft or sound-hard), $\sigma_{\mathrm{ab}} = 0$ and then $\sigma_{\mathrm{sc}} = \sigma_{\mathrm{ex}}$.

Energy is a quadratic quantity: for linear waves of (small) amplitude A, energy is proportional to A^2. Another quadratic quantity is the acoustic radiation force: for linear time-harmonic waves, it is a steady second-order force, analogous to the Stokes drift force in the context of surface water waves. The study of acoustic radiation forces has a long history, with detailed

E-mail address: pamartin@mines.edu.

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computations first made by King [1] for scattering by a small sphere. These forces have attracted more interest in recent times because they can be used to levitate and manipulate small particles. For reviews, see [2,3].

The cross-sections and the radiation force can be expressed as certain integrals of first-order quantities over a sphere of radius R, S_R, enclosing the scatterer; and they are independent of R. The usual strategy is to suppose that R is large and then far-field estimates can be used, but this is not always straightforward. Here, we adopt a brute-force approach and simply evaluate the integrals over S_R directly and exactly, having introduced standard expansions of the incident and scattered fields using spherical wavefunctions, together with appropriate Wronskians. The final results are seen to be independent of R. They are infinite series of products of coefficients from the spherical expansions. Some of these series can be expressed, exactly, in terms of far-field quantities. Finally, we connect the coefficients in the wavefunction expansions using the T-matrix, leading to a viable method for the computation of cross-sections and the radiation force.

The basic equations are introduced briefly in Section 2 and the R-independent integrals over S_R are derived in Section 3. These integrals are evaluated in Section 4 after introducing expansions in spherical wavefunctions; most of the details are relegated to an Appendix.

Section 5 is concerned with the use of far-field quantities; various pitfalls and errors are described. It is well known that $\sigma_{\rm sc}$ can be expressed exactly as an integral of the far-field pattern, and this formula is recovered. However doing the same for other quadratic quantities is awkward, mainly because they involve the incident field. After some discussion of a paper by Debye from 1909 (Section 5.3), T-matrix methods are described briefly in Section 6. The paper ends with a summary of the results obtained, covering why they are useful and what they teach us about the computation of quadratic quantities in acoustics.

2. Governing equations

The exact governing equations for a compressible inviscid fluid are

$$\tilde\rho\left(\frac{\partial\tilde{\boldsymbol v}}{\partial t}+(\tilde{\boldsymbol v}\cdot\nabla)\,\tilde{\boldsymbol v}\right)=-\operatorname{grad}\tilde p,\quad \frac{\partial\tilde\rho}{\partial t}+\operatorname{div}(\tilde\rho\tilde{\boldsymbol v})=0, \tag{2}$$

with $\tilde p=\tilde p(\tilde\rho)$, where $\tilde p(\boldsymbol r,t)$, $\tilde{\boldsymbol v}(\boldsymbol r,t)$ and $\tilde\rho(\boldsymbol r,t)$ are the pressure, velocity and density, respectively, at position $\boldsymbol r$ and time t. Introduce a small parameter ε, and expand $\tilde p$, $\tilde\rho$ and $\tilde{\boldsymbol v}$ [2, § III.F]:

$$\tilde p=p_0+\varepsilon\tilde p_1+\varepsilon^2\tilde p_2+\cdots,\quad \tilde\rho=\rho_0+\varepsilon\tilde\rho_1+\varepsilon^2\tilde\rho_2+\cdots,\quad \tilde{\boldsymbol v}=\varepsilon\tilde{\boldsymbol v}_1+\varepsilon^2\tilde{\boldsymbol v}_2+\cdots.$$

The equation of state gives $\tilde p=\tilde p(\tilde\rho)=\tilde p(\rho_0)+(\tilde\rho-\rho_0)\tilde p'(\rho_0)+\frac12(\tilde\rho-\rho_0)^2\tilde p''(\rho_0)+\cdots$. This gives $p_0=\tilde p(\rho_0)$, $\tilde p_1=c^2\tilde\rho_1$ and $\tilde p_2=c^2\tilde\rho_2+\frac12\tilde\rho_1^2\tilde p''(\rho_0)$ with $c^2=\tilde p'(\rho_0)$. We assume that p_0, ρ_0 and c^2 are constants.

2.1. Linear theory

At first order, ε^1, we obtain

$$\rho_0\frac{\partial\tilde{\boldsymbol v}_1}{\partial t}+\operatorname{grad}\tilde p_1=\boldsymbol 0,\quad \frac{\partial\tilde p_1}{\partial t}+\rho_0c^2\operatorname{div}\tilde{\boldsymbol v}_1=0. \tag{3}$$

Eliminating $\tilde{\boldsymbol v}_1$ gives the usual wave equation for $\tilde p_1$; $\tilde\rho_1$ satisfies the same equation.

Taking the scalar product of Eq. $(3)_1$ with $\tilde{\boldsymbol v}_1$, making use of Eq. $(3)_2$, we obtain the *acoustic energy equation*,

$$\frac{\partial\mathcal{E}}{\partial t}+\operatorname{div}\left(\tilde p_1\,\tilde{\boldsymbol v}_1\right)=0 \tag{4}$$

where $\mathcal{E}=\frac12\rho_0(\tilde{\boldsymbol v}_1\cdot\tilde{\boldsymbol v}_1)+\frac12\tilde p_1^2/(\rho_0c^2)$ is the acoustic energy density [4, §1.9], [5, Eq. (64.5)].

Let $\mathcal{D}$ be a fixed bounded volume with boundary $\mathcal{S}$. Integrating Eq. (4) over $\mathcal{D}$ gives

$$\frac{\mathrm d}{\mathrm dt}\int_{\mathcal D}\mathcal{E}\,\mathrm dV-\int_{\mathcal S}\tilde p_1\,\tilde{\boldsymbol v}_1\cdot\boldsymbol n\,\mathrm dS=0, \tag{5}$$

where we have used the divergence theorem and $\boldsymbol n$ is the unit normal on $\mathcal S$ pointing into $\mathcal D$. This equation has the dimensions of force $\times$ velocity, that is, power. It says that the rate of increase of energy in $\mathcal D$ is balanced by the acoustic power entering through $\mathcal S$.

Next, consider time-harmonic motions, and write

$$\tilde p_1(\boldsymbol r,t)=\operatorname{Re}\{p(\boldsymbol r)\,\mathrm e^{-\mathrm i\omega t}\}=p_R\cos\omega t+p_I\sin\omega t, \tag{6}$$

where $p_R=\operatorname{Re}p$ and $p_I=\operatorname{Im}p$ are real. Similarly, $\tilde{\boldsymbol v}_1=\operatorname{Re}\{\boldsymbol v\,\mathrm e^{-\mathrm i\omega t}\}$ and $\tilde\rho_1=\operatorname{Re}\{\rho\,\mathrm e^{-\mathrm i\omega t}\}$.

For quadratic quantities (such as energy) involving products of time-harmonic functions, it is usual to consider time averages over one period. Thus, for any function $f(\boldsymbol r,t)$, we define

$$\langle f\rangle(\boldsymbol r)=\frac1T\int_0^T f(\boldsymbol r,t)\,\mathrm dt,\quad T=\frac{2\pi}{\omega}.$$

Simple calculations give $\langle \partial\mathcal{E}/\partial t\rangle = 0$ and $\langle \tilde{p}_1\tilde{\boldsymbol{v}}_1\rangle = \frac{1}{2}\,\mathrm{Re}\{\overline{p}\,\boldsymbol{v}\}$, where the overbar denotes complex conjugation. Hence the time-averaged form of Eq. (4) is $\mathrm{Re}\,\{\mathrm{div}\,(\overline{p}\,\boldsymbol{v})\} = 0$ and the time-averaged form of Eq. (5) is

$$\mathrm{Re}\int_{\mathcal{S}} \overline{p}\,\boldsymbol{v}\cdot\boldsymbol{n}\,\mathrm{d}S = 0. \tag{7}$$

For irrotational motion, we can introduce a velocity potential $\tilde{u}_1$, with $\tilde{\boldsymbol{v}}_1 = \mathrm{grad}\,\tilde{u}_1$ and $\tilde{p}_1 = -\rho_0(\partial\tilde{u}_1/\partial t)$. Furthermore, for time-harmonic motions, we write

$$\tilde{u}_1(\boldsymbol{r},t) = (c/k)\,\mathrm{Re}\left\{u(\boldsymbol{r})\,\mathrm{e}^{-\mathrm{i}\omega t}\right\} = (c/k)\,(u_R\cos\omega t + u_I\sin\omega t)$$

where $k = \omega/c$, $u_R = \mathrm{Re}\,u$ and $u_I = \mathrm{Im}\,u$ are real, $(\nabla^2 + k^2)u = 0$, and u is dimensionless.

Some calculation gives $\langle\mathcal{E}\rangle = \langle\mathcal{K}\rangle + \langle\mathcal{V}\rangle$ where

$$\langle\mathcal{K}\rangle = \frac{\rho_0 c^2}{4k^2}\,(\mathrm{grad}\,u)\cdot(\mathrm{grad}\,\overline{u}) \quad\text{and}\quad \langle\mathcal{V}\rangle = \frac{\rho_0 c^2}{4}\,u\overline{u}; \tag{8}$$

evidently, $\langle\mathcal{K}\rangle$ is the linear approximation to the average acoustic kinetic energy density and $\langle\mathcal{V}\rangle$ is the analogous potential energy density. Also, as $\mathrm{Re}\,(\overline{p}\,\boldsymbol{v}) = c^3(\rho_0/k)\,\mathrm{Im}\,(\overline{u}\,\mathrm{grad}\,u)$, Eq. (7) becomes

$$\mathrm{Im}\int_{\mathcal{S}} \overline{u}\,\frac{\partial u}{\partial n}\,\mathrm{d}S = 0 \tag{9}$$

where $\partial u/\partial n = \boldsymbol{n}\cdot\mathrm{grad}\,u$ is the normal derivative of u on $\mathcal{S}$. The formula Eq. (9) will be used in Section 3.1.

2.2. Second-order theory

At second order, ε^2, Eq. $(2)_1$ gives

$$\rho_0\frac{\partial\tilde{\boldsymbol{v}}_2}{\partial t} + \tilde{\rho}_1\frac{\partial\tilde{\boldsymbol{v}}_1}{\partial t} + \rho_0\,(\tilde{\boldsymbol{v}}_1\cdot\nabla)\,\tilde{\boldsymbol{v}}_1 = -\,\mathrm{grad}\,\tilde{p}_2. \tag{10}$$

Multiply Eq. $(3)_2$ by $\tilde{\boldsymbol{v}}_1$ and then add the result to Eq. (10); this gives

$$\rho_0\frac{\partial\tilde{v}_i^{(2)}}{\partial t} + \frac{\partial\left(\tilde{\rho}_1\tilde{v}_i^{(1)}\right)}{\partial t} + \rho_0\frac{\partial\left(\tilde{v}_i^{(1)}\tilde{v}_j^{(1)}\right)}{\partial x_j} = -\frac{\partial\tilde{p}_2}{\partial x_i}, \quad i = 1,2,3. \tag{11}$$

where $\boldsymbol{r}$ has components x_i and we have denoted the components of $\tilde{\boldsymbol{v}}_n$ by $\tilde{v}_i^{(n)}$.

It is easy to see that $\tilde{p}_2$ has the form $\tilde{p}_2(\boldsymbol{r},t) = p_2^0(\boldsymbol{r}) + p_2^{\mathrm{c}}(\boldsymbol{r})\cos 2\omega t + p_2^{\mathrm{s}}(\boldsymbol{r})\sin 2\omega t$, with similar expressions for $\tilde{\rho}_2$ and $\tilde{\boldsymbol{v}}_2$. We are interested in the steady component of $\tilde{p}_2$, $p_2^0 = \langle\tilde{p}_2\rangle$. Extracting the steady component from Eq. (11), we obtain

$$-\frac{\partial p_2^0}{\partial x_i} = \rho_0\frac{\partial}{\partial x_j}\left\langle\tilde{v}_i^{(1)}\tilde{v}_j^{(1)}\right\rangle \tag{12}$$

$$= \frac{\rho_0}{2}\,\mathrm{Re}\,\frac{\partial(v_i\overline{v}_j)}{\partial x_j} = \frac{\rho_0 c^2}{2k^2}\,\mathrm{Re}\,\frac{\partial}{\partial x_j}\left(\frac{\partial u}{\partial x_i}\frac{\partial\overline{u}}{\partial x_j}\right) \tag{13}$$

$$= \frac{\rho_0 c^2}{4k^2}\frac{\partial}{\partial x_i}\left((\mathrm{grad}\,u)\cdot(\mathrm{grad}\,\overline{u}) - k^2 u\overline{u}\right). \tag{14}$$

We can write Eq. (12) as $(\partial/\partial x_j)\langle\Pi_{ij}\rangle = 0$ where $\Pi_{ij} = \tilde{p}_2\delta_{ij} + \rho_0\tilde{v}_i^{(1)}\tilde{v}_j^{(1)}$ [6]. The quantity $S_{ij} = -\langle\Pi_{ij}\rangle$ is known as the *acoustic radiation stress tensor*. From Eq. (13), we have

$$S_{ij} = -p_2^0\delta_{ij} - \frac{\rho_0 c^2}{2k^2}\,\mathrm{Re}\left(\frac{\partial u}{\partial x_i}\frac{\partial\overline{u}}{\partial x_j}\right).$$

Integrating Eq. (14) gives (after discarding a constant of integration)

$$-p_2^0 = \frac{\rho_0 c^2}{4k^2}\left((\mathrm{grad}\,u)\cdot(\mathrm{grad}\,\overline{u}) - k^2 u\overline{u}\right) = \langle\mathcal{K}\rangle - \langle\mathcal{V}\rangle,$$

see Eq. (8), and then

$$S_{ij} = \frac{\rho_0 c^2}{4k^2}\left\{\left((\mathrm{grad}\,u)\cdot(\mathrm{grad}\,\overline{u}) - k^2 u\overline{u}\right)\delta_{ij} - \frac{\partial u}{\partial x_i}\frac{\partial\overline{u}}{\partial x_j} - \frac{\partial\overline{u}}{\partial x_i}\frac{\partial u}{\partial x_j}\right\}. \tag{15}$$

As $(\partial/\partial x_j)S_{ij} = 0$, an application of the divergence theorem in the region $\mathcal{D}$ gives

$$\int_{\mathcal{S}} S_{ij}n_j\,\mathrm{d}S = 0. \tag{16}$$

This formula will be used in Section 3.2.

3. Scattering problems

Suppose that we have a scatterer B with boundary S. Surround the scatterer by a sphere of radius R, S_R, implying that we have chosen an origin O in B. We use spherical polar coordinates, r, θ and ϕ, so that S_R is $r = R$.

For scattering problems, we write the total potential as

$$u = u_{\text{inc}} + u_{\text{sc}}, \tag{17}$$

where $u_{\text{inc}}(\boldsymbol{r})$ is the specified incident field, $u_{\text{sc}}(\boldsymbol{r})$ is the unknown scattered field, and u_{sc} satisfies the Sommerfeld radiation condition. Recall that the wavenumber k is real: the fluid is lossless.

3.1. Cross-sections

Let $\mathcal{S} = S \cup S_R$ with $\mathcal{D}$ being the region between S and S_R. Then Eq. (9) gives

$$\operatorname{Im} \int_{S_R} \overline{u}\, \frac{\partial u}{\partial r}\, \mathrm{d}S - \operatorname{Im} \int_S \overline{u}\, \frac{\partial u}{\partial n}\, \mathrm{d}S = 0, \tag{18}$$

where the normal vector on S points out of B. Using Eq. (17), we have

$$\overline{u}\, \frac{\partial u}{\partial r} = \overline{u_{\text{inc}}}\, \frac{\partial u_{\text{inc}}}{\partial r} + \overline{u_{\text{sc}}}\, \frac{\partial u_{\text{inc}}}{\partial r} + \overline{u_{\text{inc}}}\, \frac{\partial u_{\text{sc}}}{\partial r} + \overline{u_{\text{sc}}}\, \frac{\partial u_{\text{sc}}}{\partial r}. \tag{19}$$

Substituting in the first integral in Eq. (18), the first term from Eq. (19) gives

$$\operatorname{Im} \int_{S_R} \overline{u_{\text{inc}}}\, \frac{\partial u_{\text{inc}}}{\partial r}\, \mathrm{d}S = \frac{1}{2\mathrm{i}} \int_{S_R} \left(\overline{u_{\text{inc}}}\, \frac{\partial u_{\text{inc}}}{\partial r} - u_{\text{inc}}\, \frac{\partial\, \overline{u_{\text{inc}}}}{\partial r} \right) \mathrm{d}S = 0,$$

by Green's theorem, assuming that u_{inc} is a regular solution of the Helmholtz equation everywhere inside S_R. Substituting the remaining terms from Eq. (19) in Eq. (18) gives

$$\operatorname{Im} \int_{S_R} \overline{u_{\text{sc}}}\, \frac{\partial u_{\text{sc}}}{\partial r}\, \mathrm{d}S + \operatorname{Im} \int_{S_R} \left(\overline{u_{\text{sc}}}\, \frac{\partial u_{\text{inc}}}{\partial r} - u_{\text{inc}}\, \frac{\partial\, \overline{u_{\text{sc}}}}{\partial r} \right) \mathrm{d}S - \operatorname{Im} \int_S \overline{u}\, \frac{\partial u}{\partial n}\, \mathrm{d}S = 0, \tag{20}$$

using $\operatorname{Im} \overline{w} = -\operatorname{Im} w$ for any complex quantity w.

The first term on the left-hand side of Eq. (20) involves the scattered field only; it is closely related to the *scattering cross-section*. We define

$$\sigma_{\text{sc}} = k \operatorname{Im} \int_{S_R} \overline{u_{\text{sc}}}\, \frac{\partial u_{\text{sc}}}{\partial r}\, \mathrm{d}S, \tag{21}$$

where the factor k has been inserted so that σ_{sc} is dimensionless. Physically, σ_{sc} is proportional to the radiated acoustic power.

The third term on the left-hand side of Eq. (20) involves the total field on S; it is closely related to the *absorption cross-section*. We define

$$\sigma_{\text{ab}} = -k \operatorname{Im} \int_S \overline{u}\, \frac{\partial u}{\partial n}\, \mathrm{d}S. \tag{22}$$

Physically, σ_{ab} represents the acoustic power absorbed by the scatterers (if they are lossy).

Combining Eqs. (1) and (20), we define the *extinction cross-section* by

$$\sigma_{\text{ex}} = \sigma_{\text{sc}} + \sigma_{\text{ab}} = -k \operatorname{Im} \int_{S_R} \left(\overline{u_{\text{sc}}}\, \frac{\partial u_{\text{inc}}}{\partial r} - u_{\text{inc}}\, \frac{\partial\, \overline{u_{\text{sc}}}}{\partial r} \right) \mathrm{d}S. \tag{23}$$

Sometimes, the scattering cross-section is defined as being proportional to $\lim_{R\to\infty} \sigma_{\text{sc}}$; see, for example, [7, §2.A.4]. However, as we shall see below, σ_{sc} does not depend on R. This fact was known to Twersky [8, Eq. (6)] and de Hoop [9, Eq. (4.7)], for example. Indeed, if we write Eq. (21) as

$$\sigma_{\text{sc}} = \frac{k}{2\mathrm{i}} \int_{S_R} \left(\overline{u_{\text{sc}}}\, \frac{\partial u_{\text{sc}}}{\partial r} - u_{\text{sc}}\, \frac{\partial \overline{u_{\text{sc}}}}{\partial r} \right) \mathrm{d}S,$$

we see that we can move the integration surface onto the scatterer itself,

$$\sigma_{\text{sc}} = k \operatorname{Im} \int_S \overline{u_{\text{sc}}}\, \frac{\partial u_{\text{sc}}}{\partial n}\, \mathrm{d}S. \tag{24}$$

The derivation uses Green's theorem, and so it requires that u_{sc} satisfies the Helmholtz equation everywhere between S and S_R, and that the wavenumber k is real (which it is, because the exterior medium is assumed to be lossless).

3.2. Radiation force

The steady acoustic radiation force acting on the (fixed) scatterer S is $\mathbf{F}$ with (real) components

$$F_i = \int_S S_{ij} n_j \, \mathrm{d}S,$$

where S_{ij} is defined by Eq. (15). Moreover, using Eq. (16) with $\mathcal{S} = S \cup S_R$, we can move the surface of integration from S to the sphere S_R enclosing S,

$$F_i = \int_{S_R} S_{ij} \frac{x_j}{R} \, \mathrm{d}S.$$

The fact that the integration surface can be moved is well known [10–12]. The underlying assumption is that the fluid is lossless. For viscous fluids, the situation is more complicated [13].

Let $\Lambda_0 = (\operatorname{grad} u) \cdot (\operatorname{grad} \overline{u}) - k^2 u\overline{u}$. Then, from Eq. (15),

$$F_z = \frac{\rho_0 c^2}{4k^2} \int_{S_R} \left(\Lambda_0 \cos\theta - \frac{\partial u}{\partial z}\frac{\partial \overline{u}}{\partial r} - \frac{\partial \overline{u}}{\partial z}\frac{\partial u}{\partial r} \right) \mathrm{d}S,$$

$$F_x \pm \mathrm{i}F_y = \frac{\rho_0 c^2}{4k^2} \int_{S_R} \left(\Lambda_0 \mathrm{e}^{\pm \mathrm{i}\phi} \sin\theta - \left(\frac{\partial u}{\partial x} \pm \mathrm{i}\frac{\partial u}{\partial y} \right) \frac{\partial \overline{u}}{\partial r} - \left(\frac{\partial \overline{u}}{\partial x} \pm \mathrm{i}\frac{\partial \overline{u}}{\partial y} \right) \frac{\partial u}{\partial r} \right) \mathrm{d}S.$$

In terms of spherical polar coordinates, we have

$$\frac{\partial u}{\partial z} = \cos\theta \frac{\partial u}{\partial r} - \frac{\sin\theta}{r}\frac{\partial u}{\partial \theta}, \quad \operatorname{grad} u = \frac{\partial u}{\partial r}\hat{\boldsymbol{r}} + \frac{1}{r}\frac{\partial u}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{r\sin\theta}\frac{\partial u}{\partial \phi}\hat{\boldsymbol{\phi}},$$

$$\frac{\partial u}{\partial x} \pm \mathrm{i}\frac{\partial u}{\partial y} = \mathrm{e}^{\pm \mathrm{i}\phi} \left(\sin\theta \frac{\partial u}{\partial r} + \frac{\cos\theta}{r}\frac{\partial u}{\partial \theta} \pm \frac{\mathrm{i}}{r\sin\theta}\frac{\partial u}{\partial \phi} \right).$$

Hence

$$F_z = \frac{\rho_0 c^2}{4k^2} \int_{S_R} \Lambda_z \, \mathrm{d}S \quad \text{and} \quad F_x \pm \mathrm{i}F_y = \frac{\rho_0 c^2}{4k^2} \int_{S_R} \Lambda_\pm \mathrm{e}^{\pm \mathrm{i}\phi} \, \mathrm{d}S \tag{25}$$

with

$$\begin{aligned} \Lambda_z = {} & \left(-\frac{\partial u}{\partial r}\frac{\partial \overline{u}}{\partial r} + \frac{1}{r^2}\frac{\partial u}{\partial \theta}\frac{\partial \overline{u}}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial u}{\partial \phi}\frac{\partial \overline{u}}{\partial \phi} - k^2 u\overline{u} \right) \cos\theta \\ & + \frac{\sin\theta}{r} \left(\frac{\partial u}{\partial \theta}\frac{\partial \overline{u}}{\partial r} + \frac{\partial \overline{u}}{\partial \theta}\frac{\partial u}{\partial r} \right), \end{aligned} \tag{26}$$

$$\begin{aligned} \Lambda_\pm = {} & \left(-\frac{\partial u}{\partial r}\frac{\partial \overline{u}}{\partial r} + \frac{1}{r^2}\frac{\partial u}{\partial \theta}\frac{\partial \overline{u}}{\partial \theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial u}{\partial \phi}\frac{\partial \overline{u}}{\partial \phi} - k^2 u\overline{u} \right) \sin\theta \\ & - \frac{\cos\theta}{r} \left(\frac{\partial u}{\partial \theta}\frac{\partial \overline{u}}{\partial r} + \frac{\partial \overline{u}}{\partial \theta}\frac{\partial u}{\partial r} \right) \mp \frac{\mathrm{i}}{r\sin\theta} \left(\frac{\partial u}{\partial \phi}\frac{\partial \overline{u}}{\partial r} + \frac{\partial \overline{u}}{\partial \phi}\frac{\partial u}{\partial r} \right). \end{aligned} \tag{27}$$

Formulas of this kind can be found in [6,14,15]. In most of these papers, it is assumed that S_R is a large sphere and then asymptotic estimates based on the assumption that $kR \gg 1$ are used. This is awkward because certain quantities involving u_{inc} diverge as $kR \to \infty$. For further discussion, see Section 5.1.

4. Use of spherical wavefunctions

In the vicinity of the sphere S_R, we can expand u_{inc} and u_{sc} as follows,

$$u_{\mathrm{inc}}(\boldsymbol{r}) = \sum_{n,m} D_n^m j_n(kr) \tilde{Y}_n^m(\hat{\boldsymbol{r}}), \tag{28}$$

$$u_{\mathrm{sc}}(\boldsymbol{r}) = \sum_{n,m} C_n^m h_n(kr) \tilde{Y}_n^m(\hat{\boldsymbol{r}}), \tag{29}$$

where (using the notation from [16])

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

j_n is a spherical Bessel function, $h_n \equiv h_n^{(1)}$ is a spherical Hankel function, $\tilde{Y}_n^m$ is a spherical harmonic, $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$, and D_n^m and C_n^m are coefficients. We use unnormalised spherical harmonics

$$\tilde{Y}_n^m(\hat{\boldsymbol{r}}) = P_n^m(\cos\theta)\,\mathrm{e}^{\mathrm{i}m\phi},$$

where the associated Legendre functions P_n^m satisfy the orthogonality relation

$$\int_{-1}^{1} P_n^m(t)\,P_\nu^m(t)\,\mathrm{d}t = h_n^m \delta_{n\nu} \quad \text{with} \quad h_n^m = \frac{2}{2n+1}\frac{(n+m)!}{(n-m)!}. \tag{30}$$

It is more convenient to use $\tilde{Y}_n^m$ instead of the normalised functions Y_n^m (with $Y_n^m = A_n^m \tilde{Y}_n^m$ and $A_n^m = \left(2\pi h_n^m\right)^{-1/2}$) because, when calculating $\mathbf{F}$, we shall encounter contiguous spherical harmonics, $\tilde{Y}_{n+1}^{m\pm1}$.

On S_R, we have $\mathrm{d}S = R^2\,\mathrm{d}\Omega(\hat{\boldsymbol{r}})$, where Ω is the unit sphere. The spherical harmonics are orthogonal,

$$\int_\Omega \tilde{Y}_n^m\,\overline{\tilde{Y}_\nu^\mu}\,\mathrm{d}\Omega = 2\pi h_n^m \delta_{n\nu}\,\delta_{m\mu}. \tag{31}$$

4.1. Cross-sections

Starting with Eq. (21), direct calculation (put $D_n^m = 0$ in Eq. (A.4)) gives

$$\sigma_{\mathrm{sc}} = 2\pi \sum_{n,m} h_n^m \left|C_n^m\right|^2. \tag{32}$$

Similarly, starting with Eq. (23) (put $D_n^m = E_n^m = 0$ and $F_n^m = D_n^m$ in Eq. (A.3)),

$$\sigma_{\mathrm{ex}} = -2\pi\,\mathrm{Im}\sum_{n,m} \mathrm{i}\,h_n^m\,\overline{C_n^m}\,D_n^m = -2\pi\,\mathrm{Re}\sum_{n,m} h_n^m\,C_n^m\,\overline{D_n^m}. \tag{33}$$

4.2. Radiation force: F_z

The axial component of $\mathbf{F}$, F_z, is given by Eqs. (25) and (26). Expand the total potential as

$$u = \sum_{n,m} w_n^m(kr)\,\tilde{Y}_n^m(\theta,\phi) \quad \text{with} \quad w_n^m(kr) = D_n^m\,j_n(kr) + C_n^m\,h_n(kr). \tag{34}$$

Then, inspection of Eq. (26) suggests that the simplest term in Λ_z gives the contribution

$$\begin{aligned} I_1 &\equiv \int_{S_R} k^2 u\,\bar{u}\cos\theta\,\mathrm{d}S = 2\pi(kR)^2 \sum_{n,m}\sum_{\nu=0}^{\infty} w_n^m\,\overline{w_\nu^m} \int_0^\pi P_n^m(\cos\theta)\,P_\nu^m(\cos\theta)\cos\theta\,\sin\theta\,\mathrm{d}\theta \\ &= 2\pi(kR)^2 \sum_{\nu=1}^{\infty} w_0^0\,\overline{w_\nu^0} \int_{-1}^{1} t\,P_\nu(t)\,\mathrm{d}t + 2\pi(kR)^2 \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{\nu=0}^{\infty} w_n^m\,\overline{w_\nu^m} \int_{-1}^{1} tP_n^m(t)\,P_\nu^m(t)\,\mathrm{d}t \end{aligned}$$

where $w_n^m \equiv w_n^m(kR)$ and we have separated off the contribution from $n = 0$. The first integral is $\frac{2}{3}\delta_{\nu,1}$. The second integral can be evaluated using [16, Eq. (A.13)]

$$(2\nu+1)tP_\nu^m(t) = (\nu-m+1)P_{\nu+1}^m(t) + (\nu+m)P_{\nu-1}^m(t)$$

and the orthogonality relation, Eq. (30):

$$\int_{-1}^{1} tP_n^m(t)\,P_\nu^m(t)\,\mathrm{d}t = \frac{h_n^m}{2\nu+1}\left\{(n-m)\delta_{\nu,n-1} + (n+m+1)\delta_{\nu,n+1}\right\}. \tag{35}$$

Note that the term containing $\delta_{\nu,n-1}$ is absent when $|m| = n$ because $P_\nu^m \equiv 0$ when $|m| > \nu$. Hence

$$\begin{aligned} I_1 &= \frac{4\pi}{3}(kR)^2 w_0^0\overline{w_1^0} + (kR)^2 \sum_{n=1}^{\infty}\sum_{m=-(n-1)}^{n-1} \frac{4\pi(n+m)!\,w_n^m\,\overline{w_{n-1}^m}}{(2n-1)(2n+1)(n-1-m)!} \\ &\quad + (kR)^2 \sum_{n=1}^{\infty}\sum_{m=-n}^{n} \frac{4\pi(n+m+1)!\,w_n^m\,\overline{w_{n+1}^m}}{(2n+3)(2n+1)(n-m)!} \\ &= 4\pi(kR)^2 \sum_{n,m} \mathcal{Z}_n^m \left\{w_n^m\,\overline{w_{n+1}^m} + w_{n+1}^m\overline{w_n^m}\right\}, \end{aligned} \tag{36}$$

where

$$\mathcal{Z}_n^m = \frac{(n+m+1)!}{(2n+3)(2n+1)(n-m)!}.$$

Similarly,

$$I_2 \equiv \int_{S_R} \frac{\partial u}{\partial r}\frac{\partial \overline{u}}{\partial r}\cos\theta \,\mathrm{d}S = 4\pi(kR)^2 \sum_{n,m} \mathcal{Z}_n^m \left\{ w_n^{m\prime}\,\overline{w_{n+1}^{m\prime}} + \overline{w_n^{m\prime}}\, w_{n+1}^{m\prime} \right\}. \tag{37}$$

The remaining terms in Eq. (26) make the following contributions.

$$I_3 \equiv \int_{S_R} \frac{1}{r^2}\left(\frac{\partial u}{\partial \theta}\frac{\partial \overline{u}}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial u}{\partial \phi}\frac{\partial \overline{u}}{\partial \phi}\right)\cos\theta \,\mathrm{d}S \tag{38}$$

$$= 4\pi \sum_{n,m} n(n+2)\mathcal{Z}_n^m \left\{ w_n^m\,\overline{w_{n+1}^m} + \overline{w_n^m}\, w_{n+1}^m \right\}, \tag{39}$$

$$I_4 \equiv \int_{S_R} \frac{\sin\theta}{r}\left(\frac{\partial u}{\partial \theta}\frac{\partial \overline{u}}{\partial r} + \frac{\partial u}{\partial r}\frac{\partial \overline{u}}{\partial \theta}\right)\mathrm{d}S \tag{40}$$

$$= 4\pi(kR)\sum_{n,m} \mathcal{Z}_n^m \left\{ n\left(w_n^m\overline{w_{n+1}^{m\prime}} + w_{n+1}^{m\prime}\overline{w_n^m}\right) - (n+2)\left(w_{n+1}^m\overline{w_n^{m\prime}} + w_n^{m\prime}\,\overline{w_{n+1}^m}\right)\right\}. \tag{41}$$

These integrals are evaluated in the Appendix.

From Eqs. (25) and (26), we have

$$F_z = \frac{\rho_0 c^2}{4k^2}\left(-I_1 - I_2 + I_3 + I_4\right) = -\frac{\pi\rho_0 c^2}{k^2}\sum_{n,m} \mathcal{Z}_n^m \left(\mathcal{Q}_n^m + \overline{\mathcal{Q}_n^m}\right) \tag{42}$$

where

$$\mathcal{Q}_n^m = s^2\left(w_n^m\,\overline{w_{n+1}^m} + w_n^{m\prime}\,\overline{w_{n+1}^{m\prime}}\right) - n(n+2)w_n^m\,\overline{w_{n+1}^m} - snw_n^m\overline{w_{n+1}^{m\prime}} + s(n+2)w_n^{m\prime}\,\overline{w_{n+1}^m}, \tag{43}$$

$w_n^m \equiv w_n^m(s)$ and $s = kR$. In fact, as we know that F_z does not depend on R, $\mathcal{Q}_n^m$ cannot depend on s; this provides a check on subsequent calculations.

Recall that w_n^m is given by Eq. (34). Letting z_n denote j_n or h_n, we have

$$(n+2)\,z_{n+1}(s) = s\{z_n(s) - z_{n+1}'(s)\}, \quad nz_n(s) = s\{z_n'(s) + z_{n+1}(s)\}$$

whence

$$(n+2)\,w_{n+1}^m = s\{D_{n+1}^m j_n + C_{n+1}^m h_n - w_{n+1}^{m\prime}\}, \quad nw_n^m = s\{w_n^{m\prime} + D_n^m j_{n+1} + C_n^m h_{n+1}\}. \tag{44}$$

Using these in Eq. (43),

$$\begin{aligned}
s^{-2}\mathcal{Q}_n^m &= w_n^m\,\overline{w_{n+1}^m} + w_n^{m\prime}\,\overline{w_{n+1}^{m\prime}} - \left(w_n^{m\prime} + D_n^m j_{n+1} + C_n^m h_{n+1}\right)\left(\overline{D_{n+1}^m} j_n + \overline{C_{n+1}^m h_n} - \overline{w_{n+1}^{m\prime}}\right)\\
&\quad - \left(w_n^{m\prime} + D_n^m j_{n+1} + C_n^m h_{n+1}\right)\overline{w_{n+1}^{m\prime}} + w_n^{m\prime}\left(\overline{D_{n+1}^m} j_n + \overline{C_{n+1}^m h_n} - \overline{w_{n+1}^{m\prime}}\right)\\
&= w_n^m\,\overline{w_{n+1}^m} - \left(D_n^m j_{n+1} + C_n^m h_{n+1}\right)\left(\overline{D_{n+1}^m} j_n + \overline{C_{n+1}^m h_n}\right)\\
&= \left(D_n^m j_n + C_n^m h_n\right)\left(\overline{D_{n+1}^m} j_{n+1} + \overline{C_{n+1}^m h_{n+1}}\right) - \left(D_n^m j_{n+1} + C_n^m h_{n+1}\right)\left(\overline{D_{n+1}^m} j_n + \overline{C_{n+1}^m h_n}\right)\\
&= D_n^m\,\overline{C_{n+1}^m}\left(j_n\,\overline{h_{n+1}} - j_{n+1}\overline{h_n}\right) + C_n^m\overline{D_{n+1}^m}\left(h_n j_{n+1} - h_{n+1}j_n\right) + C_n^m\overline{C_{n+1}^m}\left(h_n\overline{h_{n+1}} - h_{n+1}\overline{h_n}\right)\\
&= \mathrm{i}s^{-2}\left(D_n^m\overline{C_{n+1}^m} + C_n\overline{D_{n+1}^m} + 2C_n^m\overline{C_{n+1}^m}\right),
\end{aligned}$$

using [17, 10.50.3]. As expected, $\mathcal{Q}_n^m$ does not depend on s. In addition, the terms involving products of spherical Bessel functions cancel: there are no radiation forces without scattering.

Substitution in Eq. (42) gives

$$F_z = \frac{2\pi\rho_0 c^2}{k^2}\sum_{n,m} \mathcal{Z}_n^m \,\mathrm{Im}\left(D_n^m\,\overline{C_{n+1}^m} + C_n\overline{D_{n+1}^m} + 2C_n^m\overline{C_{n+1}^m}\right). \tag{45}$$

4.3. Radiation force: F_x and F_y

Consider $F_x \pm \mathrm{i}F_y$, defined by Eqs. (25), (27) and (34). As F_x and F_y are real, we choose to calculate $F_x - \mathrm{i}F_y$ without loss of generality. The following results are found; see the Appendix for details. First,

$$I_5 \equiv \int_{S_R} k^2 u\overline{u}\,\mathrm{e}^{-\mathrm{i}\phi}\sin\theta\,\mathrm{d}S = 4\pi(kR)^2 \sum_{n,m}\left\{\mathcal{X}_n^m\, w_{n+1}^{m+1}\,\overline{w_n^m} - \mathcal{Y}_n^m\, w_n^m\,\overline{w_{n+1}^{m-1}}\right\}, \tag{46}$$

$$I_6 \equiv \int_{S_R} \frac{\partial u}{\partial r}\frac{\partial \overline{u}}{\partial r}\,\mathrm{e}^{-\mathrm{i}\phi}\sin\theta\,\mathrm{d}S = 4\pi(kR)^2 \sum_{n,m}\left\{\mathcal{X}_n^m\, w_{n+1}^{m+1\prime}\,\overline{w_n^{m\prime}} - \mathcal{Y}_n^m\, w_n^{m\prime}\,\overline{w_{n+1}^{m-1\prime}}\right\}, \tag{47}$$

where

$$\mathcal{X}_n^m = \frac{(n+m+2)!}{(2n+3)(2n+1)(n-m)!} \quad \text{and} \quad \mathcal{Y}_n^m = \frac{(n+m)!}{(2n+3)(2n+1)(n-m)!}.$$

Two further pieces are as follows:

$$I_7 \equiv \int_{S_R} \frac{1}{r^2}\left(\frac{\partial u}{\partial\theta}\frac{\partial\overline{u}}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial u}{\partial\phi}\frac{\partial\overline{u}}{\partial\phi}\right)\mathrm{e}^{-\mathrm{i}\phi}\sin\theta\,\mathrm{d}S \tag{48}$$

$$= 4\pi\sum_{n,m} n(n+2)\left\{\mathcal{X}_n^m\, w_{n+1}^{m+1}\overline{w_n^m} - \mathcal{Y}_n^m\, w_n^m\,\overline{w_{n+1}^{m-1}}\right\}, \tag{49}$$

$$I_8 \equiv \int_{S_R}\left\{-\frac{\cos\theta}{r}\left(\frac{\partial u}{\partial\theta}\frac{\partial\overline{u}}{\partial r} + \frac{\partial\overline{u}}{\partial\theta}\frac{\partial u}{\partial r}\right) + \frac{\mathrm{i}}{r\sin\theta}\left(\frac{\partial u}{\partial\phi}\frac{\partial\overline{u}}{\partial r} + \frac{\partial\overline{u}}{\partial\phi}\frac{\partial u}{\partial r}\right)\right\}\mathrm{e}^{-\mathrm{i}\phi}\,\mathrm{d}S \tag{50}$$

$$= 4\pi kR\sum_{n,m}\mathcal{X}_n^m\left\{n w_{n+1}^{m+1\prime}\,\overline{w_n^m} - (n+2)w_{n+1}^{m+1}\overline{w_n^{m\prime}}\right\}$$
$$- 4\pi kR\sum_{n,m}\mathcal{Y}_n^m\left\{n w_n^m\,\overline{w_{n+1}^{m-1\prime}} - (n+2)w_n^{m\prime}\,\overline{w_{n+1}^{m-1}}\right\}. \tag{51}$$

From Eqs. (25) and (27), we have

$$F_x - \mathrm{i}F_y = \frac{\rho_0 c^2}{4k^2}\left(-I_5 - I_6 + I_7 + I_8\right) = -\frac{\pi\rho_0 c^2}{k^2}\sum_{n,m}\left\{\mathcal{X}_n^m\xi_n^m - \mathcal{Y}_n^m\eta_n^m\right\} \tag{52}$$

where

$$\xi_n^m = s^2\big(w_{n+1}^{m+1}\overline{w_n^m} + w_{n+1}^{m+1\prime}\,\overline{w_n^{m\prime}}\big) - n(n+2)w_{n+1}^{m+1}\overline{w_n^m} - s\big(n w_{n+1}^{m+1\prime}\,\overline{w_n^m} - (n+2)w_{n+1}^{m+1}\overline{w_n^{m\prime}}\big),$$
$$\eta_n^m = s^2\big(w_n^m\,\overline{w_{n+1}^{m-1}} + w_n^{m\prime}\,\overline{w_{n+1}^{m-1\prime}}\big) - n(n+2)\,w_n^m\,\overline{w_{n+1}^{m-1}} + s\big((n+2)w_n^{m\prime}\,\overline{w_{n+1}^{m-1}} - n w_n^m\,\overline{w_{n+1}^{m-1\prime}}\big).$$

Making use of Eqs. (34) and (44),

$$\begin{aligned}
s^{-2}\xi_n^m &= w_{n+1}^{m+1}\overline{w_n^m} + w_{n+1}^{m+1\prime}\,\overline{w_n^{m\prime}} - \{D_{n+1}^{m+1}j_n + C_{n+1}^{m+1}h_n - w_{n+1}^{m+1\prime}\}\{\overline{w_n^{m\prime}} + \overline{D_n^m}j_{n+1} + \overline{C_n^m}\,\overline{h_{n+1}}\}\\
&\quad - w_{n+1}^{m+1\prime}\{\overline{w_n^{m\prime}} + \overline{D_n^m}\,j_{n+1} + \overline{C_n^m}\,\overline{h_{n+1}}\} + \overline{w_n^{m\prime}}\{D_{n+1}^{m+1}\,j_n + C_{n+1}^{m+1}h_n - w_{n+1}^{m+1\prime}\}\\
&= w_{n+1}^{m+1}\,\overline{w_n^m} - (D_{n+1}^{m+1}\,j_n + C_{n+1}^{m+1}h_n)(\overline{D_n^m}\,j_{n+1} + \overline{C_n^m}\,\overline{h_{n+1}})\\
&= C_{n+1}^{m+1}\,\overline{D_n^m}\,(j_n h_{n+1} - j_{n+1}h_n) + \overline{C_n^m}\,D_{n+1}^{m+1}(j_{n+1}\overline{h_n} - j_n\overline{h_{n+1}})\\
&\quad + \overline{C_n^m}\,C_{n+1}^{m+1}(h_{n+1}\overline{h_n} - \overline{h_{n+1}}h_n)\\
&= -\mathrm{i}s^{-2}\left\{C_{n+1}^{m+1}\overline{D_n^m} + \overline{C_n^m}D_{n+1}^{m+1} + 2\overline{C_n^m}C_{n+1}^{m+1}\right\}.
\end{aligned} \tag{53}$$

Similarly

$$\eta_n^m = \mathrm{i}\left\{\overline{C_{n+1}^{m-1}}D_n^m + C_n^m\overline{D_{n+1}^{m-1}} + 2C_n^m\overline{C_{n+1}^{m-1}}\right\}. \tag{54}$$

Substitution in Eq. (52) then gives F_x and F_y:

$$F_x - \mathrm{i}F_y = \mathrm{i}\frac{\pi\rho_0 c^2}{k^2}\sum_{n,m}\mathcal{X}_n^m\left\{C_{n+1}^{m+1}\overline{D_n^m} + \overline{C_n^m}D_{n+1}^{m+1} + 2\overline{C_n^m}C_{n+1}^{m+1}\right\}$$
$$+ \mathrm{i}\frac{\pi\rho_0 c^2}{k^2}\sum_{n,m}\mathcal{Y}_n^m\left\{\overline{C_{n+1}^{m-1}}D_n^m + C_n^m\overline{D_{n+1}^{m-1}} + 2C_n^m\overline{C_{n+1}^{m-1}}\right\}. \tag{55}$$

4.4. Radiation force: summary and discussion

Our expressions for the components of the radiation force **F** are exact, they are applicable to scatterers of any shape, and for arbitrary incident fields (provided u_{inc} is a regular wavefunction between S and S_R). Similar formulas can be found in [18, Eqs. (11)–(13)], [15, p. 28] and [19, p. 666]. Unfortunately, the derivations in these papers contain errors; we return to these in Section 5.2.

5. Use of far-field approximations

Let us introduce the far-field pattern, $f(\hat{\boldsymbol{r}})$, defined by

$$u_{\text{sc}}(\boldsymbol{r}) \sim (\mathrm{i}kr)^{-1}\,\mathrm{e}^{\mathrm{i}kr} f(\hat{\boldsymbol{r}}) \quad \text{as } r \to \infty. \tag{56}$$

When u_{sc} is expanded as Eq. (29), we obtain

$$f(\hat{\boldsymbol{r}}) = \sum_{n,m} (-\mathrm{i})^n\, C_n^m\, \tilde{Y}_n^m(\hat{\boldsymbol{r}}). \tag{57}$$

Formally, this formula is obtained by inserting the asymptotic approximation [17, 10.52.4],

$$h_n(w) \sim (-\mathrm{i})^n (\mathrm{i}w)^{-1} \mathrm{e}^{\mathrm{i}w} \quad \text{as } w \to \infty, \tag{58}$$

into Eq. (29). However, although Eq. (57) is correct, we wrote "formally" because the approximation Eq. (58) is not uniform in n: it holds for fixed n. This difficulty was noted explicitly by Müller [20, p. 241]. For full justification, we follow Colton and Kress [21, Theorem 2.16]. First, as u_{sc} satisfies the Sommerfeld radiation condition, $f(\hat{\boldsymbol{r}})$ is well defined [21, Theorem 2.6] and it has an expansion $f(\hat{\boldsymbol{r}}) = \sum_{n,m} F_n^m \tilde{Y}_n^m(\hat{\boldsymbol{r}})$ for certain coefficients F_n^m. We want to show that $F_n^m = (-\mathrm{i})^n C_n^m$. Using Eq. (31), we obtain

$$\begin{aligned}
2\pi h_n^m F_n^m &= \int_\Omega f(\hat{\boldsymbol{r}})\, \overline{\tilde{Y}_n^m(\hat{\boldsymbol{r}})}\, \mathrm{d}\Omega = \int_\Omega \lim_{r\to\infty} \left\{ \mathrm{i}kr\, \mathrm{e}^{-\mathrm{i}kr} u_{\text{sc}}(\boldsymbol{r}) \right\} \overline{\tilde{Y}_n^m(\hat{\boldsymbol{r}})}\, \mathrm{d}\Omega \\
&= \lim_{r\to\infty} \left\{ \mathrm{i}kr\, \mathrm{e}^{-\mathrm{i}kr} \int_\Omega u_{\text{sc}}(\boldsymbol{r})\, \overline{\tilde{Y}_n^m(\hat{\boldsymbol{r}})}\, \mathrm{d}\Omega \right\} = \lim_{r\to\infty} \left\{ \mathrm{i}kr\, \mathrm{e}^{-\mathrm{i}kr} (2\pi) h_n^m C_n^m h_n(kr) \right\} \\
&= 2\pi h_n^m C_n^m \lim_{r\to\infty} \left\{ \mathrm{i}kr\, \mathrm{e}^{-\mathrm{i}kr} h_n(kr) \right\} = 2\pi h_n^m (-\mathrm{i})^n C_n^m,
\end{aligned}$$

giving the desired result.

From Eqs. (57) and (32), we obtain a well-known formula for the scattering cross-section,

$$\int_\Omega \left| f(\hat{\boldsymbol{r}}) \right|^2 \mathrm{d}\Omega = 2\pi \sum_{n,m} h_n^m \left| C_n^m \right|^2 = \sigma_{\text{sc}}. \tag{59}$$

The formula Eq. (33) for the extinction cross-section, σ_{ex}, involves the incident field through the coefficients D_n^m; we return to this complication in Section 5.1.

Next consider F_z, given by Eq. (45). One piece of this formula involves products of the coefficients C_n^m; this piece can be expressed in terms of f. Specifically, following the calculation of I_1, see Eq. (36), we find

$$\begin{aligned}
\int_\Omega \left| f(\hat{\boldsymbol{r}}) \right|^2 \cos\theta\, \mathrm{d}\Omega &= 4\pi \sum_{n,m} \mathcal{Z}_n^m \left\{ \mathrm{i} C_n^m \overline{C_{n+1}^m} + \overline{\mathrm{i} C_n^m \overline{C_{n+1}^m}} \right\} \\
&= -8\pi \sum_{n,m} \mathcal{Z}_n^m \operatorname{Im}\left(C_n^m \overline{C_{n+1}^m} \right).
\end{aligned}$$

Indeed, formally, this result can be obtained by using Eq. (36) with $u = u_{\text{sc}}$, together with Eqs. (56) and (58).

Similarly, following the calculation of I_5, see Eq. (46),

$$\int_\Omega \left| f(\hat{\boldsymbol{r}}) \right|^2 \mathrm{e}^{-\mathrm{i}\phi} \sin\theta\, \mathrm{d}\Omega = -4\pi \mathrm{i} \sum_{n,m} \left\{ \mathcal{X}_n^m \overline{C_n^m} C_{n+1}^{m+1} + \mathcal{Y}_n^m C_n^m \overline{C_{n+1}^{m-1}} \right\},$$

and it is exactly this quantity that appears in the formula for $F_x - \mathrm{i}F_y$, Eq. (55).

5.1. Direct calculations avoiding wavefunction expansions

The formula Eq. (59) giving the scattering cross-section in terms of the far-field pattern suggests a direct evaluation, using the definitions Eqs. (21) and (56). The error in Eq. (56) is $O((kr)^{-2})$ as $kr \to \infty$ so that, assuming $kR \gg 1$, Eq. (21) gives

$$\sigma_{\text{sc}} = k \operatorname{Im} \int_\Omega \left(\frac{\mathrm{e}^{-\mathrm{i}kR}}{-\mathrm{i}kR} \overline{f(\hat{\boldsymbol{r}})} + O((kR)^{-2}) \right) \left(\frac{\mathrm{e}^{\mathrm{i}kR}}{R} f(\hat{\boldsymbol{r}}) + O((kR)^{-2}) \right) R^2\, \mathrm{d}\Omega(\hat{\boldsymbol{r}});$$

taking the limit $R \to \infty$ gives Eq. (59), as expected. Similar calculations can be made for terms involving products of $u_{\rm sc}$ with itself in the formulas for the radiation force; these formulas come by substituting $u = u_{\rm sc} + u_{\rm inc}$ in Λ_z and $\Lambda_\pm$, defined by Eqs. (26) and (27), respectively. Clearly, simple calculations succeed because $u_{\rm sc}$ decays as R^{-1} on S_R whereas $\mathrm{d}S = R^2\,\mathrm{d}\Omega$: the powers of R balance.

The situation is less clear when cross terms are considered, involving products of $u_{\rm inc}$ and $u_{\rm sc}$. The simplest example of this occurs with the extinction cross-section, defined by Eq. (23), which we write as

$$\sigma_{\rm ex} = \lim_{R\to\infty} kR^2 \,\mathrm{Im} \int_\Omega \left(u_{\rm sc} \frac{\partial \overline{u_{\rm inc}}}{\partial r} - \overline{u_{\rm inc}} \frac{\partial u_{\rm sc}}{\partial r} \right) \mathrm{d}\Omega. \tag{60}$$

If we insert the far-field approximation for $u_{\rm sc}$, Eq. (56), we obtain, tentatively,

$$\sigma_{\rm ex} = \lim_{R\to\infty} kR \,\mathrm{Im} \int_\Omega \left(\frac{1}{\mathrm{i}k} \frac{\partial \overline{u_{\rm inc}}}{\partial r} - \overline{u_{\rm inc}} \right) \mathrm{e}^{\mathrm{i}kR} f(\hat{\boldsymbol{r}})\,\mathrm{d}\Omega(\hat{\boldsymbol{r}}). \tag{61}$$

At first sight, we may worry about the existence of the limit in Eq. (61) for an arbitrary regular incident wave (although we know that $\sigma_{\rm ex}$ itself does not depend on R so that the limit in Eq. (60) certainly exists), and we may worry that we should include the next term in Eq. (56), the term that decays as $(kr)^{-2}$ (which can be calculated in terms of certain derivatives of f, see [22, Corollary 3.8], for example).

It turns out that these anxieties do not cause further difficulties: the limit in Eq. (61) does exist, and the limit can be computed for quite general incident waves; and the omitted term from Eq. (56) leads to a zero contribution in the limit. Similar results can be proved for the computation of the radiation force. For more details, see [23].

5.2. Further remarks

The simplifications following from the introduction of the far-field approximation of the scattered field have encouraged some authors to introduce analogous approximations for the incident field. To examine this possibility, suppose that $u_{\rm inc}$ is a regular solution of the Helmholtz equation everywhere: we do not permit (singular) sources outside S because these would prevent moving the integration surface from S to S_R. Three examples are of interest:

1. For an incident plane wave, $u_{\rm inc}(\boldsymbol{r}) = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})$ where $\boldsymbol{k}$ is a constant vector with $|\boldsymbol{k}| = k$. Of course, plane waves do not decay as $r \to \infty$: indeed, $|u_{\rm inc}| = 1$ everywhere.
2. For an axisymmetric Bessel beam,
$$u_{\rm inc}(\boldsymbol{r}) = \exp(\mathrm{i}kr\cos\theta\cos\beta) J_0(kr\sin\theta\sin\beta),$$
where β is a real parameter and J_0 is a Bessel function. We see that $u_{\rm inc}$ decays as $(kr)^{-1/2}$ in all directions $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$ except along the axis ($\theta = 0, \pi$).
3. The incident field could be generated using a plane-wave representation (Herglotz wavefunction, angular spectral representation),
$$u_{\rm inc}(\boldsymbol{r}) = \int_\Omega q(\hat{\boldsymbol{s}})\,\mathrm{e}^{\mathrm{i}k\boldsymbol{r}\cdot\hat{\boldsymbol{s}}}\,\mathrm{d}\Omega(\hat{\boldsymbol{s}}), \tag{62}$$
where q is a chosen density function, defined on the unit sphere Ω.

When $u_{\rm inc}$ is defined by Eq. (62), its far-field behaviour depends crucially on the properties of q. If q is smooth and bounded, then

$$u_{\rm inc}(\boldsymbol{r}) \sim 2\pi q(\hat{\boldsymbol{r}}) \frac{\mathrm{e}^{\mathrm{i}kr}}{\mathrm{i}kr} - 2\pi q(-\hat{\boldsymbol{r}}) \frac{\mathrm{e}^{-\mathrm{i}kr}}{\mathrm{i}kr}, \quad \text{as } r \to \infty, \text{ for all directions } \hat{\boldsymbol{r}}. \tag{63}$$

This result is sometimes known as the *Jones lemma* [24], [25, Appendix XII]. However, if q is not smooth and bounded, then $u_{\rm inc}$ need not behave as in Eq. (63). For more examples and a detailed study, see [26].

We conclude that Eq. (63) is not always true (despite claims to the contrary [27, p. 154]). When Eq. (63) is true, it shows that $u_{\rm inc}$ behaves in the far field as the sum of an outgoing spherical wave and an incoming spherical wave.

A plausible strategy for effecting the split in Eq. (63) proceeds by substituting $2j_n = h_n + \overline{h_n} = h_n^{(1)} + h_n^{(2)}$ in the expansion Eq. (28),

$$\begin{aligned} u_{\rm inc}(\boldsymbol{r}) &= \sum_{n,m} D_n^m \left(h_n^{(1)}(kr) + h_n^{(2)}(kr) \right) \tilde{Y}_n^m(\hat{\boldsymbol{r}}) \\ &= \sum_{n,m} D_n^m h_n^{(1)}(kr) \tilde{Y}_n^m(\hat{\boldsymbol{r}}) + \sum_{n,m} D_n^m h_n^{(2)}(kr) \tilde{Y}_n^m(\hat{\boldsymbol{r}}). \end{aligned}$$

Although this seems to break $u_{\rm inc}$ into the sum of an outgoing spherical wave (first sum) and an incoming spherical wave (second sum), the second equality may be false: splitting the sum into two may result in two divergent series. To see this

clearly, consider an incident plane wave,

$$u_{\text{inc}} = \mathrm{e}^{\mathrm{i}kz} = \sum_{n=0}^{\infty}(2n+1)\,\mathrm{i}^n j_n(kr)P_n(\cos\theta). \tag{64}$$

For fixed kr, the terms in the series decay rapidly because $(2n+1)j_n(kr) \sim (kr)^n/(2n-1)!!$ as $n \to \infty$ [17, 10.52.1]; the Legendre polynomials P_n satisfy $P_n(1) = 1$, $P_n(-1) = (-1)^n$ and $P_n(\cos\theta) = O(n^{-1/2})$ as $n \to \infty$ for θ bounded away from 0 and π. On the other hand, both $h_n^{(1)}$ and $h_n^{(2)}$ grow rapidly with n [17, 10.52.2].

The error described above is often compounded by assuming further that $kr \gg 1$, so that $h_n^{(1)}(kr)$ and $h_n^{(2)}(kr)$ are replaced by their large-kr approximations (see Eq. (58)) or, equivalently, $j_n(kr)$ is replaced by $(kr)^{-1}\sin(kr - \frac{1}{2}n\pi)$ [17, 10.52.3]; see, for example, [18, Eq. (4)], [15, p. 34], [19, p. 666] and (for an analogous two-dimensional problem) [28, Eq. (20)]. Using this approximation for j_n in Eq. (64) leads to

$$u_{\text{inc}} = \mathrm{e}^{\mathrm{i}kr\cos\theta} \simeq \frac{1}{kr}\sum_{n=0}^{\infty}(2n+1)\,\mathrm{i}^n \sin\left(kr - \frac{n\pi}{2}\right)P_n(\cos\theta); \tag{65}$$

apart from the fact that the series is divergent, the factor $(kr)^{-1}$ leads to the erroneous conclusion that $u_{\text{inc}} \to 0$ as $r \to \infty$ (as stated in [15, Appendix C], for example).

5.3. Debye (1909)

It is of interest to examine Debye's famous 1909 paper [29] in which he calculated the electromagnetic radiation force due to a plane wave interacting with a sphere. His calculations are reminiscent of those in Section 4.2; compare [29, Eq. (57)] with Eq. (42). Then, whereas we used Wronskians to simply further, going from Eq. (42) to Eq. (45), Debye uses the large-argument asymptotic approximations for $j_n(kr)$ and $h_n(kr)$, giving [29, Eq. (58)], which still depends on kr. Perhaps fortunately, this is not the end of the calculation because he has to combine [29, Eq. (58)] with [29, Eq. (58′)]; the sum of these two equations does not depend on kr.

6. Use of the T-matrix

At this stage we have said very little about the scatterer S: its shape, size and constitution have not played an explicit role. However, in order to use the exact formulas presented above, we have to be able to compute the coefficients C_n^m in the expansion Eq. (29) given the coefficients D_n^m in the expansion Eq. (28). As the (first-order) scattering problem is linear, the relation between these coefficients is linear. It can be encoded in Waterman's T-matrix,

$$C_n^m = \sum_{\nu,\mu} \tilde{T}_{n\nu}^{m\mu} D_\nu^\mu; \tag{66}$$

recall that we are using unnormalised spherical harmonics, which explains the notation $\tilde{T}_{n\nu}^{m\mu}$ for the entries in the T-matrix.

Much is known about the T-matrix, including how to compute it efficiently for many kinds of scatterers. In particular, for homogeneous spherical scatterers, T is diagonal, so that we can write $C_n^m = R_n^m D_n^m$, where R_n^m depends on the details of the sphere (size, boundary condition, internal composition); see, for example, [15, Eq. (5)]. For more information and references, see [16, Chapter 7].

When Eq. (66) is substituted in Eqs. (32) and (33), we obtain

$$\sigma_{\text{sc}} = 2\pi \sum_{n,m}\sum_{\nu,\mu} h_n^m \overline{D_n^m} D_\nu^\mu \sum_{\nu',\mu'} \overline{\tilde{T}_{\nu' n}^{\mu' m}}\, \tilde{T}_{\nu'\nu}^{\mu'\mu}, \tag{67}$$

$$\sigma_{\text{ex}} = -\pi \sum_{n,m}\sum_{\nu,\mu} \overline{D_n^m} D_\nu^\mu \left(h_n^m \tilde{T}_{n\nu}^{m\mu} + h_\nu^\mu \overline{\tilde{T}_{\nu n}^{\mu m}}\right). \tag{68}$$

For lossless scatterers, the identity $\sigma_{\text{sc}} = \sigma_{\text{ex}}$ combined with the arbitrary nature of the incident field leads to a relation that must be satisfied by the T-matrix; see [16, Theorem 7.4], where the restriction to lossless scatterers was overlooked.

The far-field pattern can be expressed in terms of the T-matrix: substitute Eq. (66) in Eq. (57).

Clearly, T-matrix methods can be used to compute radiation forces by substituting Eq. (66) in Eq. (45), for example. However, although these methods have been used for computing electromagnetic radiation forces [30], we are aware of only one recent study in which T-matrix methods have been used to compute acoustic radiation forces on non-spherical scatterers [31].

7. Summary and conclusions

It is known that cross-sections and radiation forces can be expressed as integrals over a sphere of radius R, S_R, and that the values of these integrals do not depend on R. It is natural then to let $R \to \infty$ so that the integrals can be related to far-field quantities such as the far-field pattern, Eq. (56). This familiar strategy works straightforwardly for the scattering cross-section σ_{sc} (see Eqs. (21) and (59)), but this is an exceptional case: if the integrand involves the incident wave u_{inc}, extracting the limiting behaviour as $R \to \infty$ is difficult, in general; these difficulties are sketched in Section 5, with more details available elsewhere [23,26].

An alternative strategy is to evaluate the integrals over S_R directly, keeping R finite. One expands the incident field using regular spherical wavefunctions (Eq. (28) with coefficients D_n^m) and the scattered field using outgoing spherical wavefunctions (Eq. (29) with coefficients C_n^m), and then integrates with respect to the angular variables. This finite-R strategy is simple, in principle. The calculations are outlined in Section 4: inevitably, they are complicated but the final results are explicit and exact; they are also seen to be independent of R, which provides a check on the calculations themselves. The resulting formulas for the cross-sections (Eqs. (32) and (33)) and the components of the radiation force (Eqs. (45) and (55)) are useful because they do not assume a specific incident field (we just need the coefficients D_n^m) and they do not assume anything about the constitution of the scatterer (such as its shape, boundary conditions or internal properties); one has to be able to find all the C_n^m given all the D_n^m, a task that could be done using a T-matrix method (Section 6) or by any other convenient numerical method.

From a mathematical point of view, the main merit of the finite-R strategy adopted here is that it is rigorous: within the derivations, there are no divergent integrals and no divergent series. Given a desire to compute sensible physical quantities such as cross-sections and radiation forces, our goal was to do that using convergent processes: this goal was achieved herein.

Appendix. Some integrals

Suppose that

$$U(\boldsymbol{r}) = \sum_{n,m} w_n^m(kr)\tilde{Y}_n^m(\hat{\boldsymbol{r}}), \quad w_n^m(kr) = D_n^m j_n(kr) + C_n^m h_n(kr), \tag{A.1}$$

$$V(\boldsymbol{r}) = \sum_{n,m} v_n^m(kr)\tilde{Y}_n^m(\hat{\boldsymbol{r}}), \quad v_n^m(kr) = F_n^m j_n(kr) + E_n^m h_n(kr), \tag{A.2}$$

in the vicinity of a sphere $r = R$. Then [16, Lemma 6.5]

$$\int_{r=R} \left(\overline{U}\frac{\partial V}{\partial r} - V\frac{\partial \overline{U}}{\partial r} \right) \mathrm{d}S = \frac{2\pi \mathrm{i}}{k} \sum_{n,m} h_n^m \left(2\overline{C_n^m}E_n^m + \overline{C_n^m}F_n^m + \overline{D_n^m}E_n^m \right). \tag{A.3}$$

The proof makes use of the orthogonality of $\tilde{Y}_n^m$, Eq. (31), and the Wronskian for spherical Bessel functions [17, 10.50.1]. The special case $U = V$ gives

$$k\,\mathrm{Im} \int_{r=R} \overline{U}\,\frac{\partial U}{\partial r}\,\mathrm{d}S = 2\pi \sum_{n,m} h_n^m \left(\left|C_n^m\right|^2 + \mathrm{Re}\left\{\overline{D_n^m}C_n^m\right\} \right). \tag{A.4}$$

Next, consider I_3, defined by Eq. (38). Substituting Eq. (34),

$$\begin{aligned} I_3 = {} & 2\pi \sum_{n,m} \sum_{\nu=0}^{\infty} w_n^m\,\overline{w_\nu^m} \int_0^\pi P_n^{m\prime}(\cos\theta) P_\nu^{m\prime}(\cos\theta) \cos\theta \sin^3\theta\,\mathrm{d}\theta \\ & + 2\pi \sum_{n,m} \sum_{\nu=0}^{\infty} w_n^m\,\overline{w_\nu^m} \int_0^\pi m^2 P_n^m(\cos\theta) P_\nu^m(\cos\theta) \cot\theta\,\mathrm{d}\theta. \end{aligned} \tag{A.5}$$

Note that the terms with $n = m = 0$ are absent. The second integral in Eq. (A.5) is

$$m^2 \int_{-1}^{1} \frac{t}{1-t^2} P_n^m(t) P_\nu^m(t)\,\mathrm{d}t \tag{A.6}$$

whereas the first integral in Eq. (A.5) is

$$\begin{aligned} \int_{-1}^{1} t(1-t^2) P_n^{m\prime}(t) P_\nu^{m\prime}(t)\,\mathrm{d}t &= \int_{-1}^{1} \{(1-t^2)P_n^{m\prime}(t)\} \left\{ \left(tP_\nu^m(t)\right)' - P_\nu^m(t) \right\} \mathrm{d}t \\ &= \int_{-1}^{1} \{(1-t^2)P_n^{m\prime}(t)\} \left(tP_\nu^m(t)\right)'\,\mathrm{d}t - \int_{-1}^{1} (1-t^2) P_n^{m\prime}(t) P_\nu^m(t)\,\mathrm{d}t \\ &= -\int_{-1}^{1} \{(1-t^2)P_n^{m\prime}(t)\}'\,tP_\nu^m(t)\,\mathrm{d}t \end{aligned} \tag{A.7}$$

$$
\begin{aligned}
&- \frac{(n+1)(n+m)}{2n+1} \int_{-1}^{1} P_{n-1}^m(t) P_\nu^m(t)\,\mathrm{d}t + \frac{n(n-m+1)}{2n+1} \int_{-1}^{1} P_{n+1}^m(t) P_\nu^m(t)\,\mathrm{d}t \\
&= n(n+1) \int_{-1}^{1} t P_n^m(t) P_\nu^m(t)\,\mathrm{d}t - m^2 \int_{-1}^{1} \frac{t}{1-t^2} P_n^m(t) P_\nu^m(t)\,\mathrm{d}t \\
&- \frac{2(n+1)(n+m)!}{(2n+1)(2n-1)(n-1-m)!}\,\delta_{\nu,n-1} + \frac{2n(n+1+m)!}{(2n+1)(2n+3)(n-m)!}\,\delta_{\nu,n+1},
\end{aligned}
\tag{A.8}
$$

where we have used the differential equation satisfied by $P_n^m(t)$,

$$
\{(1-t^2)v'(t)\}' + \{n(n+1) - m^2/(1-t^2)\}v(t) = 0, \tag{A.9}
$$

and the formula [16, Eq. (A.14)]

$$
(2n+1)(1-t^2)P_n^{m\prime}(t) = (n+1)(n+m)P_{n-1}^m(t) - n(n-m+1)P_{n+1}^m(t). \tag{A.10}
$$

The second integral in Eq. (A.8) cancels with the second integral in Eq. (A.5), which is Eq. (A.6). Then, using Eq. (35), the sum of the two integrals in Eq. (A.5) is

$$
\frac{2n(n+2)(n+m+1)!}{(2n+1)(2n+3)(n-m)!}\,\delta_{\nu,n+1} + \frac{2(n-1)(n+1)(n+m)!}{(2n+1)(2n-1)(n-1-m)!}\,\delta_{\nu,n-1}.
$$

Hence Eq. (A.5) reduces to Eq. (39).

From Eq. (40), we obtain

$$
I_4 = -2\pi(kR) \sum_{n,m} \sum_{\nu=0}^{\infty} \left(w_n^m \overline{w_\nu^{m\prime}} + w_\nu^{m\prime}\, \overline{w_n^m} \right) \int_0^\pi P_n^{m\prime}(\cos\theta) P_\nu^m(\cos\theta) \sin^3\theta\,\mathrm{d}\theta.
$$

The integral is

$$
\int_{-1}^{1} (1-t^2) P_n^{m\prime}(t) P_\nu^m(t)\,\mathrm{d}t = \frac{2(n+1)(n+m)!}{(2n+1)(2n-1)(n-1-m)!}\,\delta_{\nu,n-1} - \frac{2n(n+1+m)!}{(2n+1)(2n+3)(n-m)!}\,\delta_{\nu,n+1};
$$

the same integral appeared in Eq. (A.7). Hence

$$
\begin{aligned}
I_4 &= -4\pi(kR) \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(w_n^m\, \overline{w_{n-1}^{m\prime}} + w_{n-1}^{m\prime}\, \overline{w_n^m} \right) \frac{(n+1)(n+m)!}{(2n+1)(2n-1)(n-1-m)!} \\
&+ 4\pi(kR) \sum_{n,m} \left(w_n^m\, \overline{w_{n+1}^{m\prime}} + w_{n+1}^{m\prime}\, \overline{w_n^m} \right) \frac{n(n+1+m)!}{(2n+1)(2n+3)(n-m)!},
\end{aligned}
$$

and this reduces to Eq. (41).

From the definition Eq. (46)

$$
\begin{aligned}
I_5 &= (kR)^2 \sum_{n,m} \sum_{\nu,\mu} w_n^m \overline{w_\nu^\mu} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m-\mu-1)\phi}\,\mathrm{d}\phi \int_0^\pi P_n^m(\cos\theta) P_\nu^\mu(\cos\theta) \sin^2\theta\,\mathrm{d}\theta \\
&= 2\pi(kR)^2 \sum_{\nu=1}^{\infty} w_0^0 \overline{w_\nu^{-1}} \int_{-1}^{1} \sqrt{1-t^2}\, P_\nu^{-1}(t)\,\mathrm{d}t \\
&+ 2\pi(kR)^2 \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \sum_{\nu=0}^{\infty} w_n^m \overline{w_\nu^{m-1}} \int_{-1}^{1} \sqrt{1-t^2}\, P_n^m(t) P_\nu^{m-1}(t)\,\mathrm{d}t
\end{aligned}
$$

after separating off the contribution from $n = 0$. The integrals can be evaluated using Eq. (30) and $(2\nu+1)\sqrt{1-t^2}\,P_\nu^{m-1}(t) = P_{\nu+1}^m(t) - P_{\nu-1}^m(t)$ [16, Eq. (A.20)]. Thus

$$
\begin{aligned}
&\int_{-1}^{1} \sqrt{1-t^2}\, P_\nu^{-1}(t)\,\mathrm{d}t = \frac{1}{2\nu+1} \int_{-1}^{1} (P_{\nu+1}(t) - P_{\nu-1}(t))\,\mathrm{d}t = -\frac{2}{3}\,\delta_{\nu,1}, \\
&\int_{-1}^{1} \sqrt{1-t^2}\, P_n^m(t) P_\nu^{m-1}(t)\,\mathrm{d}t = \frac{1}{2\nu+1} \int_{-1}^{1} \left(P_{\nu+1}^m(t) - P_{\nu-1}^m(t)\right) P_n^m(t)\,\mathrm{d}t = \frac{h_n^m}{2\nu+1} \left\{\delta_{n,\nu+1} - \delta_{n,\nu-1}\right\}.
\end{aligned}
\tag{A.11}
$$

Hence

$$I_5 = -\frac{4\pi}{3}(kR)^2 w_0^0 \overline{w_1^{-1}} + (kR)^2 \sum_{n=1}^{\infty}\sum_{m=-n}^{n} w_n^m \overline{w_{n-1}^{m-1}} \frac{4\pi\,(n+m)!}{(2n-1)(2n+1)(n-m)!}$$
$$- (kR)^2 \sum_{n=1}^{\infty}\sum_{m=-n}^{n} w_n^m \overline{w_{n+1}^{m-1}} \frac{4\pi\,(n+m)!}{(2n+3)(2n+1)(n-m)!}.$$

The first term and the second sum can be combined. In the first sum, replace n by $n+1$ and m by $m+1$. Hence we obtain Eq. (46). Similar arguments apply to I_6, see Eq. (47).

From the definition Eq. (48),

$$I_7 = \sum_{n,m}\sum_{\nu,\mu} w_n^m \overline{w_\nu^\mu} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m-\mu-1)\phi}\,\mathrm{d}\phi \int_0^{\pi} P_n^{m\,\prime}(\cos\theta) P_\nu^{\mu\,\prime}(\cos\theta)\sin^4\theta\,\mathrm{d}\theta$$
$$+ \sum_{n,m}\sum_{\nu,\mu} w_n^m \overline{w_\nu^\mu}\, m\mu \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m-\mu-1)\phi}\,\mathrm{d}\phi \int_0^{\pi} P_n^m(\cos\theta) P_\nu^\mu(\cos\theta)\,\mathrm{d}\theta.$$

The contributions from $n = m = 0$ and from $\nu = \mu = 0$ are absent. Hence

$$I_7 = 2\pi \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{\nu=1}^{\infty} w_n^m \overline{w_\nu^{m-1}} \int_0^{\pi} P_n^{m\,\prime}(\cos\theta) P_\nu^{m-1\,\prime}(\cos\theta)\sin^4\theta\,\mathrm{d}\theta$$
$$+ 2\pi \sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{\nu=1}^{\infty} w_n^m \overline{w_\nu^{m-1}} \int_0^{\pi} m(m-1) P_n^m(\cos\theta) P_\nu^{m-1}(\cos\theta)\,\mathrm{d}\theta.$$

The second integral is

$$\mathcal{I}_2 \equiv m(m-1)\int_{-1}^{1} P_n^m(t) P_\nu^{m-1}(t)\,\frac{\mathrm{d}t}{\sqrt{1-t^2}} \tag{A.12}$$

whereas the first integral is

$$\mathcal{I}_1 \equiv \int_{-1}^{1} (1-t^2)^{3/2} P_n^{m\,\prime}(t) P_\nu^{m-1\,\prime}(t)\,\mathrm{d}t = \int_{-1}^{1} \left\{(1-t^2)P_n^{m\,\prime}(t)\right\}\sqrt{1-t^2}\,P_\nu^{m-1\,\prime}(t)\,\mathrm{d}t$$
$$= \int_{-1}^{1} \left\{(1-t^2)P_n^{m\,\prime}(t)\right\}\left(\sqrt{1-t^2}\,P_\nu^{m-1}(t)\right)'\,\mathrm{d}t + \int_{-1}^{1} t\sqrt{1-t^2}\,P_n^{m\,\prime}(t) P_\nu^{m-1}(t)\,\mathrm{d}t$$
$$= -\int_{-1}^{1} \left\{(1-t^2)P_n^{m\,\prime}(t)\right\}'\sqrt{1-t^2}\,P_\nu^{m-1}(t)\,\mathrm{d}t + \int_{-1}^{1} t(1-t^2)P_n^{m\,\prime}(t) P_\nu^{m-1}(t)\,\frac{\mathrm{d}t}{\sqrt{1-t^2}},$$

using $\sqrt{1-t^2}P_\nu^{m-1\,\prime}(t) = \left(\sqrt{1-t^2}P_\nu^{m-1}(t)\right)' + t(1-t^2)^{-1/2}P_\nu^{m-1}(t)$. Now use the differential equation Eq. (A.9) and [16, Eq. (A.12)]

$$t(1-t^2)P_n^{m\,\prime}(t) = -(n-m+1)(n+m)t\sqrt{1-t^2}\,P_n^{m-1}(t) + m(t^2-1)P_n^m(t) + mP_n^m(t). \tag{A.13}$$

Thus

$$\mathcal{I}_1 = \int_{-1}^{1}\left\{n(n+1) - \frac{m^2}{1-t^2}\right\} P_n^m(t)\sqrt{1-t^2}\,P_\nu^{m-1}(t)\,\mathrm{d}t$$
$$- \int_{-1}^{1}\left\{(n-m+1)(n+m)t\,P_n^{m-1}(t) + m\sqrt{1-t^2}\,P_n^m(t) - \frac{m}{\sqrt{1-t^2}}P_n^m(t)\right\} P_\nu^{m-1}(t)\,\mathrm{d}t$$
$$= \{n(n+1)-m\}\int_{-1}^{1}\sqrt{1-t^2}\,P_n^m(t)P_\nu^{m-1}(t)\,\mathrm{d}t$$
$$- (n+m)(n-m+1)\int_{-1}^{1} tP_n^{m-1}(t)P_\nu^{m-1}(t)\,\mathrm{d}t - m(m-1)\int_{-1}^{1} P_n^m(t)P_\nu^{m-1}(t)\frac{\mathrm{d}t}{\sqrt{1-t^2}}.$$

The last term cancels with Eq. (A.12). The first integral can be evaluated using Eq. (A.11) and the second integral can be evaluated using Eq. (35). Hence

$$\mathcal{I} \equiv \mathcal{I}_1 + \mathcal{I}_2 = \{n(n+1) - m\}\frac{h_n^m}{2\nu+1}\left\{\delta_{n,\nu+1} - \delta_{n,\nu-1}\right\}$$
$$- \frac{h_n^m}{2\nu+1}\left\{(\nu - m + 2)\delta_{n,\nu+1} + (\nu + m - 1)\delta_{n,\nu-1}\right\}$$
$$= \frac{h_n^m}{2\nu+1}\left\{(n^2-1)\delta_{\nu,n-1} - n(n+2)\delta_{\nu,n+1}\right\}$$

and

$$I_7 = \sum_{n=1}^{\infty}\sum_{m=-n}^{n} w_n^m \overline{w_{n-1}^{m-1}} \frac{4\pi(n^2-1)(n+m)!}{(2n-1)(2n+1)(n-m)!} - \sum_{n=1}^{\infty}\sum_{m=-n}^{n} w_n^m \overline{w_{n+1}^{m-1}} \frac{4\pi n(n+2)(n+m)!}{(2n+3)(2n+1)(n-m)!}.$$

In the first sum, replace n by $n+1$ and m by $m+1$. Hence we obtain Eq. (49).

Finally, consider I_8, defined by Eq. (50). We have

$$\begin{aligned} I_8 = {} & kR\sum_{n,m}\sum_{\nu,\mu} w_n^m \overline{w_\nu^{\mu\,\prime}} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m-\mu-1)\phi}\,\mathrm{d}\phi \int_0^{\pi} P_n^{m\,\prime}(\cos\theta) P_\nu^\mu(\cos\theta)\cos\theta\sin^2\theta\,\mathrm{d}\theta \\ & + kR\sum_{n,m}\sum_{\nu,\mu} w_n^{m\,\prime} \overline{w_\nu^{\mu}} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m-\mu-1)\phi}\,\mathrm{d}\phi \int_0^{\pi} P_n^{m}(\cos\theta) P_\nu^{\mu\,\prime}(\cos\theta)\cos\theta\sin^2\theta\,\mathrm{d}\theta \\ & - kR\sum_{n,m}\sum_{\nu,\mu} w_n^m \overline{w_\nu^{\mu\,\prime}} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m-\mu-1)\phi}\,\mathrm{d}\phi \int_0^{\pi} m\,P_n^{m}(\cos\theta) P_\nu^{\mu}(\cos\theta)\,\mathrm{d}\theta \\ & + kR\sum_{n,m}\sum_{\nu,\mu} w_n^{m\,\prime} \overline{w_\nu^{\mu}} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(m-\mu-1)\phi}\,\mathrm{d}\phi \int_0^{\pi} \mu\,P_n^{m}(\cos\theta) P_\nu^{\mu}(\cos\theta)\,\mathrm{d}\theta. \end{aligned} \tag{A.14}$$

The first and third lines combine as

$$2\pi kR\sum_{n=1}^{\infty}\sum_{m=-n}^{n}\sum_{\nu=0}^{\infty} w_n^m \overline{w_\nu^{m-1\,\prime}}\,\mathcal{J}_1$$

where

$$\begin{aligned} \mathcal{J}_1 &= \int_{-1}^{1}\left\{t(1-t^2)P_n^{m\,\prime}(t) - mP_n^m(t)\right\} P_\nu^{m-1}(t)\,\frac{\mathrm{d}t}{\sqrt{1-t^2}} \\ &= -(n+m)(n-m+1)\int_{-1}^{1} tP_n^{m-1}(t)P_\nu^{m-1}(t)\,\mathrm{d}t - m\int_{-1}^{1}\sqrt{1-t^2}\,P_n^m(t)P_\nu^{m-1}(t)\,\mathrm{d}t \\ &= -\frac{h_n^m}{2\nu+1}\left\{(n+1)\delta_{\nu,n-1} + n\delta_{\nu,n+1}\right\}, \end{aligned}$$

using Eqs. (A.13), (35) and (A.11). Similarly, the second and fourth lines in Eq. (A.14) combine as

$$2\pi kR\sum_{n,m}\sum_{\nu=1}^{\infty} w_n^{m\,\prime}\overline{w_\nu^{m-1}}\,\mathcal{J}_2$$

where

$$\begin{aligned} \mathcal{J}_2 &= \int_{-1}^{1}\left\{t(1-t^2)P_\nu^{m-1\,\prime}(t) + (m-1)P_\nu^{m-1}(t)\right\} P_n^m(t)\,\frac{\mathrm{d}t}{\sqrt{1-t^2}} \\ &= \int_{-1}^{1} tP_n^m(t)P_\nu^m(t)\,\mathrm{d}t + (m-1)\int_{-1}^{1}\sqrt{1-t^2}\,P_n^m(t)P_\nu^{m-1}(t)\,\mathrm{d}t \\ &= \frac{h_n^m}{2\nu+1}\left\{(n-1)\delta_{\nu,n-1} + (n+2)\delta_{\nu,n+1}\right\}, \end{aligned}$$

using [16, Eq. (A.11)]

$$t(1-t^2)P_\nu^{\mu\,\prime}(t) + \mu P_\nu^\mu(t) = t\sqrt{1-t^2}\,P_\nu^{\mu+1}(t) + \mu(1-t^2)P_\nu^\mu(t),$$

with $\mu = m-1$ together with Eqs. (35) and (A.11). Thus

$$
\begin{aligned}
I_8 = &-kR\sum_{n=1}^{\infty}\sum_{m=-n}^{n} w_n^m \overline{w_{n-1}^{m-1\,\prime}}\,\frac{4\pi(n+1)(n+m)!}{(2n-1)(2n+1)(n-m)!}\\
&-kR\sum_{n=1}^{\infty}\sum_{m=-n}^{n} w_n^m \overline{w_{n+1}^{m-1\,\prime}}\,\frac{4\pi n(n+m)!}{(2n+3)(2n+1)(n-m)!}\\
&+kR\sum_{n=2}^{\infty}\sum_{m=-n}^{n} w_n^{m\,\prime} \overline{w_{n-1}^{m-1}}\,\frac{4\pi(n-1)(n+m)!}{(2n-1)(2n+1)(n-m)!}\\
&+kR\sum_{n,m} w_n^{m\,\prime} \overline{w_{n+1}^{m-1}}\,\frac{4\pi(n+2)(n+m)!}{(2n+3)(2n+1)(n-m)!}.
\end{aligned}
$$

As before, replace n by $n+1$ and m by $m+1$ in the first and third sums, giving Eq. (51).

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