Project on

NV-centered nanodiamond for QGEM

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Table of Contents

List of Figures **6**

1 Laser light heating of NV-centre nanodiamond (Rayleigh regime) **7**

1.1 Heat absorption in an optically trapped nanodiamond as an electric dipole . . . 7

1.1.1 Polarizability and Dipole Moment: 7

1.1.2 Polarizability of a Dielectric Sphere 8

1.2 Heat dissipated in the nanodiamond due to thermal collisions 13

1.3 Heat dissipated by the nanodiamond through black body radiation: 15

1.4 Net heating of the nanodiamond 19

1.5 Dimentional analysis of Eq. (1.5) 19

1.5.1 Basic dimensions 19

1.5.2 Left-hand side 20

1.6 Laser absorption term 20

1.6.1 Gas collisional cooling term 20

1.6.2 Black-body radiation exchange term 21

1.6.3 Conclusion 22

2 Power absorption for beyond Rayleigh size particles: Integral equation form of Mie scattering **23**

2.1 Setup 23

2.2 Derivation of the Optical Theorem Power Balance: $P_{\text{abs}} = P_{\text{ext}} - P_{\text{sca}}$ 24

2.2.1 Time Averaged Poynting Theorem . . . 24
2.2.2 Decomposing into the Power Flux . . . 24
2.2.3 Analysing Each Flux Integral . . . 25
2.2.4 Assemble the Result . . . 26
2.3 The Electric-Field Integral Equation (EFIE) . . . 26
2.3.1 Setup and Conventions . . . 26
2.3.2 The Vector Wave Equation for $\vec{E}$ . . . 27
2.3.3 Green's Vector Identity (Levine–Schwinger trick) . . . 27
2.3.4 The Dyadic Green's Function . . . 28
2.3.5 Applying the Vector Green's Identity . . . 29
2.3.6 Derivation of the Surface Integral Term . . . 30
2.3.7 Electric field in terms of Scalar Green's Function . . . 32
2.3.8 Far-Field Asymptotics of G and ∇G . . . 33
2.3.9 Evaluating the First Volume Integral in the Far Field . . . 34
2.3.10 Evaluating the Second (Gradient) Term in the Far Field . . . 35
2.3.11 Combining the Pieces to Find the Scattering Electric Field . . . 35
2.4 The Magnetic-Field Integral Equation (MFIE) . . . 37
2.4.1 Setup and Conventions . . . 37
2.4.2 Rewrite the Magnetic Wave Equation into "Source" Form . . . 37
2.4.3 Obtain the Volume Integral Equation via Green's Identity . . . 38
2.4.4 The Far-Field Limit and Scattering Amplitude $\vec{A}_2$ . . . 40
2.4.5 Physical Interpretation of the Contributions . . . 41

3 Power absorption for beyond Rayleigh size particles: Gordon's approximation and spherical basis 42

3.1 Conventions and Maxwell equations . . . 42
3.2 Scattered electric field using Gordon's ansatz . . . 43
3.2.1 Setup . . . 43
3.2.2 Computing $\vec{P}(\hat{s})$ . . . 44

3.2.3 Far-field projection and $\vec{E}_{\text{sctd}}$ . . . 45
3.2.4 Electric field in different polarisation bases . . . 46
3.3 Scattered magnetic field using Gordon's ansatz . . . 46
3.3.1 Internal fields (Gordon ansatz) . . . 46
3.3.2 Far-field magnetic scattering via volume integrals . . . 47
3.4 Summary of the scattered fields: . . . 50
3.4.1 Checks . . . 51
3.5 Spherical coordinates transformation . . . 51
3.6 Polarisation basis tied to the scattering plane . . . 52
3.7 Incident plane wave, labelled in the spherical scattering basis . . . 53
3.8 Far-field scattered fields for arbitrary (θ, ϕ) . . . 54

4 Mie theory and Rayleigh limit **55**
4.1 Maxwell's Problem and Separation in Spherical Waves . . . 55
4.1.1 Maxwell to the Vector Helmholtz Equation and Transversality . . . 56
4.1.2 Scalar Helmholtz Separation in Spherical Coordinates . . . 56
4.1.3 Building Transverse Vector Solutions from Scalar Ones . . . 57
4.1.4 Explicit VSWFs and Their Radial Behavior . . . 58
4.1.5 Why These Span the Maxwell Solutions . . . 59
4.1.6 Plane Wave Expansion and Mie Scattering Solution . . . 60
4.2 Boundary conditions at the spherical interface (derivation and 2×2 systems) . . . 60
4.2.1 From VSWFs to the angle–resolved amplitudes $S_1(\theta), S_2(\theta)$ . . . 62
4.2.2 From far field to differential and integrated cross-sections . . . 63
4.2.3 Optical theorem and extinction (derivation in our normalization) . . . 65

5 Appendix A **70**
5.1 Derivation of black body radiation energy density per unit frequency formula in a system with harmonic interaction . . . 70
5.1.1 Density of States for Photons . . . 70

5.1.2 Energy per Photon Mode . . . 72
5.1.3 Energy Density . . . 72
5.1.4 Notes . . . 72

6 Appendix B **74**
6.1 Derivation of the Time-Domain Poynting Theorem . . . 74
6.2 Time-Averaged Poynting Theorem and Ohmic Loss . . . 75
6.2.1 Phasor Time-Average Calculation . . . 76
6.2.2 Derivation of Complex Permittivity in Phasor Form . . . 77
6.3 Proof of zero divergence for the incident Poynting vector . . . 78
6.3.1 Convention . . . 78
6.3.2 Derivation . . . 78
6.4 Free-space Helmholtz Green's function and Sommerfeld condition . . . 81
6.4.1 Setup . . . 81
6.4.2 Green's function method . . . 81
6.4.3 Fourier transform and retarded prescription . . . 81
6.4.4 Inverse transform reducing to one oscillatory integral) . . . 82
6.4.5 Evaluating scalar Helmholtz Equation Green's function by Sokhotski-Plemelj . . . 82
6.4.6 Sommerfeld radiation condition . . . 84
6.5 Dyadic Green's function from the scalar Helmholtz Green's function . . . 84
6.5.1 Setting and notation . . . 84
6.5.2 Proof of (6.35) . . . 85
6.5.3 Proof of reciprocity (6.36) . . . 87
6.5.4 Remarks . . . 87

List of Figures

3.1 $\hat{s}_0$ and $\hat{s}$ are unit vectors in the incident and scattering directions. $\mathbf{r}'$ is a position vector of a point within the scattering sphere of radius a. P is the point at which the scattered radiation is observed. The position vector of P is $\mathbf{r}$. In the text it is assumed that $r \gg a$. 43

Chapter 1

Laser light heating of NV-centre nanodiamond (Rayleigh regime)

1.1 Heat absorption in an optically trapped nanodiamond as an electric dipole

We know that for a nanodiamond illuminated (optically levitated or dipole trapping) by light, the power absorbed E_{abs} is given by:

$$\frac{dE_{\text{abs}}}{dt} = C_x I \tag{1.1}$$

where C_x is the absorption cross-section and I is the intensity of light at the focus.

1.1.1 Polarizability and Dipole Moment:

When the laser's electric field ($\mathbf{E}$) acts on the nanodiamond, it polarizes the material, creating an induced dipole moment ($\mathbf{p} = \alpha\mathbf{E}$).

The polarizability α depends on the nanodiamond's material properties (ϵ) and size (V). For an NV-centred nanodiamond, the NV centres (defects with electronic transitions) increase ϵ_i, the dielectric constant making α complex: $\alpha = \alpha_r + i\alpha_i$, where α_i (the imaginary part) relates to energy loss.

1.1.2 Polarizability of a Dielectric Sphere

The polarizability arises from electrostatics in the Rayleigh regime, where the nanoparticle is much smaller than the wavelength of light ($r \ll \lambda$), so the electric field is approximately uniform across the particle. We'll derive this using the electrostatic solution for a dielectric sphere in a uniform electric field, assuming SI units for clarity, as used in the previous derivation of the absorption cross-section.

Considering a dielectric sphere of radius r, volume $V = \frac{4}{3}\pi r^3$, and relative dielectric constant $\epsilon = \epsilon_r + i\epsilon_i$ (complex to account for absorption, as in "Equations.pdf"). The sphere is placed in a medium with dielectric constant $\epsilon_m\epsilon_0$ (where $\epsilon_m \approx 1$ for air or vacuum, and ϵ_0 is the permittivity of free space). A uniform external electric field $\mathbf{E}_0 = E_0\hat{z}$ is applied (e.g., from the laser).

The dipole moment induced in the sphere is:

$$\mathbf{p} = \alpha \mathbf{E}_0$$

Our task is to find α by solving for the electric fields inside and outside the sphere and calculating the induced dipole moment.

Electrostatic Solution for a Dielectric Sphere

In the Rayleigh regime, we use the quasi-static approximation (ignoring time-dependent effects since $r \ll \lambda$). The electric field is described by the electric potential Φ, which satisfies Laplace's equation ($\nabla^2\Phi = 0$) in regions with no free charges. We define two regions:

- **Inside the sphere** ($r < a$, where a is the radius): Permittivity is $\epsilon\epsilon_0$.
- **Outside the sphere** ($r > a$): Permittivity is $\epsilon_m\epsilon_0 \approx \epsilon_0$ (since $\epsilon_m = 1$).

The boundary conditions are:

1. The potential is continuous at $r = a$.
2. The normal component of the displacement field $\mathbf{D} = \epsilon\epsilon_0\mathbf{E}$ is continuous at $r = a$.
3. Far from the sphere ($r \to \infty$), the field is $\mathbf{E}_0 = -\nabla\Phi$, corresponding to $\Phi = -E_0 z = -E_0 r\cos\theta$ in spherical coordinates.

We solve Laplace's equation in spherical coordinates, using the general solution for the potential:

$$\Phi(r,\theta) = \sum_{l=0}^{\infty}\left(A_l r^l + \frac{B_l}{r^{l+1}}\right)P_l(\cos\theta)$$

where P_l are Legendre polynomials. For a uniform field, the $l = 1$ term (dipole term) dominates due to symmetry.

Inside the sphere ($r < a$):

$$\Phi_{\text{in}} = Ar\cos\theta$$

(The r^{-2} term is excluded to avoid singularity at $r = 0$.)

Outside the sphere ($r > a$):

$$\Phi_{\text{out}} = \left(-E_0 r + \frac{B}{r^2}\right)\cos\theta$$

The $-E_0 r\cos\theta$ term gives the applied field $\mathbf{E}_0 = E_0\hat{z}$, and $\frac{B}{r^2}\cos\theta$ represents the dipole field of the sphere.

Boundary Conditions:

1. **Continuity of potential** at $r = a$:

$$\Phi_{\text{in}}(r = a) = \Phi_{\text{out}}(r = a)$$

$$Aa\cos\theta = \left(-E_0 a + \frac{B}{a^2}\right)\cos\theta$$

$$Aa = -E_0 a + \frac{B}{a^2} \quad (1)$$

2. **Continuity of the normal displacement field:** The normal component of $\mathbf{D} = \epsilon\epsilon_0\mathbf{E}$ is continuous. Since $\mathbf{E} = -\nabla\Phi$, the radial component is $E_r = -\frac{\partial\Phi}{\partial r}$.

Inside:

$$E_{r,\text{in}} = -\frac{\partial\Phi_{\text{in}}}{\partial r} = -A\cos\theta$$

$$D_{r,\text{in}} = \epsilon\epsilon_0 E_{r,\text{in}} = -\epsilon\epsilon_0 A\cos\theta$$

Outside:

$$E_{r,\text{out}} = -\frac{\partial\Phi_{\text{out}}}{\partial r} = -\left(-E_0 - \frac{2B}{r^3}\right)\cos\theta$$

At $r = a$:

$$E_{r,\text{out}} = \left(E_0 + \frac{2B}{a^3}\right)\cos\theta$$

$$D_{r,\text{out}} = \epsilon_m\epsilon_0 E_{r,\text{out}} = \epsilon_m\epsilon_0\left(E_0 + \frac{2B}{a^3}\right)\cos\theta$$

Continuity of D_r:

$$\epsilon\epsilon_0(-A) = \epsilon_m\epsilon_0\left(E_0 + \frac{2B}{a^3}\right)$$

$$-\epsilon A = \epsilon_m\left(E_0 + \frac{2B}{a^3}\right) \quad (2)$$

Solving for the equations (1) and (2):

From (1):

$$Aa = -E_0 a + \frac{B}{a^2}$$

$$B = a^3(A + E_0) \quad (3)$$

From (2):

$$-\epsilon A = \epsilon_m \left(E_0 + \frac{2B}{a^3} \right)$$

Substitute $B = a^3(A + E_0)$:

$$-\epsilon A = \epsilon_m \left(E_0 + \frac{2a^3(A + E_0)}{a^3} \right) = \epsilon_m(E_0 + 2A + 2E_0) = \epsilon_m(3E_0 + 2A)$$

$$-\epsilon A = \epsilon_m(2A + 3E_0)$$

$$-\epsilon A = 2\epsilon_m A + 3\epsilon_m E_0$$

$$-(\epsilon + 2\epsilon_m)A = 3\epsilon_m E_0$$

$$A = -\frac{3\epsilon_m E_0}{\epsilon + 2\epsilon_m}$$

Now find B:

$$B = a^3 \left(-\frac{3\epsilon_m E_0}{\epsilon + 2\epsilon_m} + E_0 \right) = a^3 E_0 \left(\frac{-3\epsilon_m + (\epsilon + 2\epsilon_m)}{\epsilon + 2\epsilon_m} \right) = a^3 E_0 \frac{\epsilon - \epsilon_m}{\epsilon + 2\epsilon_m}$$

The potential outside includes a dipole term:

$$\Phi_{\text{out}} = -E_0 r \cos\theta + \frac{B \cos\theta}{r^2}$$

The dipole field is $\Phi_{\text{dipole}} = \frac{p\cos\theta}{4\pi\epsilon_m\epsilon_0 r^2}$, so:

$$\frac{B\cos\theta}{r^2} = \frac{p\cos\theta}{4\pi\epsilon_m\epsilon_0 r^2}$$

$$p = 4\pi\epsilon_m\epsilon_0 B$$

Substitute B:

$$p = 4\pi\epsilon_m\epsilon_0 \cdot a^3 E_0 \frac{\epsilon - \epsilon_m}{\epsilon + 2\epsilon_m}$$

Since $p = \alpha E_0$:

$$\alpha = \frac{p}{E_0} = 4\pi\epsilon_m\epsilon_0 a^3 \frac{\epsilon - \epsilon_m}{\epsilon + 2\epsilon_m}$$

Since $V = \frac{4}{3}\pi a^3$, we have $a^3 = \frac{3V}{4\pi}$, so:

$$\alpha = 4\pi\epsilon_m\epsilon_0 \cdot \frac{3V}{4\pi}\frac{\epsilon - \epsilon_m}{\epsilon + 2\epsilon_m} = 3\epsilon_m\epsilon_0 V \frac{\epsilon - \epsilon_m}{\epsilon + 2\epsilon_m}$$

For air or vacuum, $\epsilon_m = 1$:

$$\alpha = 3\epsilon_0 V \frac{\epsilon - 1}{\epsilon + 2}$$

This is the desired polarizability, where ϵ is the relative dielectric constant of the nanoparticle.

Energy Absorption from the Dipole:

The power absorbed by the dipole is given by the work done by the electric field on the oscillating dipole, averaged over time: $P_{\text{abs}} = \frac{\omega}{2}\operatorname{Im}(\mathbf{p} \cdot \mathbf{E}^*)$

Since $\mathbf{p} = \alpha\mathbf{E}$ and $\mathbf{E} = \mathbf{E}_0 e^{-i\omega t}$ (with $\mathbf{E}^*$ as its complex conjugate), the dot product becomes: $\mathbf{p} \cdot \mathbf{E}^* = \alpha|\mathbf{E}|^2$

The imaginary part of α ($\operatorname{Im}(\alpha)$) accounts for energy dissipation (absorption) but not elastic scattering. So: $P_{\text{abs}} = \frac{\omega}{2}\,\text{Im}(\alpha)|\mathbf{E}|^2$

Relating to Intensity:

The laser intensity I is the power per unit area, related to the electric field by $I = \frac{1}{2}c\epsilon_0|\mathbf{E}|^2$, where c is the speed of light. Thus: $|\mathbf{E}|^2 = \frac{2I}{c\epsilon_0}$

Substitute into the power equation: $P_{\text{abs}} = \frac{\omega}{2}\,\text{Im}(\alpha)\cdot\frac{2I}{c\epsilon_0} = \frac{\omega}{c\epsilon_0}\,\text{Im}(\alpha)I$

Since $\omega = ck$ (where $k = \frac{2\pi}{\lambda}$ is the wave number): $P_{\text{abs}} = \frac{k}{\epsilon_0}\,\text{Im}(\alpha)I$

Deriving the Absorption Cross-Section:

The absorption cross-section C_x is defined as the ratio of absorbed power to intensity: $P_{\text{abs}} = C_x I$

Equate the two expressions for P_{abs}: $C_x I = \frac{k}{\epsilon_0}\,\text{Im}(\alpha)I$

Thus: $C_x = \frac{k}{\epsilon_0}\,\text{Im}(\alpha)$

Substitute $\alpha = 3\epsilon_0 V\frac{\epsilon-1}{\epsilon+2}$. The imaginary part is: $\text{Im}(\alpha) = \text{Im}\left(3\epsilon_0 V\frac{\epsilon-1}{\epsilon+2}\right) = 3\epsilon_0 V\,\text{Im}\left(\frac{\epsilon-1}{\epsilon+2}\right)$

So:

$$C_x = \frac{k}{\epsilon_0}\,\text{Im}(\alpha) = \frac{k}{\epsilon_0}\cdot 3\epsilon_0 V\,\text{Im}\left(\frac{\epsilon-1}{\epsilon+2}\right) = 3kV\,\text{Im}\left(\frac{\epsilon-1}{\epsilon+2}\right) \tag{1.2}$$

1.2 Heat dissipated in the nanodiamond due to thermal collisions

From the equipartition theorem, for a system of particles within a harmonic oscillator potential (Debye model), the average energy in three dimensions is given by (N is the number of molecules which are colliding):

$$\langle E\rangle = 3Nk_BT \quad (a)$$

Replacing N with the rate of collisions will give us the rate of energy dissipated.

In our case, we have a treatment of air surrounding the nanodiamond similar to the an ideal gas. We denote the internal temperature as T and the gas temperature as T_0 Energy transfer occurs during collisions, proportional to the temperature difference $T - T_0$. The mean energy transferred per collision is $\alpha_g k_B(T - T_0)$, where α_g is the fraction of energy accommodated.

The rate of collisions the levitated nanoparticle receives is:

$$N_c = \frac{1}{2}\bar{v}nA, \quad (b)$$

where:

- $\bar{v} = \sqrt{\frac{8k_BT_0}{\pi m}}$ is the mean speed of the gas molecules,
- $A = 4\pi r^2$ is the surface area of the nanoparticle,
- m is the mass of a gas molecule,
- T_0 is the gas temperature.

Using the pressure-number density relation (similar to the ideal gas equation), the number density of gas molecules is:

$$N = N_0\frac{p}{p_0} \quad (c)$$

,

where N_0 is the number density at atmospheric pressure p_0. p is the pressure of the gas surrounding the nanodiamond (in the vacuum chamber).

From substituting the values of A, replacing T_0 with $T - T_0$, we get the rate of energy dissipated from substituting (c) and (b) in equation (a) (which now gives energy dissipation rate by taking N_c collisions per unit time instead of number of particles), we get:

$$\frac{dE_{gas}}{dt} = -6\alpha_g\pi r^2\bar{v}N_0\frac{p}{p_0}k_B(T - T_0), \tag{1.3}$$

where α_g is a constant called the accommodation coefficient. $0 \leq \alpha_g \leq 1$ represents the fraction of the maximum possible energy exchange that occurs during a collision.

1.3 Heat dissipated by the nanodiamond through black body radiation:

To derive the equation for the rate of absorption of blackbody radiation by a dielectric nanosphere, as presented in Chang et al.'s paper, we start with the blackbody radiation law and the provided absorption cross-section. The goal is to obtain the expression:

$$\frac{dE}{dt} = \frac{72\zeta(5)}{\pi^2}\frac{V}{c^3\hbar^4}\,\mathrm{Im}\left(\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}\right)(k_BT)^5$$

where V is the volume of the nanosphere, c is the speed of light, $\hbar$ is the reduced Planck constant, ϵ_{bb} is the permittivity of the nanosphere across the blackbody radiation spectrum, k_B is the Boltzmann constant, T is the background temperature, and $\zeta(5)$ is the Riemann zeta function evaluated at 5.

Blackbody Radiation Energy Density

The blackbody radiation energy density per unit frequency interval at frequency ω and temperature T is given by the Planck distribution 5.1:

$$u(\omega,T) = \frac{\hbar\omega^3}{\pi^2c^3}\frac{1}{e^{\hbar\omega/k_BT}-1}$$

This represents the energy per unit volume per unit frequency for electromagnetic radiation in thermal equilibrium at temperature T. The spectral energy density $u(\omega,T)$ has units of energy per unit volume per unit frequency (e.g., $\mathrm{J/m^3{\cdot}Hz}$).

Absorption Cross-Section

The absorption cross-section for a dielectric nanosphere in the Rayleigh scattering regime ($r \ll \lambda$) is provided as:

$$C_x = 3kV\,\mathrm{Im}\left(\frac{\epsilon-1}{\epsilon+2}\right)$$

where $k = \omega/c$ is the wave number, V is the volume of the nanosphere, and ϵ is the relative permittivity of the nanosphere. For blackbody radiation, we assume the permittivity is approximately constant across the relevant frequency spectrum and denote it as ϵ_{bb}. Thus, the absorption cross-section becomes:

$$C_x(\omega) = 3\frac{\omega}{c}V \,\mathrm{Im}\left(\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}\right)$$

The imaginary part $\mathrm{Im}\left(\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}\right)$ accounts for the absorptive properties of the material, and $C_x(\omega)$ has units of area (m^2).

Power Absorbed from Blackbody Radiation

The power absorbed by the nanosphere at a given frequency ω is the product of the energy flux of the blackbody radiation and the absorption cross-section. The energy flux (energy per unit area per unit time per unit frequency) is related to the energy density by:

$$\mathrm{Flux} = u(\omega, T) \cdot c$$

This is because the energy density $u(\omega, T)$ is isotropic, and the flux through a surface is obtained by multiplying the energy density by the speed of light c. Thus, the power absorbed per unit frequency is:

$$\frac{dP}{d\omega} = C_x(\omega) \cdot u(\omega, T) \cdot c$$

Substituting the expressions for $C_x(\omega)$ and $u(\omega, T)$:

$$\frac{dP}{d\omega} = \left[3\frac{\omega}{c}V \,\mathrm{Im}\left(\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}\right)\right] \cdot \left[\frac{\hbar\omega^3}{\pi^2 c^3}\frac{1}{e^{\hbar\omega/k_B T}-1}\right] \cdot c$$

Simplify the expression:

$$\frac{dP}{d\omega} = 3V \,\mathrm{Im}\left(\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}\right) \cdot \frac{\hbar\omega^4}{\pi^2 c^3} \cdot \frac{1}{e^{\hbar\omega/k_B T}-1}$$

Integrating over all frequencies for the total power absorbed:

$$\frac{dE}{dt} = \int_0^\infty \frac{dP}{d\omega}\,d\omega = \int_0^\infty 3V \,\mathrm{Im}\left(\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}\right) \cdot \frac{\hbar\omega^4}{\pi^2 c^3} \cdot \frac{1}{e^{\hbar\omega/k_B T}-1}\,d\omega$$

Assuming the permittivity ϵ_{bb} is approximately constant across the blackbody spectrum (a common approximation for small particles in the Rayleigh regime), we can factor out the frequency-independent terms:

$$\frac{dE}{dt} = 3V\,\mathrm{Im}\left(\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2}\right) \cdot \frac{\hbar}{\pi^2 c^3} \int_0^\infty \frac{\omega^4}{e^{\hbar\omega/k_B T}-1}\,d\omega$$

Thus the integral to evaluate is:

$$\int_0^\infty \frac{\omega^4}{e^{\hbar\omega/k_B T}-1}\,d\omega$$

Making the substitution $x = \frac{\hbar\omega}{k_B T}$, so $\omega = \frac{k_B T}{\hbar}x$, $d\omega = \frac{k_B T}{\hbar}dx$. The exponent becomes:

$$\frac{\hbar\omega}{k_B T} = x$$

and the frequency term:

$$\omega^4 = \left(\frac{k_B T}{\hbar}x\right)^4 = \left(\frac{k_B T}{\hbar}\right)^4 x^4$$

The differential transforms as:

$$d\omega = \frac{k_B T}{\hbar}dx$$

Thus, the integral becomes:

$$\int_0^\infty \frac{\omega^4}{e^{\hbar\omega/k_B T}-1}\,d\omega = \int_0^\infty \frac{\left(\frac{k_B T}{\hbar}x\right)^4}{e^x-1} \cdot \frac{k_B T}{\hbar}\,dx$$

$$= \left(\frac{k_B T}{\hbar}\right)^4 \cdot \frac{k_B T}{\hbar} \int_0^\infty \frac{x^4}{e^x-1}\,dx$$

$$= \left(\frac{k_B T}{\hbar}\right)^5 \int_0^\infty \frac{x^4}{e^x-1}\,dx$$

The integral $\int_0^\infty \frac{x^4}{e^x-1}\,dx$ is a standard form related to the Riemann zeta function. It is known that:

$$\int_0^\infty \frac{x^{n-1}}{e^x - 1}\, dx = \Gamma(n)\zeta(n)$$

For $n = 5$ (since the exponent of x is 4, so $n - 1 = 4$, $n = 5$):

$$\int_0^\infty \frac{x^4}{e^x - 1}\, dx = \Gamma(5)\zeta(5)$$

The gamma function for an integer n is $\Gamma(n) = (n-1)!$, so:

$$\Gamma(5) = 4! = 24$$

Thus:

$$\int_0^\infty \frac{x^4}{e^x - 1}\, dx = 24\zeta(5)$$

Substitute back into the power expression:

$$\frac{dE}{dt} = 3V\,\mathrm{Im}\left(\frac{\epsilon_{bb} - 1}{\epsilon_{bb} + 2}\right) \cdot \frac{\hbar}{\pi^2 c^3} \cdot \left(\frac{k_B T}{\hbar}\right)^5 \cdot 24\zeta(5)$$

$$= 3V\,\mathrm{Im}\left(\frac{\epsilon_{bb} - 1}{\epsilon_{bb} + 2}\right) \cdot \frac{\hbar}{\pi^2 c^3} \cdot \frac{(k_B T)^5}{\hbar^5} \cdot 24\zeta(5)$$

$$= 3V\,\mathrm{Im}\left(\frac{\epsilon_{bb} - 1}{\epsilon_{bb} + 2}\right) \cdot \frac{(k_B T)^5}{\pi^2 c^3 \hbar^4} \cdot 24\zeta(5)$$

$$= \frac{72\zeta(5)V}{\pi^2 c^3 \hbar^4}\,\mathrm{Im}\left(\frac{\epsilon_{bb} - 1}{\epsilon_{bb} + 2}\right)(k_B T)^5$$

The derived expression matches the form given in the *Equations.pdf*:

$$\frac{dE_{bb}}{dt} = -\frac{72\zeta(5)}{\pi^2}\frac{V}{c^3\hbar^4}\,\mathrm{Im}\left(\frac{\epsilon_{bb} - 1}{\epsilon_{bb} + 2}\right)(k_B T)^5 \tag{1.4}$$

1.4 Net heating of the nanodiamond

From Eqs. (1.2), (1.3), and (1.4), we get the net heat absorbed, which is equal to the volumetric heat capacity C_V, multiplied by the temperature difference, i.e.,

$$V\frac{d[C_V(T-T_0)]}{dt} = 3IkV\,\mathrm{Im}\,\frac{\epsilon-1}{\epsilon+2} - 6\alpha_g \pi r^2 \bar{v} N_0 \frac{p}{p_0} k_B(T-To) - \frac{72\zeta(5)V}{\pi^2 c^3 \hbar^4}(\mathrm{Im}\,\frac{\epsilon_{bb}-1}{\epsilon_{bb}+2})k_B^5 T^5 \tag{1.5}$$

where r is the radius of the nanosphere V is the volume of the nanosphere, c is the speed of light, $\hbar$ is the reduced Planck constant, ϵ_{bb} is the permittivity of the nanosphere across the blackbody radiation spectrum, k_B is the Boltzmann constant, T_0 is the background temperature, and $\zeta(5)$ is the Riemann zeta function evaluated at 5. $k = \frac{2\pi}{\lambda}$ is the wave number of incident light and ϵ is the relative dielectric constant of the nanosphere. $\bar{v}$ is the mean speed of nanoparticle molecules. Finally T is the temperature of the diamond. N_0 is the number density at atmospheric pressure p_0 and p is the total pressure on the nanosphere (atmospheric pressure plus radiation pressure). α_g is a constant called the accommodation coefficient. $0 \leq \alpha_g \leq 1$.

1.5 Dimentional analysis of Eq. (1.5)

Dimensions are denoted as $[\cdot]$.

1.5.1 Basic dimensions

- $[V] = \mathrm{m}^3$
- $[C_V] = \mathrm{J\,m^{-3}\,K^{-1}}$ (volumetric heat capacity; see note at the end)
- $[T] = \mathrm{K}$, $[t] = \mathrm{s}$
- $[I] = \mathrm{W\,m^{-2}} = \mathrm{J\,s^{-1}\,m^{-2}}$
- $[k] = \mathrm{m}^{-1}$

- $[\varepsilon]$, $[\varepsilon_{\text{bb}}]$, $\text{Im}(\cdot)$, $\zeta(5)$, π, numerical factors, α_g, p/p_0 are dimensionless
- $[r] = \text{m}$
- $[\bar{v}] = \text{m}\,\text{s}^{-1}$
- $[N_0] = \text{m}^{-3}$ (number density at p_0)
- $[k_B] = \text{J}\,\text{K}^{-1}$
- $[c] = \text{m}\,\text{s}^{-1}$
- $[\hbar] = \text{J}\,\text{s}$

1.5.2 Left-hand side

The expression is:

$$V\frac{d[C_V(T-T_0)]}{dt}$$

The dimensions are:

$$[\text{m}^3]\cdot[\text{J}\,\text{m}^{-3}\,\text{K}^{-1}]\cdot[\text{K}\,\text{s}^{-1}] = \text{J}\,\text{s}^{-1} = \text{W}$$

1.6 Laser absorption term

The expression is:

$$3IkV\,\text{Im}\left[\frac{\varepsilon-1}{\varepsilon+2}\right]$$

The dimensions are:

$$[\text{W}\,\text{m}^{-2}]\cdot[\text{m}^{-1}]\cdot[\text{m}^3]\cdot[\text{dimensionless}] = \text{W}$$

1.6.1 Gas collisional cooling term

The expression is:

$$6\alpha_g\pi r^2\bar{v}N_0(p/p_0)k_B(T-T_0)$$

Units piece by piece: First, for the term $r^2\bar{v}N$:

$$[\mathrm{m}^2] \cdot [\mathrm{m\,s^{-1}}] \cdot [\mathrm{m^{-3}}] = \mathrm{m}^{2+1-3}\mathrm{s}^{-1} = \mathrm{s}^{-1}$$

So $r^2\bar{v}N$ has units of s^{-1} (a collision rate scale when multiplied by area).

Now multiply by k_B and $(T - T_0)$:

$$[\mathrm{s}^{-1}] \cdot [\mathrm{J\,K^{-1}}] \cdot [\mathrm{K}] = \mathrm{J\,s^{-1}} = \mathrm{W}$$

The dimensionless multipliers $(6, \alpha_g, \pi, p/p_0)$ do not change the units. So Term 2 is in Watts.

1.6.2 Black-body radiation exchange term

The expression is:

$$\frac{72\zeta(5)V}{\pi^2 c^3 \hbar^4}\mathrm{Im}\left[\frac{\varepsilon_{\mathrm{bb}} - 1}{\varepsilon_{\mathrm{bb}} + 2}\right] k_B^5 T^5$$

Dimensions of the coefficient:

$$\left[\frac{V}{c^3\hbar^4}\right] \cdot [k_B^5 T^5]$$

$\left[\frac{V}{c^3\hbar^4}\right]$

$$[c^3] = (\mathrm{m\,s^{-1}})^3 = \mathrm{m^3\,s^{-3}} \tag{1.6}$$

$$[\hbar^4] = (\mathrm{J\,s})^4 = \mathrm{J^4\,s^4} \tag{1.7}$$

$$\implies [c^3\hbar^4] = (\mathrm{m^3\,s^{-3}})(\mathrm{J^4\,s^4}) = \mathrm{m^3\,J^4\,s} \tag{1.8}$$

Hence:

$$\left[\frac{V}{c^3\hbar^4}\right] = \frac{\mathrm{m}^3}{\mathrm{m^3\,J^4\,s}} = \mathrm{J^{-4}\,s^{-1}}$$

$[k_B^5 T^5]$

$$[k_B^5 T^5] = (\mathrm{J\,K^{-1}})^5 (\mathrm{K})^5 = \mathrm{J}^5$$

Total units for Term 3

Multiplying the two parts:

$$(\mathrm{J}^{-4}\,\mathrm{s}^{-1}) \cdot (\mathrm{J}^{5}) = \mathrm{J}\,\mathrm{s}^{-1} = \mathrm{W}$$

Again, the remaining factors are dimensionless. So Term 3 is in Watts.

1.6.3 Conclusion

Every term has units of power (W), matching the left-hand side $V\,\frac{d[C_V(T-T_0)]}{dt}$. The equation is dimensionally consistent.

Chapter 2

Power absorption for beyond Rayleigh size particles: Integral equation form of Mie scattering

2.1 Setup

We consider a time-harmonic electromagnetic wave, with time dependence $e^{-i\omega t}$, incident on a scattering particle.

- The exterior medium is homogeneous and lossless, with real permittivity ε_m and permeability μ_0.
- The total electric and magnetic fields outside the particle are a superposition of the incident and scattered fields: $\mathbf{E} = \mathbf{E}_{\text{inc}} + \mathbf{E}_{\text{sca}}$ and $\mathbf{H} = \mathbf{H}_{\text{inc}} + \mathbf{H}_{\text{sca}}$.
- The time-averaged Poynting vector is defined as $\mathbf{S} := \frac{1}{2}\,\mathrm{Re}(\mathbf{E} \times \mathbf{H}^*)$.

Our goal is to prove the relationship between absorbed, scattered, and extinction powers.

2.2 Derivation of the Optical Theorem Power Balance: $P_{\mathbf{abs}} = P_{\mathbf{ext}} - P_{\mathbf{sca}}$

2.2.1 Time Averaged Poynting Theorem

The time-averaged Poynting theorem states that the net power flowing out of a closed surface is equal to the negative of the power dissipated (absorbed) within the volume enclosed by that surface. Let's consider a large sphere S_R of radius R that encloses the scattering particle. The net power flux out of this sphere is (derived in Appendix B Eq. (6.16)):

$$\oint_{S_R} \langle \mathbf{S} \rangle \cdot \hat{\mathbf{r}}\, dA = -P_{\text{abs}} \tag{2.1}$$

Here, $P_{\text{abs}} = \frac{\omega}{2} \int_{\text{particle}} \varepsilon'' |\mathbf{E}|^2\, dV$ is the total power absorbed by the particle. The left-hand side represents the total power leaving the sphere; if the particle absorbs energy, this net flux must be negative (i.e., more power flows in than out).

2.2.2 Decomposing into the Power Flux

We now express the total Poynting vector $\langle \mathbf{S} \rangle$ in terms of the incident and scattered fields.

$$\begin{aligned}
\mathbf{E} \times \mathbf{H}^* &= (\mathbf{E}_{\text{inc}} + \mathbf{E}_{\text{sca}}) \times (\mathbf{H}_{\text{inc}} + \mathbf{H}_{\text{sca}})^* && (2.2)\\
&= (\mathbf{E}_{\text{inc}} + \mathbf{E}_{\text{sca}}) \times (\mathbf{H}^*_{\text{inc}} + \mathbf{H}^*_{\text{sca}}) && (2.3)\\
&= \underbrace{\mathbf{E}_{\text{inc}} \times \mathbf{H}^*_{\text{inc}}}_{\text{Incident}} + \underbrace{\mathbf{E}_{\text{sca}} \times \mathbf{H}^*_{\text{sca}}}_{\text{Scattered}} + \underbrace{\mathbf{E}_{\text{inc}} \times \mathbf{H}^*_{\text{sca}} + \mathbf{E}_{\text{sca}} \times \mathbf{H}^*_{\text{inc}}}_{\text{Interference (Extinction)}} && (2.4)
\end{aligned}$$

By taking $\frac{1}{2}\,\mathrm{Re}\{\cdot\}$ of each term, we can split the total Poynting vector $\langle \mathbf{S} \rangle$ into three meaningful components:

$$\langle \mathbf{S}_{\mathrm{inc}} \rangle := \frac{1}{2}\,\mathrm{Re}(\mathbf{E}_{\mathrm{inc}} \times \mathbf{H}^*_{\mathrm{inc}}) \tag{2.5}$$

$$\langle \mathbf{S}_{\mathrm{sca}} \rangle := \frac{1}{2}\,\mathrm{Re}(\mathbf{E}_{\mathrm{sca}} \times \mathbf{H}^*_{\mathrm{sca}}) \tag{2.6}$$

$$\langle \mathbf{S}_{\mathrm{int}} \rangle := \frac{1}{2}\,\mathrm{Re}(\mathbf{E}_{\mathrm{inc}} \times \mathbf{H}^*_{\mathrm{sca}} + \mathbf{E}_{\mathrm{sca}} \times \mathbf{H}^*_{\mathrm{inc}}) \tag{2.7}$$

The total flux is the sum of the fluxes from these three parts:

$$\oint_{S_R} \langle \mathbf{S} \rangle \cdot \hat{\mathbf{r}}\, dA = \oint_{S_R} \langle \mathbf{S}_{\mathrm{inc}} \rangle \cdot \hat{\mathbf{r}}\, dA + \oint_{S_R} \langle \mathbf{S}_{\mathrm{sca}} \rangle \cdot \hat{\mathbf{r}}\, dA + \oint_{S_R} \langle \mathbf{S}_{\mathrm{int}} \rangle \cdot \hat{\mathbf{r}}\, dA \tag{2.8}$$

2.2.3 Analysing Each Flux Integral

We now evaluate each of the three integrals on the right-hand side of Eq. (2.8).

Incident Flux: The incident fields $(\mathbf{E}_{\mathrm{inc}}, \mathbf{H}_{\mathrm{inc}})$ are a source-free solution to Maxwell's equations everywhere inside the sphere S_R (since the sources are at infinity). For such fields in a lossless medium,$\langle \nabla \cdot \mathbf{S}_{\mathrm{inc}} \rangle = 0$. By the divergence theorem, the flux through any closed surface must be zero (derived in Appendix B, Eq. (6.29)).

$$\oint_{S_R} \langle \mathbf{S}_{\mathrm{inc}} \cdot \hat{\mathbf{r}} \rangle\, dA = \int_{V_R} \langle (\nabla \cdot \mathbf{S}_{\mathrm{inc}}) \rangle\, dV = 0 \tag{2.9}$$

Scattered Flux: The scattered fields originate from the particle. The integral of $\mathbf{S}_{\mathrm{sca}}$ over the sphere gives the total power radiated by the particle in all directions. This is, by definition, the **scattered power**, P_{sca}.

$$\oint_{S_R} \langle \mathbf{S}_{\mathrm{sca}} \cdot \hat{\mathbf{r}} \rangle\, dA = P_{\mathrm{sca}} \tag{2.10}$$

Interference Flux: The third integral, involving the cross-terms, represents the interference between the incident and scattered waves. This term accounts for the total power removed from the incident beam by both absorption and scattering. We define the **extinction power**,

P_{ext}, as the negative of this interference flux.

$$\oint_{S_R} \langle \mathbf{S}_{\text{int}} \cdot \hat{\mathbf{r}} \rangle \, dA = -P_{\text{ext}} \tag{2.11}$$

This definition is the basis of the optical theorem, which relates the extinction power to the imaginary part of the forward-scattering amplitude.

2.2.4 Assemble the Result

We now substitute our findings for each of the three flux integrals back into Eq. (2.8):

$$\oint_{S_R} \langle \mathbf{S} \rangle \cdot \hat{\mathbf{r}} \, dA = 0 + P_{\text{sca}} - P_{\text{ext}} \tag{2.12}$$

Finally, we equate this result with our starting point from the Poynting theorem, Eq. (2.1):

$$-P_{\text{abs}} = P_{\text{sca}} - P_{\text{ext}} \tag{2.13}$$

Rearranging this equation gives the final, celebrated result:

$$\boxed{P_{\text{abs}} = P_{\text{ext}} - P_{\text{sca}}} \tag{2.14}$$

This demonstrates the conservation of energy: the total power removed from the incident beam (*extinction*) is precisely the sum of the power that is re-radiated (*scattering*) and the power that is dissipated as heat (*absorption*).

2.3 The Electric-Field Integral Equation (EFIE)

2.3.1 Setup and Conventions

Time dependence $\sim e^{-i\omega t}$ is assumed. We use Gaussian units and $\mu = 1$. Define $k_0 = \omega/c$ and $\kappa^2(\vec{r}) = \varepsilon(\vec{r})k_0^2$. The incident field $\vec{E}_{\text{inc}}$ is what we would have in free space ($\varepsilon = 1$) without scatterers; the scattered field is what arises because $\varepsilon(\vec{r}) \neq 1$ in a finite region. Maxwell's equations are:

$$\nabla \times \vec{E} = \frac{i\omega}{c}\vec{H}, \qquad \nabla \times \vec{H} = -\frac{i\omega}{c}\,\varepsilon(\vec{r})\vec{E}.$$

2.3.2 The Vector Wave Equation for $\vec{E}$

Take the curl of $\nabla \times \vec{E} = (i\omega/c)\vec{H}$:

$$\nabla \times \nabla \times \vec{E} = \frac{i\omega}{c}\,\nabla \times \vec{H} = -\frac{\omega^2}{c^2}\,\varepsilon(\vec{r})\vec{E} = -k_0^2\,\varepsilon(\vec{r})\vec{E}.$$

Bringing the RHS to the left:

$$\nabla \times \nabla \times \vec{E} - \varepsilon(\vec{r})k_0^2\vec{E} = 0. \tag{2.15}$$

Comment on divergence: From $\nabla \cdot (\varepsilon\vec{E}) = 0$ (no free charge) we get:

$$\nabla \cdot \vec{E} = -\frac{1}{\varepsilon}\,\vec{E} \cdot \nabla\varepsilon. \tag{2.16}$$

Using the identity $\nabla \times \nabla \times \vec{E} = \nabla(\nabla \cdot \vec{E}) - \nabla^2\vec{E}$, you can rewrite Eq. (2.15) as:

$$\nabla^2\vec{E} + \nabla\left[\frac{1}{\varepsilon}\,\vec{E} \cdot \nabla\varepsilon\right] + \varepsilon k_0^2\vec{E} = 0. \tag{2.17}$$

. We won't actually solve Eq. (2.17); it just tells us the divergence is not zero when $\nabla\varepsilon \neq 0$.

2.3.3 Green's Vector Identity (Levine–Schwinger trick)

For any smooth $\vec{A}, \vec{B}$ on a volume V with boundary S, the identity

$$\int_S d\vec{s} \cdot \left[\vec{B} \times (\nabla \times \vec{A}) - \vec{A} \times (\nabla \times \vec{B})\right] = \int_V dV\left[\vec{A} \cdot (\nabla \times \nabla \times \vec{B}) - \vec{B} \cdot (\nabla \times \nabla \times \vec{A})\right] \tag{2.18}$$

follows from $\nabla \cdot (\vec{C} \times \vec{D}) = \vec{D} \cdot (\nabla \times \vec{C}) - \vec{C} \cdot (\nabla \times \vec{D})$ plus Gauss' theorem. We will apply Eq. (2.18) with

$$\vec{A}(\vec{r}') = \mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e} \quad \text{and}$$
$$\vec{B}(\vec{r}') = \vec{E}_{int}(\vec{r}'),$$

where $\vec{e}$ is any fixed constant vector and $\mathbf{\Gamma}$ is the dyadic (tensor) Green's function defined next.

2.3.4 The Dyadic Green's Function

$$\nabla \times \nabla \times \mathbf{\Gamma}(\vec{r}, \vec{r}') - k^2 \, \mathbf{\Gamma}(\vec{r}, \vec{r}') = \mathbf{I} \, \delta(\vec{r} - \vec{r}'). \tag{2.19}$$

Here k is chosen as the exterior wavenumber (free space), so $k = k_0$. $\mathbf{I}$ is the identity dyad. Two key identities we will need:

Divergence of Eq. (2.19). Taking $\nabla \cdot$ with respect to $\vec{r}$:

$$k^2 \, \nabla \cdot \mathbf{\Gamma}(\vec{r}, \vec{r}') = -\nabla \delta(\vec{r} - \vec{r}') = \nabla' \delta(\vec{r} - \vec{r}'). \tag{2.20}$$

Link to the scalar Green's function $G(\vec{r}, \vec{r}') = \dfrac{e^{ik|\vec{r} - \vec{r}'|}}{4\pi |\vec{r} - \vec{r}'|}$, (from Eq. (6.31)) which satisfies:

$$(\nabla^2 + k^2) G(\vec{r}, \vec{r}') = -\delta(\vec{r} - \vec{r}'). \tag{2.21}$$

Using $\nabla \times \nabla \times = -\nabla^2 + \nabla\nabla\cdot$, we find that (From Eq. (6.34) :

$$\mathbf{\Gamma}(\vec{r}, \vec{r}') = \left(\mathbf{I} - \frac{1}{k^2} \nabla \nabla' \right) G(\vec{r}, \vec{r}') \quad \text{and} \quad \tilde{\mathbf{\Gamma}}(\vec{r}', \vec{r}) = \mathbf{\Gamma}(\vec{r}, \vec{r}'). \tag{2.22}$$

where, $\nabla\nabla'$ represents the Hessian matrix.

2.3.5 Applying the Vector Green's Identity

We apply the vector Green's identity from the previous section (equation Eq. (2.18)) over all space $V = \mathbb{R}^3$. We choose our vectors to be $\vec{A}(\vec{r}') = \mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e}$ and $\vec{B}(\vec{r}') = \vec{E}_{int}(\vec{r}')$. The core idea is that the surface integral at infinity will yield the incident field, while the volume integral will relate the total field $\vec{E}$ to the scattering source.

Right-Hand Side (Volume Integral): We substitute the wave equations for $\vec{E}$ and $\mathbf{\Gamma}$:

- From Eq. (2.15): $\nabla' \times \nabla' \times \vec{E}_{int}(\vec{r}') = \varepsilon(\vec{r}')k_0^2\vec{E}_{int}(\vec{r}')$
- From Eq. (2.19) : $\nabla' \times \nabla' \times \mathbf{\Gamma}(\vec{r}', \vec{r}) = k^2\mathbf{\Gamma}(\vec{r}', \vec{r}) + \mathbf{I}\delta(\vec{r}' - \vec{r})$

The volume integral becomes:

$$\begin{aligned}
&\int_{\mathbb{R}^3} dV' \Big[(\mathbf{\Gamma} \cdot \vec{e}) \cdot (\nabla' \times \nabla' \times \vec{E}) - \vec{E} \cdot (\nabla' \times \nabla' \times (\mathbf{\Gamma} \cdot \vec{e}))\Big] \\
&= \int_{\mathbb{R}^3} dV' \Big[(\mathbf{\Gamma} \cdot \vec{e}) \cdot (\varepsilon k_0^2 \vec{E}) - \vec{E} \cdot \Big(k^2(\mathbf{\Gamma} \cdot \vec{e}) + \mathbf{I}\delta(\vec{r}' - \vec{r}) \cdot \vec{e}\Big)\Big] \\
&= \int_V dV' \,[\varepsilon(\vec{r}')k_0^2 - k^2]\, \vec{E}_{int}(\vec{r}') \cdot \mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e} - \int_{\mathbb{R}^3} dV' \,\vec{E}_{int}(\vec{r}') \cdot \mathbf{I}\delta(\vec{r}' - \vec{r}) \cdot \vec{e} \\
&= \int_V dV' \,[\varepsilon(\vec{r}')k_0^2 - k^2]\, \vec{E}_{int}(\vec{r}') \cdot \mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e} - \vec{E}(\vec{r}) \cdot \vec{e}
\end{aligned}$$

Here, the integral domain V can be restricted to the region where $\varepsilon(\vec{r}') \neq 1$.

Left-Hand Side (Surface Integral): With an outgoing Green's function, the surface integral at infinity gives the incident field: $\int_S \cdots = -\vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e}$.

Combining Both Sides: Equating the left and right sides and rearranging gives:

$$\vec{E}(\vec{r}) \cdot \vec{e} = \vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e} + \int_V dV' \left[\varepsilon(\vec{r}')k_0^2 - k^2\right] \vec{E}_{int}(\vec{r}') \cdot \mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e}. \tag{2.23}$$

We choose the Green's function for free space, so $k = k_0$. The term in brackets simplifies to $[\varepsilon(\vec{r}') - 1]k_0^2$. Since the constant vector $\vec{e}$ is arbitrary, we can write the dyadic equation:

$$\boxed{\vec{E}(\vec{r}) = \vec{E}_{\text{inc}}(\vec{r}) + \int_V k_0^2\,[\varepsilon(\vec{r}') - 1]\,\mathbf{\Gamma}(\vec{r},\vec{r}') \cdot \vec{E}_{int}(\vec{r}')\,dV'.} \tag{2.24}$$

This famous result is the **Lippmann-Schwinger equation** for vector fields. It states that the total field is the incident field plus the field radiated by the equivalent polarization currents $\vec{J}_{\text{eq}}(\vec{r}') \equiv k_0^2[\varepsilon(\vec{r}') - 1]\vec{E}_{int}(\vec{r}')$.

2.3.6 Derivation of the Surface Integral Term

Let's walk through the derivation of Eq. (2.23) more slowly to see exactly where the incident field term comes from.

Goal

Starting from Green's vector identity, show that:

$$\boxed{\vec{E}(\vec{r})\cdot\vec{e} = \vec{E}_{\text{inc}}(\vec{r})\cdot\vec{e} + \int_V \left[\varepsilon(\vec{r}')k_0^2 - k^2\right] \vec{E}_{int}(\vec{r}')\cdot\mathbf{\Gamma}(\vec{r}',\vec{r})\cdot\vec{e}\,dV'.}$$

Here $k_0 = \omega/c$, k is the wavenumber used to build $\mathbf{\Gamma}$, and $\mathbf{\Gamma}$ solves:

$$\nabla' \times \nabla' \times \mathbf{\Gamma}(\vec{r}',\vec{r}) - k^2\mathbf{\Gamma}(\vec{r}',\vec{r}) = \mathbf{I}\,\delta(\vec{r}' - \vec{r}). \tag{2.25}$$

Start from Green's Identity

The identity (with derivatives w.r.t. $\vec{r}'$) is:

$$\int_S d\vec{s}'\cdot\left[\vec{B}\times(\nabla'\times\vec{A}) - \vec{A}\times(\nabla'\times\vec{B})\right] = \int_V dV'\left[\vec{A}\cdot(\nabla'\times\nabla'\times\vec{B}) - \vec{B}\cdot(\nabla'\times\nabla'\times\vec{A})\right]. \tag{2.26}$$

Choose $\vec{A}(\vec{r}') = \mathbf{\Gamma}(\vec{r}',\vec{r})\cdot\vec{e}$ and $\vec{B}(\vec{r}') = \vec{E}_{int}(\vec{r}')$.

Evaluate the Volume (RHS) Integral

We use the wave equations for the fields inside the integral:

- Maxwell's equations give: $\nabla' \times \nabla' \times \vec{E}_{int}(\vec{r}') = \varepsilon(\vec{r}')k_0^2\, \vec{E}_{int}(\vec{r}')$.
- The definition of $\mathbf{\Gamma}$ gives: $\nabla' \times \nabla' \times (\mathbf{\Gamma} \cdot \vec{e}) = k^2(\mathbf{\Gamma} \cdot \vec{e}) + \vec{e}\,\delta(\vec{r}' - \vec{r})$.

Plugging these into the RHS of Eq. (2.26) gives:

$$\begin{aligned} &\int_V dV' \left[(\mathbf{\Gamma} \cdot \vec{e}) \cdot (\varepsilon k_0^2 \vec{E}) - \vec{E} \cdot \left(k^2 \mathbf{\Gamma} \cdot \vec{e} + \vec{e}\,\delta\right)\right] \\ &= \int_V dV' \left(\varepsilon(\vec{r}')k_0^2 - k^2\right) \vec{E}_{int}(\vec{r}') \cdot (\mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e}) - \vec{E}(\vec{r}) \cdot \vec{e}. \end{aligned} \tag{2.27}$$

So, Green's identity now reads:

$$\underbrace{\int_S d\vec{s}' \cdot \left[\vec{E} \times (\nabla' \times (\mathbf{\Gamma} \cdot \vec{e})) - (\mathbf{\Gamma} \cdot \vec{e}) \times (\nabla' \times \vec{E})\right]}_{\mathcal{S}} = \int_V \left(\varepsilon k_0^2 - k^2\right) \vec{E} \cdot (\mathbf{\Gamma} \cdot \vec{e})\, dV' - \vec{E}(\vec{r}) \cdot \vec{e}. \tag{2.28}$$

Rearranging for $\vec{E}(\vec{r}) \cdot \vec{e}$ gives:

$$\vec{E}(\vec{r}) \cdot \vec{e} = \int_V \left(\varepsilon k_0^2 - k^2\right) \vec{E} \cdot (\mathbf{\Gamma} \cdot \vec{e})\, dV' - \mathcal{S}. \tag{2.29}$$

To finish, we must show that the surface term $\mathcal{S}$ is equal to $-\vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e}$.

Evaluate the Surface Term $\mathcal{S}$

Let the total field be $\vec{E} = \vec{E}_{\text{inc}} + \vec{E}_{\text{sct}}$. The surface integral splits into two parts: $\mathcal{S} = \mathcal{S}_{\text{inc}} + \mathcal{S}_{\text{sct}}$.

(a) **The scattered part vanishes.** Both $\vec{E}_{\text{sct}}$ and $\mathbf{\Gamma}$ represent outgoing waves. They obey the Sommerfeld radiation condition, meaning they decay as e^{ikR}/R at large distances R. This causes the integrand to decay faster than the surface area (R^2) grows, so $\mathcal{S}_{\text{sct}} \to 0$ as the surface S is taken to infinity.

(b) **The incident part gives the result.** Let's evaluate $\mathcal{S}_{\text{inc}}$ by applying Green's identity a second time, but for the incident field $\vec{E}_{\text{inc}}$ and $\mathbf{\Gamma}$ in a volume free of scatterers (where

$\varepsilon = 1$ and $k = k_0$). The volume integral is:

$$\int_V dV' \left[\vec{E}_{\text{inc}} \cdot (\nabla' \times \nabla' \times (\mathbf{\Gamma} \cdot \vec{e})) - (\mathbf{\Gamma} \cdot \vec{e}) \cdot (\nabla' \times \nabla' \times \vec{E}_{\text{inc}})\right].$$

In free space, $\nabla' \times \nabla' \times \vec{E}_{\text{inc}} = k^2 \vec{E}_{\text{inc}}$, and from Eq. (2.25) , $\nabla' \times \nabla' \times (\mathbf{\Gamma} \cdot \vec{e}) = k^2 (\mathbf{\Gamma} \cdot \vec{e}) + \vec{e}\delta$. The k^2 terms cancel perfectly! The volume integral simplifies to:

$$\int_V dV' \, \vec{E}_{\text{inc}}(\vec{r}') \cdot (\vec{e}\delta(\vec{r}' - \vec{r})) = \vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e}.$$

This volume integral is equal to the surface integral from Green's identity:

$$\int_S d\vec{s}' \cdot \left[\vec{E}_{\text{inc}} \times (\nabla' \times (\mathbf{\Gamma} \cdot \vec{e})) - (\mathbf{\Gamma} \cdot \vec{e}) \times (\nabla' \times \vec{E}_{\text{inc}})\right] = \vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e}.$$

Notice the terms in the bracket are in the opposite order of our original definition of $\mathcal{S}_{\text{inc}}$. Therefore, $\mathcal{S}_{\text{inc}} = -\vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e}$.

Combining the terms above, we find the total surface term is $\mathcal{S} = \mathcal{S}_{\text{inc}} + \mathcal{S}_{\text{sct}} = -\vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e}$.

Final Assembly

Inserting our result for $\mathcal{S}$ back into equation Eq. (2.29) , we get:

$$\vec{E}(\vec{r}) \cdot \vec{e} = \int_V \left(\varepsilon k_0^2 - k^2\right) \vec{E}_{int}(\vec{r}') \cdot \mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e} \, dV' - (-\vec{E}_{\text{inc}}(\vec{r}) \cdot \vec{e}),$$

which is exactly the target equation Eq. (2.23) .

2.3.7 Electric field in terms of Scalar Green's Function

We now substitute the expression for $\mathbf{\Gamma}$ from Eq. (2.22) into our final result Eq. (2.24) :

$$\mathbf{\Gamma}(\vec{r}, \vec{r}') = \left(\mathbf{I} - \frac{1}{k_0^2} \nabla\nabla'\right) G(\vec{r}, \vec{r}').$$

The integral becomes, with $\vec{E}_{int}(\vec{r}')$ representing the Electric field inside the volume of the sphere:

$$\begin{aligned}\vec{E}(\vec{r}) &= \vec{E}_{\mathrm{inc}}(\vec{r}) + \int_V k_0^2\,[\varepsilon(\vec{r}') - 1]\left(\mathbf{I} - \frac{1}{k_0^2}\nabla\nabla'\right) G(\vec{r},\vec{r}')\cdot\vec{E}_{int}(\vec{r}')\,dV' \\ &= \vec{E}_{\mathrm{inc}}(\vec{r}) + k_0^2\int_V [\varepsilon(\vec{r}') - 1]\,G(\vec{r},\vec{r}')\,\vec{E}_{int}(\vec{r}')\,dV' \\ &\quad - \int_V [\varepsilon(\vec{r}') - 1]\,(\nabla\nabla' G(\vec{r},\vec{r}'))\cdot\vec{E}_{int}(\vec{r}')\,dV'. \end{aligned} \tag{2.30}$$

Since ∇ acts on $\vec{r}$ and not $\vec{r}'$, we can pull it outside the integral:

$$\begin{aligned}\vec{E}(\vec{r}) = \vec{E}_{\mathrm{inc}}(\vec{r}) &+ k_0^2\int_V [\varepsilon(\vec{r}') - 1]\,G(\vec{r},\vec{r}')\,\vec{E}_{int}(\vec{r}')\,dV' \\ &- \nabla\int_V [\varepsilon(\vec{r}') - 1]\left[\nabla' G(\vec{r},\vec{r}')\cdot\vec{E}_{int}(\vec{r}')\right]dV'. \end{aligned} \tag{2.31}$$

This is the electric-field volume integral equation in its scalar-Green form. The outgoing boundary condition is automatically satisfied because it's built into G.

2.3.8 Far-Field Asymptotics of G and ∇G

Let $\hat{s} := \vec{r}/r$ be the unit vector pointing from the origin (assumed to be inside the scatterer) to the observer. The scatterer is contained in a bounded volume V, so for any source point $\vec{r}' \in V$, we have $r \gg r' = |\vec{r}'|$. We can then approximate the distance $|\vec{r} - \vec{r}'|$:

$$|\vec{r} - \vec{r}'| = \sqrt{(\vec{r} - \vec{r}')\cdot(\vec{r} - \vec{r}')} = \sqrt{r^2 - 2\vec{r}\cdot\vec{r}' + r'^2} = r\sqrt{1 - \frac{2\hat{s}\cdot\vec{r}'}{r} + \frac{r'^2}{r^2}} \approx r - \hat{s}\cdot\vec{r}'.$$

In the denominator of G, we can simply use $|\vec{r} - \vec{r}'| \approx r$. In the exponent (the phase), the second term is crucial. This gives the far-field approximation for G:

$$G(\vec{r},\vec{r}') = \frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} \approx \frac{e^{ik(r-\hat{s}\cdot\vec{r}')}}{4\pi r} = \frac{e^{ikr}}{4\pi r}\,e^{-ik\,\hat{s}\cdot\vec{r}'}. \tag{2.32}$$

Next, we need the gradients. For ∇ (derivatives w.r.t. $\vec{r}$), the dominant contribution comes from differentiating the rapidly oscillating e^{ikr} term:

$$\nabla\left(\frac{e^{ikr}}{4\pi r}\right) = \hat{s}\frac{d}{dr}\left(\frac{e^{ikr}}{4\pi r}\right) = \hat{s}\left(\frac{ike^{ikr}}{4\pi r} - \frac{e^{ikr}}{4\pi r^2}\right) = ik\,\hat{s}\,\frac{e^{ikr}}{4\pi r}\left(1+\frac{i}{kr}\right).$$

In the far field ($kr \gg 1$), we keep only the leading order term in $1/r$:

$$\nabla G(\vec{r},\vec{r}') \approx \nabla\left(\frac{e^{ikr}}{4\pi r}\right)e^{-ik\,\hat{s}\cdot\vec{r}'} \approx ik\,\hat{s}\,\frac{e^{ikr}}{4\pi r}e^{-ik\,\hat{s}\cdot\vec{r}'}. \tag{2.33}$$

Similarly, for ∇' (derivatives w.r.t. $\vec{r}'$), the only term that depends on $\vec{r}'$ in the far-field form is the phase $e^{-ik\,\hat{s}\cdot\vec{r}'}$.

$$\nabla' e^{-ik\,\hat{s}\cdot\vec{r}'} = -ik\,\hat{s}e^{-ik\,\hat{s}\cdot\vec{r}'}.$$

So, the gradient with respect to the source coordinates is:

$$\nabla' G(\vec{r},\vec{r}') \approx \frac{e^{ikr}}{4\pi r}\nabla'\left(e^{-ik\,\hat{s}\cdot\vec{r}'}\right) \approx -ik\,\hat{s}\,\frac{e^{ikr}}{4\pi r}\,e^{-ik\,\hat{s}\cdot\vec{r}'}. \tag{2.34}$$

2.3.9 Evaluating the First Volume Integral in the Far Field

Using approximation Eq. (2.32) for G in the first integral of Eq. (2.31) :

$$\begin{aligned} k^2\int_V [\varepsilon(\vec{r}')-1]\,\vec{E}_{int}(\vec{r}')\,G\,dV' &\approx k^2\int_V [\varepsilon(\vec{r}')-1]\,\vec{E}_{int}(\vec{r}')\left(\frac{e^{ikr}}{4\pi r}\,e^{-ik\,\hat{s}\cdot\vec{r}'}\right)dV' \\ &\approx \frac{e^{ikr}}{r}\,\frac{k^2}{4\pi}\int_V e^{-ik\,\hat{s}\cdot\vec{r}'}[\varepsilon(\vec{r}')-1]\,\vec{E}_{int}(\vec{r}')\,dV' \\ &=: \frac{e^{ikr}}{r}\,\vec{P}(\hat{s}). \end{aligned} \tag{2.35}$$

This defines the vector amplitude $\vec{P}(\hat{s})$, which is essentially the Fourier transform of the equivalent polarisation current. If we assume the internal electric field isn't dependent on the position inside the sphere, it has a fixed direction, then, $\vec{P}(\hat{s})$ in the direction of the internal electric field $\vec{E}_{int}(\vec{r}')$:

$$\boxed{\vec{P}(\hat{s}) = \frac{k^2}{4\pi} \int_V e^{-ik\,\hat{s}\cdot\vec{r}'} \left[\varepsilon(\vec{r}') - 1\right] \vec{E}_{int}(\vec{r}')\, dV'.} \tag{2.36}$$

2.3.10 Evaluating the Second (Gradient) Term in the Far Field

Let's call the scalar integral inside the gradient term $I(\vec{r})$:

$$I(\vec{r}) := \int_V \left[\nabla' G(\vec{r}, \vec{r}') \cdot \vec{E}_{int}(\vec{r}')\right] \left[\varepsilon(\vec{r}') - 1\right] dV'. \tag{2.37}$$

Using approximation Eq. (2.34) for $\nabla' G$:

$$\begin{aligned} I(\vec{r}) &\approx \int_V \left[\left(-ik\,\hat{s}\,\frac{e^{ikr}}{4\pi r}\, e^{-ik\,\hat{s}\cdot\vec{r}'}\right) \cdot \vec{E}_{int}(\vec{r}')\right] \left[\varepsilon(\vec{r}') - 1\right] dV' \\ &= -\frac{ik\, e^{ikr}}{4\pi r}\,\hat{s} \cdot \int_V e^{-ik\,\hat{s}\cdot\vec{r}'} \left[\varepsilon(\vec{r}') - 1\right] \vec{E}_{int}(\vec{r}')\, dV' \\ &= -\frac{ik\, e^{ikr}}{r} \left(\frac{1}{k^2}\right) \hat{s} \cdot \vec{P}(\hat{s}) = -\frac{e^{ikr}}{r}\,\frac{i}{k}\,\hat{s} \cdot \vec{P}(\hat{s}). \end{aligned} \tag{2.38}$$

Now we apply $-\nabla$ to this result. Using approximation Eq. (2.33) for the gradient of the outgoing spherical wave:

$$\begin{aligned} -\nabla I(\vec{r}) &\approx -\nabla\left[\frac{e^{ikr}}{r}\right] \left(-\frac{i}{k}\,\hat{s} \cdot \vec{P}(\hat{s})\right) \\ &\approx -\left(ik\,\hat{s}\,\frac{e^{ikr}}{r}\right) \left(-\frac{i}{k}\,\hat{s} \cdot \vec{P}(\hat{s})\right) \\ &= -\frac{e^{ikr}}{r}\,\hat{s}\left(\hat{s} \cdot \vec{P}(\hat{s})\right). \end{aligned} \tag{2.39}$$

2.3.11 Combining the Pieces to Find the Scattering Electric Field

The total scattered field $\vec{E}_{\mathrm{sctd}}$ is the sum of the results from (Eq. (2.35)) and (Eq. (2.39)):

$$\begin{aligned} \vec{E}_{\mathrm{sctd}}(\vec{r}) &\approx \frac{e^{ikr}}{r}\,\vec{P}(\hat{s}) - \frac{e^{ikr}}{r}\,\hat{s}\left(\hat{s} \cdot \vec{P}(\hat{s})\right) \\ &= \frac{e^{ikr}}{r}\left[\vec{P}(\hat{s}) \;-\; \hat{s}\left(\hat{s} \cdot \vec{P}(\hat{s})\right)\right]. \end{aligned}$$

This gives the final form for the scattered field:

$$\boxed{\vec{E}_{\text{sctd}}(\vec{r}) \;\approx\; \frac{e^{ikr}}{r}\left[\,\vec{P}(\hat{s}) \;-\; \hat{s}\left(\hat{s}\cdot\vec{P}(\hat{s})\right)\right].} \tag{2.40}$$

The term in the brackets is the component of the vector $\vec{D}$ that is transverse to the direction of propagation $\hat{s}$, which is exactly what we expect for an electromagnetic wave. We can express this using the transverse projector dyadic $\mathbf{P}_{\perp}(\hat{s}) = \mathbf{I} - \hat{s}\hat{s}^{\top}$:

$$\vec{E}_{\text{sctd}}(\vec{r}) \approx \frac{e^{ikr}}{r}\,\mathbf{P}_{\perp}(\hat{s})\,\vec{P}(\hat{s}). \tag{2.41}$$

A more common way to write this transverse projection is using the vector triple product identity $\vec{A} - \hat{s}(\hat{s}\cdot\vec{A}) = \hat{s}\times(\vec{A}\times\hat{s})$. Applying this, we arrive at the standard form for the scattered field in terms of the scattering amplitude $\vec{F}_1$:

$$\boxed{\vec{E}_{\text{sctd}}(\vec{r}) \;\approx\; \frac{e^{ikr}}{r}\,\vec{F}_1(\hat{s}) \quad \text{with} \quad \vec{F}_1(\hat{s}) = \hat{s}\times\left(\vec{P}(\hat{s})\times\hat{s}\right),} \tag{2.42}$$

where $\vec{P}(\hat{s}) = \frac{k^2}{4\pi}\int_V e^{-ik\,\hat{s}\cdot\vec{r}'}\,[\varepsilon(\vec{r}') - 1]\,\vec{E}_{int}(\vec{r}')\,dV'$ and $\hat{s} := \vec{r}/r$ is the unit vector pointing from the origin (assumed to be inside the scatterer) to the observer.

Remarks:

- The direction of $\vec{F}_1(\hat{s})$ is dependent on the direction of $\vec{P}(\hat{s})$ which is in the direction of the internal electric field $\vec{E}_{int}(\vec{r}')$. This is if we assume that the internal electric field isn't dependent on the position of the point inside the sphere and is constant.

- The final result is manifestly transverse, as $\hat{s}\cdot\vec{F}_1 = \hat{s}\cdot(\hat{s}\times(\dots)) = 0$.

2.4 The Magnetic-Field Integral Equation (MFIE)

2.4.1 Setup and Conventions

We use Gaussian units with $\mu = 1$. The time-dependence is $e^{-i\omega t}$. The free-space wavenumber is $k_0 = \omega/c$, and the position-dependent wavenumber is $\kappa^2(\vec{r}) = \varepsilon(\vec{r})k_0^2$. The dyadic Green's function for free space, $\mathbf{\Gamma}$, satisfies:

$$\nabla \times \nabla \times \mathbf{\Gamma}(\vec{r}, \vec{r}') - k_0^2\, \mathbf{\Gamma}(\vec{r}, \vec{r}') = \mathbf{I}\, \delta(\vec{r} - \vec{r}'),$$

and can be expressed in terms of the scalar Green's function $G(\vec{r}, \vec{r}') = \dfrac{e^{ik_0|\vec{r}-\vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|}$ as:

$$\mathbf{\Gamma}(\vec{r}, \vec{r}') = \left(\mathbf{I} - \frac{1}{k_0^2}\nabla\nabla'\right) G(\vec{r}, \vec{r}').$$

2.4.2 Rewrite the Magnetic Wave Equation into "Source" Form

We start from the second-order wave equation for the magnetic field $\vec{H}$ in an inhomogeneous medium (Eq. (2.3.1)):

$$\nabla \times \left[\frac{1}{\varepsilon(\vec{r})}\, \nabla \times \vec{H}(\vec{r})\right] - k_0^2\, \vec{H}(\vec{r}) = 0.$$

Our first goal is to rearrange this into a form that looks like a standard Helmholtz equation with an explicit source term. We begin by applying the vector product rule $\nabla \times (f\vec{A}) = f(\nabla \times \vec{A}) + (\nabla f) \times \vec{A}$:

$$\nabla \times \left(\frac{1}{\varepsilon}\, \nabla \times \vec{H}\right) = \frac{1}{\varepsilon}\, \nabla \times \nabla \times \vec{H} + \nabla\left(\frac{1}{\varepsilon}\right) \times (\nabla \times \vec{H}).$$

Next, we simplify the two terms on the right. For the second term, we use Maxwell's equation for the curl of $\vec{H}$ and the chain rule for $\nabla(1/\varepsilon)$:

- $\nabla \times \vec{H} = -\dfrac{i\omega}{c}\, \varepsilon\, \vec{E} = -ik_0\, \varepsilon\, \vec{E}$
- $\nabla(1/\varepsilon) = -\dfrac{\nabla\varepsilon}{\varepsilon^2}$

Substituting these in gives:

$$\nabla\left(\frac{1}{\varepsilon}\right) \times (\nabla \times \vec{H}) = -\frac{\nabla\varepsilon}{\varepsilon^2} \times \big(- ik_0\, \varepsilon\, \vec{E}\big) = \frac{ik_0}{\varepsilon}\, \nabla\varepsilon \times \vec{E}.$$

Plugging this result back into the wave equation and multiplying the entire equation by $\varepsilon(\vec{r})$ yields:

$$\nabla \times \nabla \times \vec{H} + ik_0\, \nabla\varepsilon(\vec{r}) \times \vec{E}(\vec{r}) - \varepsilon(\vec{r})k_0^2\, \vec{H}(\vec{r}) = 0.$$

Rearranging this to isolate the Helmholtz operator acting on $\vec{H}$ (and recalling $\kappa^2 = \varepsilon k_0^2$), we get our desired "source" form:

$$\boxed{\nabla \times \nabla \times \vec{H}(\vec{r}) - \kappa^2(\vec{r})\vec{H}(\vec{r}) = -ik_0\, \nabla\varepsilon(\vec{r}) \times \vec{E}(\vec{r}).} \tag{2.43}$$

This powerful result shows that for the magnetic field, the "source" driving the scattering is not just the presence of the dielectric ($\varepsilon \neq 1$), but specifically the *gradient* of the permittivity, $\nabla\varepsilon$.

2.4.3 Obtain the Volume Integral Equation via Green's Identity

We now use the Levine-Schwinger vector Green's identity to convert our differential equation into an integral equation. The identity is:

$$\int_S d\vec{s}' \cdot \big[\vec{B} \times (\nabla' \times \vec{A}) - \vec{A} \times (\nabla' \times \vec{B})\big] = \int_V dV' \,\big[\vec{A} \cdot (\nabla' \times \nabla' \times \vec{B}) - \vec{B} \cdot (\nabla' \times \nabla' \times \vec{A})\big].$$

We make the following choices for our vector fields:

$$\vec{A}(\vec{r}') = \mathbf{\Gamma}(\vec{r}', \vec{r}) \cdot \vec{e}, \qquad \vec{B}(\vec{r}') = \vec{H}(\vec{r}'),$$

where $\vec{e}$ is an arbitrary constant vector.

Right-Hand Side (Volume Term). We substitute our "source" equation for $\nabla' \times \nabla' \times \vec{H}$ and the defining equation for $\mathbf{\Gamma}$:

$$\begin{aligned}
\nabla' \times \nabla' \times \vec{H}(\vec{r}') &= \kappa^2(\vec{r}')\vec{H}(\vec{r}') - ik_0 \nabla'\varepsilon(\vec{r}') \times \vec{E}_{int}(\vec{r}'), \\
\nabla' \times \nabla' \times (\mathbf{\Gamma} \cdot \vec{e}) &= k_0^2(\mathbf{\Gamma} \cdot \vec{e}) + \vec{e}\,\delta(\vec{r}' - \vec{r}).
\end{aligned}$$

The volume integral becomes:

$$\begin{aligned}
\text{RHS} &= \int_V \Big[(\mathbf{\Gamma} \cdot \vec{e}) \cdot (\kappa^2 \vec{H} - ik_0 \nabla'\varepsilon \times \vec{E}) - \vec{H} \cdot \big(k_0^2(\mathbf{\Gamma} \cdot \vec{e}) + \vec{e}\,\delta\big)\Big]\, dV' \\
&= \int_V (\kappa^2 - k_0^2)\, \vec{H} \cdot (\mathbf{\Gamma} \cdot \vec{e})\, dV' - ik_0 \int_V (\mathbf{\Gamma} \cdot \vec{e}) \cdot (\nabla'\varepsilon \times \vec{E})\, dV' - \vec{H}(\vec{r}) \cdot \vec{e}.
\end{aligned}$$

Left-Hand Side (Surface Term). Just as in the electric-field case, the surface integral at infinity, $\mathcal{S}_H$, evaluates to the incident field. The scattered field $\vec{H}_{\text{sct}}$ satisfies the Sommerfeld radiation condition, causing its contribution to vanish. A second application of Green's identity shows that the incident field part gives $\mathcal{S}_H^{(\text{inc})} = -\vec{H}_{\text{inc}}(\vec{r}) \cdot \vec{e}$.

Combining and Solving. Equating the LHS and RHS and rearranging to solve for $\vec{H}(\vec{r}) \cdot \vec{e}$, we find:

$$\vec{H}(\vec{r}) \cdot \vec{e} = \vec{H}_{\text{inc}}(\vec{r}) \cdot \vec{e} + \int_V (\kappa^2 - k_0^2)\, \vec{H} \cdot (\mathbf{\Gamma} \cdot \vec{e})\, dV' - ik_0 \int_V (\mathbf{\Gamma} \cdot \vec{e}) \cdot (\nabla'\varepsilon \times \vec{E})\, dV'.$$

Since $\vec{e}$ is arbitrary, we can promote this to a vector equation. Using $\kappa^2 - k_0^2 = k_0^2(\varepsilon - 1)$, we arrive at the final Magnetic-Field Integral Equation:

$$\boxed{\begin{aligned}
\vec{H}(\vec{r}) = \vec{H}_{\text{inc}}(\vec{r}) &+ \int_V k_0^2\,(\varepsilon(\vec{r}') - 1)\,\mathbf{\Gamma}(\vec{r}, \vec{r}') \cdot \vec{H}(\vec{r}')\, dV' \\
&- ik_0 \int_V \mathbf{\Gamma}(\vec{r}, \vec{r}') \cdot \big[\nabla'\varepsilon(\vec{r}') \times \vec{E}_{int}(\vec{r}')\big]\, dV'.
\end{aligned}} \tag{2.44}$$

2.4.4 The Far-Field Limit and Scattering Amplitude $\vec{A}_2$

To find the scattered field at a large distance ($r = |\vec{r}| \to \infty$), we use the asymptotic form of the Green's function. Let $\hat{s} = \vec{r}/r$.

$$G(\vec{r}, \vec{r}') \approx \frac{e^{ik_0 r}}{4\pi r}\, e^{-ik_0\, \hat{s}\cdot\vec{r}'} \qquad \text{and} \qquad \nabla\nabla' G \approx (-ik_0)^2 \hat{s}\hat{s}^\top G.$$

This leads to the far-field approximation for the dyadic Green's function:

$$\mathbf{\Gamma}(\vec{r}, \vec{r}') = \Big(\mathbf{I} - \frac{1}{k_0^2}\nabla\nabla'\Big) G \xrightarrow{\text{far field}} \Big(\mathbf{I} - \hat{s}\hat{s}^\top\Big) \frac{e^{ik_0 r}}{4\pi r}\, e^{-ik_0\, \hat{s}\cdot\vec{r}'} = \mathbf{P}_\perp(\hat{s}) G(\vec{r}, \vec{r}').$$

Applying this to the two integrals in the MFIE:

- **First Term:**

$$\int_V k_0^2(\varepsilon - 1)\, \mathbf{\Gamma} \cdot \vec{H}\, dV' \approx \frac{e^{ik_0 r}}{r}\, \mathbf{P}_\perp(\hat{s}) \underbrace{\left[\frac{k_0^2}{4\pi} \int_V e^{-ik_0\, \hat{s}\cdot\vec{r}'}\, (\varepsilon - 1)\, \vec{H}(\vec{r}')\, dV'\right]}_{:=\ \vec{P}'(\hat{s})}.$$

- **Second Term:**

$$-ik_0 \int_V \mathbf{\Gamma} \cdot \big(\nabla'\varepsilon \times \vec{E}\big)\, dV' \approx \frac{e^{ik_0 r}}{r}\, \mathbf{P}_\perp(\hat{s}) \underbrace{\left[-\frac{ik_0}{4\pi} \int_V e^{-ik_0\, \hat{s}\cdot\vec{r}'}\, \nabla'\varepsilon(\vec{r}') \times \vec{E}_{int}(\vec{r}')\, dV'\right]}_{:=\ \vec{P}''(\hat{s})}.$$

The total scattered field $\vec{H}_{\text{sctd}} = \vec{H} - \vec{H}_{\text{inc}}$ is the sum of these two contributions:

$$\boxed{\vec{H}_{\text{sctd}}(\vec{r}) \;\approx\; \frac{e^{ik_0 r}}{r}\, \mathbf{P}_\perp(\hat{s})\, [\, \vec{P}'(\hat{s}) + \vec{P}''(\hat{s})\,].} \tag{2.45}$$

Using the identity $\mathbf{P}_\perp(\hat{s})\vec{A} = -\hat{s} \times (\hat{s} \times \vec{A})$, we can define the magnetic scattering amplitude $\vec{A}_2$:

$$\boxed{\vec{H}_{\text{sctd}}(\vec{r}) = \frac{e^{ik_0 r}}{r}\, \vec{F}_2(\hat{s}), \qquad \text{where} \quad \vec{F}_2(\hat{s}) = -\hat{s} \times \Big[\hat{s} \times \Big(\vec{P}'(\hat{s}) + \vec{P}''(\hat{s})\Big)\Big].} \tag{2.46}$$

The vector amplitudes are given by:

$$\boxed{\begin{aligned} \vec{P}'(\hat{s}) &= \frac{k_0^2}{4\pi}\int_V e^{-ik_0\,\hat{s}\cdot\vec{r}'}\,[\varepsilon(\vec{r}')-1]\;\vec{H}(\vec{r}')\,dV', \\ \vec{P}''(\hat{s}) &= -\frac{ik_0}{4\pi}\int_V e^{-ik_0\,\hat{s}\cdot\vec{r}'}\;\nabla'\varepsilon(\vec{r}')\times\vec{E}_{int}(\vec{r}')\,dV'. \end{aligned}} \tag{2.47}$$

2.4.5 Physical Interpretation of the Contributions

The two terms in the scattering amplitude, $\vec{P}'$ and $\vec{P}''$, have distinct physical origins.

- $\tilde{\mathbf{P}}'(\hat{\mathbf{s}})$ represents the radiation from the bulk of the material, driven by the contrast current proportional to $(\varepsilon-1)\vec{H}$. This is analogous to the source term in the E-field equation.
- $\tilde{\mathbf{P}}''(\hat{\mathbf{s}})$ is a unique feature of the MFIE. It represents radiation generated only where the material properties change, i.e., where $\nabla\varepsilon \neq 0$. This term is sourced by the term $\nabla\varepsilon\times\vec{E}$, which can be thought of as an effective magnetic surface current at interfaces.

This second term is crucial because it accounts for polarisation effects that are not present in the simpler E-field formulation. The cross product with $\nabla\varepsilon$ can rotate the polarisation of the internal E-field, leading to a more complex polarisation pattern in the scattered magnetic field. For a homogeneous object, this term becomes a surface integral over the object's boundary.

Chapter 3

Power absorption for beyond Rayleigh size particles: Gordon's approximation and spherical basis

3.1 Conventions and Maxwell equations

Time dependence is $e^{-i\omega t}$. We use Gaussian units with $\mu = 1$. The fields satisfy

$$\nabla \times \mathbf{E} = \frac{i\omega}{c}\,\mathbf{H}, \qquad \nabla \times \mathbf{H} = -\frac{i\omega}{c}\,\varepsilon\,\mathbf{E}. \tag{3.1}$$

Inside a homogeneous dielectric sphere of radius a, we set $\varepsilon = m^2$ (constant). Define the vacuum wavenumber $k_0 = \omega/c$. In the exterior (vacuum) $|\mathbf{k}| = k_0$, while in the homogeneous interior $|\mathbf{k}| = mk_0$.

For any plane wave $\mathbf{E} = \hat{n}\,E_0\,e^{i\mathbf{k}\cdot\mathbf{r}}$ with $\mathbf{k} = k\,\hat{s}$,

$$\mathbf{H} = \frac{c}{\omega}\,\mathbf{k} \times \mathbf{E} = \frac{k}{k_0}\,\hat{s} \times \mathbf{E}. \tag{3.2}$$

Hence, in the interior ($k = mk_0$) one has $\mathbf{H} = m\,\hat{s} \times \mathbf{E}$, so $|\mathbf{H}| = m\,|\mathbf{E}|$. In vacuum ($k = k_0$) one has $\mathbf{H} = \hat{s} \times \mathbf{E}$ and $|\mathbf{H}| = |\mathbf{E}|$.

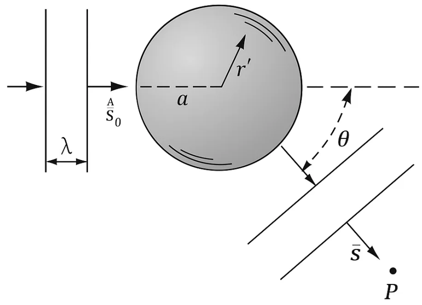

Figure 3.1: $\hat{s}_0$ and $\hat{s}$ are unit vectors in the incident and scattering directions. $\mathbf{r}'$ is a position vector of a point within the scattering sphere of radius a. P is the point at which the scattered radiation is observed. The position vector of P is $\mathbf{r}$. In the text it is assumed that $r \gg a$.

3.2 Scattered electric field using Gordon's ansatz

3.2.1 Setup

We start from the far-field relation

$$\boxed{\vec{E}_{\text{sctd}}(\vec{r}) = \frac{e^{ikr}}{r}\,\vec{F}_1(\hat{s}), \qquad \vec{F}_1(\hat{s}) = \hat{s} \times \big(\vec{P}(\hat{s}) \times \hat{s}\big) = \vec{P}(\hat{s}) - \hat{s}\,\big(\hat{s}\cdot\vec{P}(\hat{s})\big)} \tag{3.3}$$

with

$$\vec{P}(\hat{s}) = \frac{k^2}{4\pi}\int_V e^{-ik\,\hat{s}\cdot\vec{r}'}\,[\varepsilon(\vec{r}') - 1]\,\vec{E}_{\text{int}}(\vec{r}')\,d^3r', \qquad \hat{s} := \frac{\vec{r}}{r}. \tag{3.4}$$

For a homogeneous sphere of radius a centred at the origin we set $\varepsilon(\vec{r}') = m^2$ inside and 1 outside, so the integral extends over $|\vec{r}'| \le a$.

We take the internal-field ansatz (Gordon type)

$$\vec{E}_{\text{int}}(\vec{r}') = \hat{n}_0\,e^{imk\,\hat{s}_0\cdot\vec{r}'} + \hat{n}\,\gamma\,e^{ik\,\hat{s}\cdot\vec{r}'}, \tag{3.5}$$

where $\hat{s}_0$ is the incident propagation direction, $\hat{n}_0$ its polarization, and $\hat{n}$ is a unit polarization transverse to $\hat{s}$ (see Fig. 3.1).

We assume the amplitude of the incident electric field to be 1.

3.2.2 Computing $\vec{P}(\hat{s})$

Insert the ansatz into $\vec{P}(\hat{s})$:

$$\begin{aligned}\vec{P}(\hat{s}) &= \frac{k^2}{4\pi}(m^2-1)\int_{|\vec{r}'|\le a} e^{-ik\,\hat{s}\cdot\vec{r}'}\left[\hat{n}_0\, e^{imk\,\hat{s}_0\cdot\vec{r}'} + \hat{n}\,\gamma\, e^{ik\,\hat{s}\cdot\vec{r}'}\right] d^3r' \\ &= \frac{k^2}{4\pi}(m^2-1)\left[\hat{n}_0\int_{|\vec{r}'|\le a} e^{-i\boldsymbol{q}\cdot\vec{r}'}\, d^3r' \;+\; \hat{n}\,\gamma\int_{|\vec{r}'|\le a} 1\, d^3r'\right],\end{aligned} \tag{3.6}$$

with the mismatch wavevector

$$\boldsymbol{q} := k(\hat{s}-m\hat{s}_0), \qquad q := |\boldsymbol{q}|, \qquad qa = ka\sqrt{1+m^2-2m\cos\theta}, \qquad \cos\theta = \hat{s}\cdot\hat{s}_0.$$

Integral over a ball

We need

$$I(\boldsymbol{q}) := \int_{|\vec{r}'|\le a} e^{-i\,\boldsymbol{q}\cdot\vec{r}'}\, d^3r' \;=\; 4\pi a^3\,\frac{j_1(qa)}{qa}, \tag{3.7}$$

where j_1 is the spherical Bessel function $j_1(z) = \dfrac{\sin z - z\cos z}{z^2}$.

Derivation of (3.7) in detail. Choose spherical coordinates with polar axis along $\boldsymbol{q}$, so $\boldsymbol{q}\cdot\vec{r}' = qr'\cos\theta$ and $d^3r' = r'^2\sin\theta\, d\theta\, d\phi\, dr'$:

$$\begin{aligned}I(q) &= \int_0^a\int_0^{2\pi}\int_0^{\pi} e^{-iqr'\cos\theta}\, r'^2\sin\theta\, d\theta\, d\phi\, dr' = 2\pi\int_0^a r'^2\left[\int_{-1}^{1} e^{-iqr'\mu}\, d\mu\right] dr' \\ &= 2\pi\int_0^a r'^2\left[\frac{e^{-iqr'}-e^{iqr'}}{-iqr'}\right] dr' = \frac{4\pi}{q}\int_0^a r'\sin(qr')\, dr' \\ &= \frac{4\pi}{q}\left[-\frac{a\cos(qa)}{q}+\frac{\sin(qa)}{q^2}\right] = 4\pi\,\frac{\sin(qa)-qa\cos(qa)}{q^3} \\ &= 4\pi a^3\,\frac{j_1(qa)}{qa}.\end{aligned} \tag{3.8}$$

As $qa \to 0$, $j_1(qa) \sim (qa)/3$ so $I \to 4\pi a^3/3$, the sphere volume.

Final expression $\vec{P}$

Using (3.7) and $\int_{|\vec{r}'|\leq a} d^3r' = \frac{4\pi a^3}{3}$:

$$\begin{aligned}\vec{P}(\hat{s}) &= \frac{k^2}{4\pi}(m^2-1)\left[\hat{n}_0 \cdot 4\pi a^3 \frac{j_1(qa)}{qa} \;+\; \hat{n}\,\gamma \cdot \frac{4\pi a^3}{3}\right] \\ &= k^2(m^2-1)\left[a^3\frac{j_1(x)}{x}\,\hat{n}_0 + \frac{a^3}{3}\,\gamma\,\hat{n}\right] = k^2\frac{(m^2-1)a^3}{3}\left\{\left[\frac{3j_1(x)}{x}\right]\hat{n}_0 + \gamma\,\hat{n}\right\},\end{aligned} \tag{3.9}$$

with

$$x := qa = ka\sqrt{1+m^2-2m\cos\theta}, \qquad \cos\theta = \hat{s}\cdot\hat{s}_0.$$

3.2.3 Far-field projection and $\vec{E}_{\mathbf{sctd}}$

The radiation pattern is the transverse projection

$$\vec{F}_1(\hat{s}) = \hat{s}\times(\vec{P}\times\hat{s}) = \vec{P} - \hat{s}(\hat{s}\cdot\vec{P}).$$

Assuming $\hat{n}\perp\hat{s}$ (transverse polarization of the scattered wave), we get

$$\hat{s}\cdot\vec{P} = k^2\frac{(m^2-1)a^3}{3}\left\{\left[\frac{3j_1(x)}{x}\right](\hat{s}\cdot\hat{n}_0) + \gamma\,(\hat{s}\cdot\hat{n})\right\} = k^2\frac{(m^2-1)a^3}{3}\left[\frac{3j_1(x)}{x}\right](\hat{s}\cdot\hat{n}_0), \tag{3.10}$$

and hence

$$\boxed{\vec{F}_1(\hat{s}) = k^2\frac{(m^2-1)a^3}{3}\left\{\left[\frac{3j_1(x)}{x}\right]\left[\hat{n}_0 - \hat{s}(\hat{s}\cdot\hat{n}_0)\right] + \gamma\,\hat{n}\right\}.} \tag{3.11}$$

Therefore the scattered field is

$$\boxed{\vec{E}_{\text{sctd}}(\vec{r}) = \frac{e^{ikr}}{r}\,k^2\frac{(m^2-1)a^3}{3}\left\{\left[\frac{3j_1(x)}{x}\right]\left[\hat{n}_0 - \hat{s}(\hat{s}\cdot\hat{n}_0)\right] + \gamma\,\hat{n}\right\}.} \tag{3.12}$$

with

$$x := ka\sqrt{1+m^2-2m\cos\theta}, \qquad \cos\theta = \hat{s}\cdot\hat{s}_0.$$

3.2.4 Electric field in different polarisation bases

Let the scattering plane be spanned by $\hat{s}_0$ and $\hat{s}$, with scattering angle θ:

$$\hat{e}_\perp = \frac{\hat{s} \times \hat{s}_0}{\sin\theta}, \qquad \hat{e}_\parallel = \frac{\hat{s}_0 - \cos\theta\,\hat{s}}{\sin\theta}.$$

Both obey $\hat{s} \cdot \hat{e}_{\perp,\parallel} = 0$. For either incident polarization choice $\hat{n}_0 \in \{\hat{e}_\perp, \hat{e}_\parallel\}$ and taking $\hat{n} = \hat{n}_0$, one gets

$$\vec{E}^{(\perp \text{ or } \parallel)}_{\text{sctd}}(\vec{r}) = \frac{e^{ikr}}{r}\, k^2 \frac{(m^2-1)a^3}{3} \left[\frac{3j_1(x)}{x} + \gamma\right] \hat{n}_0. \tag{3.13}$$

with

$$x := ka\sqrt{1 + m^2 - 2m\cos\theta}, \qquad \cos\theta = \hat{s} \cdot \hat{s}_0.$$

3.3 Scattered magnetic field using Gordon's ansatz

3.3.1 Internal fields (Gordon ansatz)

Take the internal electric field as

$$\mathbf{E}_{\text{int}}(\mathbf{r}') = \hat{n}_0\, e^{imk_0\,\hat{s}_0\cdot\mathbf{r}'} + \gamma\,\hat{n}\, e^{ik_0\,\hat{s}\cdot\mathbf{r}'}, \tag{3.14}$$

where $\hat{s}_0$ is the incident direction, $\hat{n}_0$ its polarization, and $\hat{n} \perp \hat{s}$ a unit polarization for the scattered channel. Using $\mathbf{H} = (c/\omega)\nabla \times \mathbf{E}$,

$$\boxed{\mathbf{H}_{\text{int}}(\mathbf{r}') = m\,(\hat{s}_0 \times \hat{n}_0)\, e^{imk_0\,\hat{s}_0\cdot\mathbf{r}'} \;+\; \gamma\,(\hat{s} \times \hat{n})\, e^{ik_0\,\hat{s}\cdot\mathbf{r}'}.} \tag{3.15}$$

Note: the magnitude ratio inside the medium is $|\mathbf{H}^{(1)}_{\text{int}}|/|\mathbf{E}^{(1)}_{\text{int}}| = m$ for the first term; for the "vacuum-phase" leakage term the factor is 1.

3.3.2 Far-field magnetic scattering via volume integrals

The scattered magnetic field in the far zone is written as

$$\mathbf{H}_{\text{sctd}}(\mathbf{r}) = \frac{e^{ik_0 r}}{r}\,\mathbf{F}_2(\hat{s}), \qquad \mathbf{F}_2(\hat{s}) = -\hat{s}\times\Big[\hat{s}\times\big(\mathbf{P}'(\hat{s})+\mathbf{P}''(\hat{s})\big)\Big], \tag{3.16}$$

with

$$\mathbf{P}'(\hat{s}) = \frac{k_0^2}{4\pi}\int_V e^{-ik_0\,\hat{s}\cdot\mathbf{r}'}\,[\varepsilon(\mathbf{r}')-1]\,\mathbf{H}(\mathbf{r}')\,d^3r', \qquad \mathbf{P}''(\hat{s}) = -\frac{ik_0}{4\pi}\int_V e^{-ik_0\,\hat{s}\cdot\mathbf{r}'}\,\nabla'\varepsilon(\mathbf{r}')\times\mathbf{E}_{\text{int}}(\mathbf{r}')\,d^3r'. \tag{3.17}$$

Inserting $\mathbf{H}_{\text{int}}$ in $\mathbf{P}'(\hat{s})$ and splitting the integral into two parts:

mismatch (interior-phase) term:

$$\begin{aligned}\int_{|\mathbf{r}'|\le a} e^{-ik_0\,\hat{s}\cdot\mathbf{r}'}\,m(\hat{s}_0\times\hat{n}_0)\,e^{imk_0\,\hat{s}_0\cdot\mathbf{r}'}\,d^3r' &= m(\hat{s}_0\times\hat{n}_0)\int_{|\mathbf{r}'|\le a} e^{-i\mathbf{q}\cdot\mathbf{r}'}\,d^3r' \\ &= m(\hat{s}_0\times\hat{n}_0)\,4\pi a^3\,\frac{j_1(x)}{x},\end{aligned} \tag{3.18}$$

where $\mathbf{q} = k_0(\hat{s} - m\hat{s}_0)$, $x := |\mathbf{q}|a = k_0 a\sqrt{1+m^2-2m\cos\theta}$, and $\cos\theta = \hat{s}\cdot\hat{s}_0$. Here $j_1(z) = (\sin z - z\cos z)/z^2$.

in-phase (vacuum-phase) term:

$$\int_{|\mathbf{r}'|\le a} e^{-ik_0\,\hat{s}\cdot\mathbf{r}'}\,\gamma(\hat{s}\times\hat{n})\,e^{ik_0\,\hat{s}\cdot\mathbf{r}'}\,d^3r' = \gamma(\hat{s}\times\hat{n})\,\frac{4\pi a^3}{3}. \tag{3.19}$$

Therefore

$$\boxed{\mathbf{P}'(\hat{s}) = k_0^2\,\frac{(m^2-1)a^3}{3}\left\{m\left[\frac{3j_1(x)}{x}\right](\hat{s}_0\times\hat{n}_0) + \gamma\,(\hat{s}\times\hat{n})\right\}.} \tag{3.20}$$

Explicit evaluation of the surface term $\mathbf{P}''$ and the cancellation of m

We start from the far-field magnetic amplitude (Gaussian units)

$$\mathbf{H}_{\text{sctd}}(\mathbf{r}) = \frac{e^{ik_0 r}}{r}\,\mathbf{F}_2(\hat{s}), \qquad \mathbf{F}_2(\hat{s}) = -\hat{s}\times\big[\hat{s}\times(\mathbf{P}'(\hat{s})+\mathbf{P}''(\hat{s}))\big],$$

with

$$\mathbf{P}'(\hat{s}) = \frac{k_0^2}{4\pi}\int_V e^{-ik_0\hat{s}\cdot\mathbf{r}'}\,[\varepsilon(\mathbf{r}')-1]\,\mathbf{H}_{\text{int}}(\mathbf{r}')\,d^3r', \qquad \mathbf{P}''(\hat{s}) = -\frac{ik_0}{4\pi}\int_V e^{-ik_0\hat{s}\cdot\mathbf{r}'}\,\nabla'\varepsilon(\mathbf{r}')\times\mathbf{E}_{\text{int}}(\mathbf{r}')\,d^3r'. \tag{3.21}$$

Setup for a homogeneous sphere. Let $\varepsilon(\mathbf{r}') = m^2$ inside the sphere $|\mathbf{r}'| \le a$ and 1 outside. Then

$$\nabla\varepsilon(\mathbf{r}') = (\varepsilon_{\text{out}} - \varepsilon_{\text{in}})\,\hat{s}'\,\delta_S = (1-m^2)\,\hat{s}'\,\delta_S = -(m^2-1)\,\hat{s}'\,\delta_S,$$

where $\hat{s}' = \hat{r}'$ is the outward normal and δ_S is the surface delta supported on $|\mathbf{r}'| = a$. Hence the *volume* integral in $\mathbf{P}''$ reduces to a *surface* integral with a *plus* sign:

$$\boxed{\mathbf{P}''(\hat{s}) = \frac{ik_0}{4\pi}\,(m^2-1)\oint_{|\mathbf{r}'|=a} e^{-ik_0\hat{s}\cdot\mathbf{r}'}\,\big(\hat{s}'\times\mathbf{E}_{\text{int}}(\mathbf{r}')\big)\,dS'.} \tag{3.22}$$

Internal-field ansatz and split of terms. With

$$\mathbf{E}_{\text{int}}(\mathbf{r}') = \hat{n}_0\,e^{imk_0\hat{s}_0\cdot\mathbf{r}'} + \gamma\,\hat{n}\,e^{ik_0\hat{s}\cdot\mathbf{r}'},$$

the surface integral splits into a "mismatch" term (phases $mk_0\hat{s}_0$ vs $k_0\hat{s}$) and an "in-phase" term:

$$\mathbf{P}''(\hat{s}) = \frac{ik_0}{4\pi}(m^2-1)\left[\oint e^{-ik_0\hat{s}\cdot\mathbf{r}'}\,\hat{s}'\times\hat{n}_0\,e^{imk_0\hat{s}_0\cdot\mathbf{r}'}\,dS' \;+\; \gamma\oint e^{-ik_0\hat{s}\cdot\mathbf{r}'}\,\hat{s}'\times\hat{n}\,e^{ik_0\hat{s}\cdot\mathbf{r}'}\,dS'\right]. \tag{3.23}$$

The second integral vanishes from Gauss's theorem, $\mathbf{a}\cdot\left(\oint\hat{s}'\,dS'\right) = \oint\hat{s}'\cdot\mathbf{a}\,dS' = \iiint\nabla\cdot\mathbf{a}\,dV' = 0$, where $\mathbf{a}$ is any constant vector.

Vector surface integral on the sphere. Let $\mathbf{q} := k_0(\hat{s} - m\hat{s}_0)$ and $x := qa = k_0 a\sqrt{1 + m^2 - 2m\cos\theta}$ with $\cos\theta = \hat{s}\cdot\hat{s}_0$. Using the identity

$$\oint_{|\mathbf{r}'|=a} e^{-i\mathbf{q}\cdot\mathbf{r}'}\,\hat{s}'\,dS' = a^2\int d\Omega_{\hat{r}'}\,\hat{r}'\,e^{-iqa\,\hat{q}\cdot\hat{r}'} = -\,4\pi i\,a^2\,j_1(x)\,\hat{q}, \qquad \hat{q} = \frac{\mathbf{q}}{q}, \tag{3.24}$$

we obtain, for constant $\hat{n}_0$,

$$\oint e^{-i\mathbf{q}\cdot\mathbf{r}'}\,(\hat{s}'\times\hat{n}_0)\,dS' = \left(\oint e^{-i\mathbf{q}\cdot\mathbf{r}'}\,\hat{s}'\,dS'\right)\times\hat{n}_0 = \big[-\,4\pi i\,a^2\,j_1(x)\,\hat{q}\big]\times\hat{n}_0.$$

Therefore

$$\boxed{\mathbf{P}''(\hat{s}) = k_0\,(m^2-1)\,a^2\,j_1(x)\,(\hat{q}\times\hat{n}_0), \qquad \hat{q} = \frac{\hat{s} - m\hat{s}_0}{\sqrt{1+m^2-2m\cos\theta}}.} \tag{3.25}$$

Volume term for comparison. From the volume current term in (3.21) one finds (using the previously derived scalar form-factor $4\pi a^3 j_1(x)/x$ and $\mathbf{H}_{\text{int}} = m(\hat{s}_0\times\hat{n}_0)e^{imk_0\hat{s}_0\cdot\mathbf{r}'} + \cdots$)

$$\boxed{\mathbf{P}'(\hat{s})\Big|_{\text{mismatch}} = k_0^2\,\frac{(m^2-1)a^3}{3}\,m\left[\frac{3j_1(x)}{x}\right](\hat{s}_0\times\hat{n}_0).} \tag{3.26}$$

Projecting to the radiative (transverse) subspace. The far-field operator $-\hat{s}\times(\hat{s}\times\cdot)$ projects any vector to its component $\perp\hat{s}$. For either polarization channel $\hat{n}_0\in\{\hat{e}_\perp,\hat{e}_\parallel\}$ (defined about the scattering plane), the following geometric identities hold:

$$\big[(\hat{s}_0\times\hat{n}_0)\big]_{\perp\hat{s}} = \cos\theta\,(\hat{s}\times\hat{n}_0), \tag{3.27}$$

$$\big[(\hat{q}\times\hat{n}_0)\big]_{\perp\hat{s}} = (\hat{q}\cdot\hat{s})\,(\hat{s}\times\hat{n}_0) = \frac{1-m\cos\theta}{\sqrt{1+m^2-2m\cos\theta}}\,(\hat{s}\times\hat{n}_0) = \frac{k_0 a}{x}\,(1-m\cos\theta)\,(\hat{s}\times\hat{n}_0). \tag{3.28}$$

Cancellation of the spurious m and the final amplitude. Using (3.25)–(3.27) and $x = qa$, the *mismatch* parts of the projected amplitudes become

$$\big[\mathbf{P}'(\hat{s})\big]_{\perp\hat{s}} = k_0^2\frac{(m^2-1)a^3}{3}\,m\left[\frac{3j_1(x)}{x}\right]\cos\theta\,(\hat{s}\times\hat{n}_0),$$

$$\left[\mathbf{P}''(\hat{s})\right]_{\perp\hat{s}} = k_0(m^2-1)a^2\, j_1(x)\cdot\frac{k_0 a}{x}(1-m\cos\theta)\,(\hat{s}\times\hat{n}_0) = k_0^2\frac{(m^2-1)a^3}{3}\,\left[\frac{3j_1(x)}{x}\right](1-m\cos\theta)\,(\hat{s}\times\hat{n}_0).$$

Summing,

$$\left[\mathbf{P}'(\hat{s}) + \mathbf{P}''(\hat{s})\right]_{\perp\hat{s}} = k_0^2\frac{(m^2-1)a^3}{3}\left[\frac{3j_1(x)}{x}\right]\underbrace{\left(m\cos\theta + 1 - m\cos\theta\right)}_{=1}(\hat{s}\times\hat{n}_0),$$

so the offending m factor cancels *exactly*:

$$\boxed{\left[\mathbf{P}'(\hat{s}) + \mathbf{P}''(\hat{s})\right]_{\perp\hat{s}} = k_0^2\frac{(m^2-1)a^3}{3}\left[\frac{3j_1(x)}{x}\right](\hat{s}\times\hat{n}_0).} \tag{3.29}$$

Adding the in-phase (γ) piece (which contributes only via $\mathbf{P}'$ and is already transverse), the total far-field magnetic amplitude is

$$\mathbf{F}_2(\hat{s}) = \left[\mathbf{P}'(\hat{s}) + \mathbf{P}''(\hat{s})\right]_{\perp\hat{s}} = K\left[\frac{3j_1(x)}{x} + \gamma\right](\hat{s}\times\hat{n}_0), \qquad K := k_0^2\frac{(m^2-1)a^3}{3}.$$

Hence

$$\boxed{\mathbf{H}_{\text{sctd}}(\mathbf{r}) = \frac{e^{ik_0 r}}{r}\,K\left[\frac{3j_1(x)}{x} + \gamma\right](\hat{s}\times\hat{n}_0).} \tag{3.30}$$

Since in the vacuum exterior $\mathbf{H}_{\text{sctd}} = \hat{s}\times\mathbf{E}_{\text{sctd}}$, this coincides with the electric-field result and guarantees $|\mathbf{H}_{\text{sctd}}| = |\mathbf{E}_{\text{sctd}}|$ outside the particle.

3.4 Summary of the scattered fields:

Defining the orthonormal basis about the scattering plane spanned by $\hat{s}_0$ and $\hat{s}$:

$$\hat{e}_\perp = \frac{\hat{s}\times\hat{s}_0}{\sin\theta}, \qquad \hat{e}_\parallel = \frac{\hat{s}_0 - \cos\theta\,\hat{s}}{\sin\theta}, \qquad \hat{s}\cdot\hat{e}_{\perp,\parallel} = 0, \quad \theta = \arccos(\hat{s}\cdot\hat{s}_0). \tag{3.31}$$

choosing either incident polarization $\hat{n}_0 \in \{\hat{e}_\perp, \hat{e}_\parallel\}$ and set isotropic sphere approximaton:$\hat{n} = \hat{n}_0$ (so $\hat{s} \cdot \hat{n}_0 = 0$). Time dependence is $e^{-i\omega t}$. We use Gaussian units with $\mu = 1$. Then

$$\boxed{\mathbf{E}^{(\perp\text{ or }\parallel)}_{\text{sctd}}(\mathbf{r}) = \frac{e^{ik_0 r}}{r} F(\theta)\, \hat{n}_0, \qquad F(\theta) := K\left[\frac{3j_1(x)}{x} + \gamma\right], \quad x = k_0 a\sqrt{1 + m^2 - 2m\cos\theta}.} \tag{3.32}$$

$$\mathbf{H}^{(\perp)}_{\text{sctd}}(\mathbf{r}) = \frac{e^{ik_0 r}}{r} F(\theta)\, (\hat{s} \times \hat{e}_\perp) = \frac{e^{ik_0 r}}{r} F(\theta)\, (-\hat{e}_\parallel), \tag{3.33}$$

$$\mathbf{H}^{(\parallel)}_{\text{sctd}}(\mathbf{r}) = \frac{e^{ik_0 r}}{r} F(\theta)\, (\hat{s} \times \hat{e}_\parallel) = \frac{e^{ik_0 r}}{r} F(\theta)\, \hat{e}_\perp, \tag{3.34}$$

here,

$$K := k_0^2 \frac{(m^2 - 1)a^3}{3}$$

and j_1 is the spherical Bessel function $j_1(z) = \dfrac{\sin z - z\cos z}{z^2}$. The magnitudes are $|\mathbf{H}_{\text{sctd}}| = |\mathbf{E}_{\text{sctd}}|$ outside (Gaussian units), while inside the dielectric $|\mathbf{H}| = m\,|\mathbf{E}|$.

3.4.1 Checks

(i) transversality: $\hat{s} \cdot \mathbf{H}_{\text{sctd}} = 0$ and $\hat{s} \cdot \mathbf{E}_{\text{sctd}} = 0$.

(ii) energy flow: in the interior, with $D = m^2 E$ and $B = H$, one finds $|\mathbf{S}|/u = c/m$, as expected.

3.5 Spherical coordinates transformation

Time dependence $e^{-i\omega t}$, Gaussian units with $\mu = 1$. Incident direction $\hat{s}_0 = \hat{x}$. Observation direction $\hat{s} = \hat{\boldsymbol{r}}$ is the spherical radial unit.

Spherical basis (physics convention):

$$\hat{\boldsymbol{r}} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta), \quad \hat{\boldsymbol{\theta}} = (\cos\theta\cos\phi,\ \cos\theta\sin\phi,\ -\sin\theta), \quad \hat{\boldsymbol{\phi}} = (-\sin\phi,\ \cos\phi,\ 0).$$

Right-handedness: $\hat{\boldsymbol{r}} \times \hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\phi}}$, $\hat{\boldsymbol{\theta}} \times \hat{\boldsymbol{\phi}} = \hat{\boldsymbol{r}}$, $\hat{\boldsymbol{\phi}} \times \hat{\boldsymbol{r}} = \hat{\boldsymbol{\theta}}$.

Scattering angle between $\hat{s}_0 = \hat{x}$ and $\hat{s} = \hat{\mathbf{r}}$

Writing the unit vectors. In standard spherical coordinates,

$$\hat{\mathbf{r}} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta), \qquad \hat{s}_0 = \hat{x} = (1, 0, 0).$$

Computing $\cos\psi$ from the dot product. By definition,

$$\cos\psi = \hat{s}_0 \cdot \hat{s} = \hat{x} \cdot \hat{\mathbf{r}} = (1, 0, 0) \cdot (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta) = \sin\theta\cos\phi.$$

Hence

$$\boxed{\cos\psi = \sin\theta\cos\phi}.$$

Obtaining $\sin\psi$. Using $\sin^2\psi = 1 - \cos^2\psi$,

$$\sin\psi = \sqrt{1 - \cos^2\psi} = \sqrt{1 - \sin^2\theta\cos^2\phi}\,.$$

Thus

$$\boxed{\sin\psi = \sqrt{1 - \sin^2\theta\cos^2\phi}}.$$

3.6 Polarisation basis tied to the scattering plane

Defining the orthonormal pair in the plane orthogonal to $\hat{s}$:

$$\hat{e}_\perp = \frac{\hat{s} \times \hat{s}_0}{\sin\psi}, \qquad \hat{e}_\parallel = \frac{\hat{s}_0 - (\hat{s}_0 \cdot \hat{s})\,\hat{s}}{\sin\psi}.$$

In spherical components (note there is no $\hat{\boldsymbol{r}}$ component):

$$\boxed{\hat{e}_\perp = \frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} + \frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}, \qquad \hat{e}_\parallel = \frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} - \frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}.}$$

By construction $\hat{e}_{\perp,\parallel} \perp \hat{s}$ and $\hat{e}_\perp \times \hat{e}_\parallel = \hat{s}$.

Remark (degenerate directions). When $\sin\psi = 0$ (forward/backward along $\hat{x}$), the scattering plane is undefined. Use a limiting procedure in ψ if needed; the scattered amplitudes remain well behaved.

3.7 Incident plane wave, labelled in the spherical scattering basis

The incident phase is $k_0 x = k_0 R \sin\theta\cos\phi$. Using your scattering-basis labeling, take

$$\boldsymbol{E}_{\mathrm{inc}}^{(\perp)} = e^{ik_0 R\sin\theta\cos\phi}\ \hat{e}_{\perp}, \qquad \boldsymbol{E}_{\mathrm{inc}}^{(\parallel)} = e^{ik_0 R\sin\theta\cos\phi}\ \hat{e}_{\parallel}.$$

Thus, explicitly in spherical components:

$$\boxed{\begin{aligned} \boldsymbol{E}_{\mathrm{inc}}^{(\perp)} &= e^{ik_0 R\sin\theta\cos\phi}\left(\frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} + \frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}\right), \\ \boldsymbol{E}_{\mathrm{inc}}^{(\parallel)} &= e^{ik_0 R\sin\theta\cos\phi}\left(\frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} - \frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}\right). \end{aligned}}$$

The incident magnetic fields follow from $\boldsymbol{H}_{\mathrm{inc}} = \hat{s}_0 \times \boldsymbol{E}_{\mathrm{inc}}$. The decomposition identities we use are

$$\hat{x}\times\hat{\boldsymbol{\theta}} = \sin\phi\,\hat{\boldsymbol{r}} + \sin\theta\cos\phi\,\hat{\boldsymbol{\phi}}, \qquad \hat{x}\times\hat{\boldsymbol{\phi}} = \cos\theta\cos\phi\,\hat{\boldsymbol{r}} - \sin\theta\cos\phi\,\hat{\boldsymbol{\theta}}.$$

Therefore

$$\boxed{\begin{aligned} \boldsymbol{H}_{\mathrm{inc}}^{(\perp)} &= e^{ik_0 R\sin\theta\cos\phi}\left[\frac{\sin\phi}{\sin\psi}\big(\sin\phi\,\hat{\boldsymbol{r}} + \sin\theta\cos\phi\,\hat{\boldsymbol{\phi}}\big) + \frac{\cos\theta\cos\phi}{\sin\psi}\big(\cos\theta\cos\phi\,\hat{\boldsymbol{r}} - \sin\theta\cos\phi\,\hat{\boldsymbol{\theta}}\big)\right], \\ \boldsymbol{H}_{\mathrm{inc}}^{(\parallel)} &= e^{ik_0 R\sin\theta\cos\phi}\left[\frac{\cos\theta\cos\phi}{\sin\psi}\big(\sin\phi\,\hat{\boldsymbol{r}} + \sin\theta\cos\phi\,\hat{\boldsymbol{\phi}}\big) - \frac{\sin\phi}{\sin\psi}\big(\cos\theta\cos\phi\,\hat{\boldsymbol{r}} - \sin\theta\cos\phi\,\hat{\boldsymbol{\theta}}\big)\right]. \end{aligned}}$$

These expressions are exact and fully in the spherical basis.

Plane-wave orthogonality check (incident). Since $\boldsymbol{H}_{\mathrm{inc}} = \hat{s}_0 \times \boldsymbol{E}_{\mathrm{inc}}$ and $\hat{s}_0 \perp \boldsymbol{E}_{\mathrm{inc}}$, we have $\hat{\boldsymbol{E}}_{\mathrm{inc}} \times \hat{\boldsymbol{H}}_{\mathrm{inc}} = \hat{s}_0$.

3.8 Far-field scattered fields for arbitrary (θ, ϕ)

Our far-field ansatz (with $R = |\boldsymbol{r}|$) is

$$\boldsymbol{E}_{\text{sctd}}^{(\perp\ /\ \parallel)}(R,\theta,\phi) = \frac{e^{ik_0R}}{R}\,F(\psi)\,\hat{n}_0, \qquad \boldsymbol{H}_{\text{sctd}} = \hat{s}\times\boldsymbol{E}_{\text{sctd}}, \quad \hat{s} = \hat{\boldsymbol{r}},$$

with

$$F(\psi) = K\left[\frac{3\,j_1(x)}{x} + \gamma\right], \quad K = k_0^2\frac{(m^2-1)a^3}{3}, \quad x = k_0a\sqrt{1+m^2-2m\cos\psi}, \quad \cos\psi = \sin\theta\cos\phi.$$

Using the spherical forms of $\hat{e}_{\perp,\parallel}$ above, we get the explicit components:

$$\boxed{\begin{aligned} \boldsymbol{E}_{\text{sctd}}^{(\perp)} &= \frac{e^{ik_0R}}{R}\,F(\psi)\left(\frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} + \frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}\right), \\ \boldsymbol{H}_{\text{sctd}}^{(\perp)} = \hat{\boldsymbol{r}}\times\boldsymbol{E}_{\text{sctd}}^{(\perp)} &= \frac{e^{ik_0R}}{R}\,F(\psi)\left(-\frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} + \frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}\right), \end{aligned}}$$

$$\boxed{\begin{aligned} \boldsymbol{E}_{\text{sctd}}^{(\parallel)} &= \frac{e^{ik_0R}}{R}\,F(\psi)\left(\frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} - \frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}\right), \\ \boldsymbol{H}_{\text{sctd}}^{(\parallel)} = \hat{\boldsymbol{r}}\times\boldsymbol{E}_{\text{sctd}}^{(\parallel)} &= \frac{e^{ik_0R}}{R}\,F(\psi)\left(\frac{\sin\phi}{\sin\psi}\,\hat{\boldsymbol{\theta}} + \frac{\cos\theta\cos\phi}{\sin\psi}\,\hat{\boldsymbol{\phi}}\right). \end{aligned}}$$

Radiation-zone checks (scattered). Transversality holds identically:

$$\hat{\boldsymbol{r}}\cdot\boldsymbol{E}_{\text{sctd}} = 0, \qquad \hat{\boldsymbol{r}}\cdot\boldsymbol{H}_{\text{sctd}} = 0.$$

Moreover, with $\boldsymbol{H}_{\text{sctd}} = \hat{\boldsymbol{r}}\times\boldsymbol{E}_{\text{sctd}}$ and $|\hat{e}_{\perp,\parallel}| = 1$, the Poynting direction is

$$\hat{\boldsymbol{E}}_{\text{sctd}}\times\hat{\boldsymbol{H}}_{\text{sctd}} = \hat{e}_{(\cdot)}\times(\hat{\boldsymbol{r}}\times\hat{e}_{(\cdot)}) = (\hat{e}\cdot\hat{e})\,\hat{\boldsymbol{r}} - (\hat{e}\cdot\hat{\boldsymbol{r}})\,\hat{e} = \hat{\boldsymbol{r}},$$

so the energy flux points along the propagation direction $\hat{s} = \hat{\boldsymbol{r}}$.

Chapter 4

Mie theory and Rayleigh limit

We now use standard Mie scattering to show the Rayleigh limit and calculate higher-order terms.

We introduce x, the expansion parameter

$$x \equiv k_0 a,$$

4.1 Maxwell's Problem and Separation in Spherical Waves

We seek the fields for a plane wave incident on a sphere of radius a. We adopt the $e^{-i\omega t}$ time dependence throughout.

In each homogeneous region (host: subscript m; particle: subscript p), the frequency-domain Maxwell equations imply the vector Helmholtz equation:

$$\nabla \times \nabla \times \mathbf{E} - k^2 \mathbf{E} = 0, \qquad k = \omega\sqrt{\varepsilon\mu},$$

and the same equation holds for $\mathbf{H}$.

4.1.1 Maxwell to the Vector Helmholtz Equation and Transversality

In a homogeneous, isotropic, source-free region with constant permittivity ε and permeability μ, the frequency-domain Maxwell equations are:

$$\nabla \times \mathbf{E} = i\omega\mu\,\mathbf{H}, \qquad \nabla \times \mathbf{H} = -i\omega\varepsilon\,\mathbf{E},$$

$$\nabla \cdot (\varepsilon\mathbf{E}) = 0, \qquad \nabla \cdot (\mu\mathbf{H}) = 0.$$

Since ε is constant within the region and there is no free charge, $\nabla \cdot \mathbf{E} = 0$; likewise, in the absence of magnetic charge and for constant μ, $\nabla \cdot \mathbf{H} = 0$.

Taking the curl of Faraday's law and using the vector identity $\nabla \times \nabla \times \mathbf{E} = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E}$:

$$\nabla \times \nabla \times \mathbf{E} = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E} = -\nabla^2\mathbf{E} = i\omega\mu\,(\nabla \times \mathbf{H})$$

$$= i\omega\mu(-i\omega\varepsilon)\mathbf{E} = \omega^2\mu\varepsilon\,\mathbf{E}.$$

Hence each component of $\mathbf{E}$ satisfies the vector Helmholtz equation:

$$\nabla \times \nabla \times \mathbf{E} - k^2\mathbf{E} = 0 \quad \Longleftrightarrow \quad (\nabla^2 + k^2)\mathbf{E} = 0, \qquad k \equiv \omega\sqrt{\mu\varepsilon},$$

and the same holds for $\mathbf{H}$; moreover $\nabla \cdot \mathbf{E} = 0 = \nabla \cdot \mathbf{H}$ (transverse fields).

4.1.2 Scalar Helmholtz Separation in Spherical Coordinates

The scalar Helmholtz equation $(\nabla^2 + k^2)\psi = 0$ separates in spherical coordinates with solutions:

$$\psi_{\ell m}^{(q)}(r,\theta,\phi) = z_\ell^{(q)}(kr)\,Y_{\ell m}(\theta,\phi), \qquad \ell = 0,1,2,\ldots,\; m = -\ell,\ldots,\ell,$$

where $Y_{\ell m}$ are scalar spherical harmonics, and the radial functions $z_\ell^{(q)}$ are chosen from:

$$z_\ell^{(1)}(kr) = j_\ell(kr) \quad \text{(regular at the origin)},$$

$$z_\ell^{(3)}(kr) = h_\ell^{(1)}(kr) \quad \text{(outgoing at infinity).}$$

The asymptotics justify these labels:

$$j_\ell(\rho) \sim \frac{\rho^\ell}{(2\ell+1)!!} \quad (\rho \to 0), \qquad h_\ell^{(1)}(\rho) \sim (-i)^{\ell+1}\frac{e^{i\rho}}{\rho} \quad (\rho \to \infty),$$

and $h_\ell^{(1)}$ satisfies the Sommerfeld radiation condition.

4.1.3 Building Transverse Vector Solutions from Scalar Ones

Let ψ be any scalar solution of $(\nabla^2 + k^2)\psi = 0$.

Define the (dimensionless) orbital angular-momentum operator:

$$\mathbf{L} = -i\,\mathbf{r} \times \nabla, \qquad \mathbf{L}^2 = -\nabla_\Omega^2.$$

where ∇_Ω^2 the symbol indicates it acts only on angular variables and commutes with the Laplacian: $[\nabla^2, \mathbf{L}] = 0$.

Consider the two vector fields:

$$\mathbf{M} \equiv \nabla \times (\mathbf{r}\,\psi), \qquad \mathbf{N} \equiv \frac{1}{k}\nabla \times \mathbf{M}.$$

With the above convention for $\mathbf{L}$, one has $\mathbf{M} = i\,\mathbf{L}\psi$.

These are the solenoidal vector spherical wave functions (VSWFs) once $\psi = z_\ell^{(q)}(kr)Y_{\ell m}(\hat{\mathbf{r}})$ is specified.

Transversality. Since divergence of a curl is zero,

$$\nabla \cdot \mathbf{M} = 0, \qquad \nabla \cdot \mathbf{N} = \frac{1}{k}\nabla \cdot (\nabla \times \mathbf{M}) = 0.$$

Hence both $\mathbf{M}$ and $\mathbf{N}$ are transverse (solenoidal), as required by Maxwell in a homogeneous, source-free region.

Vector Helmholtz equation. Because $[\nabla^2, \mathbf{L}] = 0$ and $(\nabla^2 + k^2)\psi = 0$,

$$(\nabla^2 + k^2)\mathbf{M} = (\nabla^2 + k^2)\,\mathbf{L}\psi = \mathbf{L}\,(\nabla^2 + k^2)\psi = 0.$$

Using $\nabla^2\nabla\times = \nabla\times\nabla^2$ for smooth fields,

$$(\nabla^2 + k^2)\mathbf{N} = \frac{1}{k}(\nabla^2 + k^2)\,\nabla\times\mathbf{M} = \frac{1}{k}\,\nabla\times\big[(\nabla^2 + k^2)\mathbf{M}\big] = 0.$$

Thus $\mathbf{M}$ and $\mathbf{N}$ each satisfy the vector Helmholtz equation.

First-order curl relations. Directly from the definitions and the scalar Helmholtz equation,

$$\nabla\times\mathbf{M} = k\,\mathbf{N}, \qquad \nabla\times\mathbf{N} = k\,\mathbf{M},$$

whenever ψ solves $(\nabla^2 + k^2)\psi = 0$. Consequently,

$$\nabla\times\nabla\times\mathbf{M} = k^2\mathbf{M}, \qquad \nabla\times\nabla\times\mathbf{N} = k^2\mathbf{N},$$

which is exactly the vector Helmholtz form $\nabla\times\nabla\times\mathbf{F} - k^2\mathbf{F} = 0$.

4.1.4 Explicit VSWFs and Their Radial Behavior

Choose $\psi^{(q)}_{\ell m}(r,\theta,\phi) = z^{(q)}_\ell(kr)Y_{\ell m}(\theta,\phi)$. Then:

$$\boxed{\mathbf{M}^{(q)}_{\ell m}(k\mathbf{r}) = \nabla\times\big[\mathbf{r}\,z^{(q)}_\ell(kr)Y_{\ell m}(\hat{\mathbf{r}})\big]\ , \qquad \mathbf{N}^{(q)}_{\ell m}(k\mathbf{r}) = \frac{1}{k}\nabla\times\mathbf{M}^{(q)}_{\ell m}(k\mathbf{r})}\,.$$

Writing the purely tangential vector harmonic:

$$\mathbf{X}_{\ell m}(\hat{\mathbf{r}}) \equiv \frac{1}{\sqrt{\ell(\ell+1)}}\,\mathbf{L}Y_{\ell m}(\hat{\mathbf{r}}),$$

one finds the standard decompositions:

$$\mathbf{M}_{\ell m}^{(q)} = z_\ell^{(q)}(kr)\,\sqrt{\ell(\ell+1)}\,\mathbf{X}_{\ell m},$$

$$\mathbf{N}_{\ell m}^{(q)} = \frac{\ell(\ell+1)}{kr}\,z_\ell^{(q)}(kr)\,Y_{\ell m}\,\hat{\mathbf{r}} + \frac{1}{r}\frac{d}{d(kr)}\big[(kr)z_\ell^{(q)}(kr)\big]\,\mathbf{W}_{\ell m},$$

where $\mathbf{W}_{\ell m} \equiv \hat{\mathbf{r}} \times \mathbf{X}_{\ell m}$ is also tangential.

From these forms:

$$\hat{\mathbf{r}} \cdot \mathbf{M}_{\ell m}^{(q)} = 0 \quad \text{(TE w.r.t. } \hat{\mathbf{r}}),$$

$$\hat{\mathbf{r}} \times \mathbf{N}_{\ell m}^{(q)} \neq 0,\ \hat{\mathbf{r}} \cdot \mathbf{N}_{\ell m}^{(q)} \propto z_\ell^{(q)}(kr) \text{ (TM).}$$

Regularity and radiation follow from $z_\ell^{(q)}$: choose j_ℓ for fields finite at $r \to 0$ (interior problem), and $h_\ell^{(1)}$ for fields satisfying the outgoing radiation condition at $r \to \infty$ (scattered field).

4.1.5 Why These Span the Maxwell Solutions

Any divergence-free vector solution of $(\nabla^2+k^2)\mathbf{F} = 0$ on a spherical surface admits an expansion in the orthonormal basis $\{\mathbf{X}_{\ell m}, \mathbf{W}_{\ell m}\}$ for each (ℓ, m). The radial dependence is then constrained by the scalar radial Helmholtz equation, whose independent solutions are $j_\ell(kr)$ and $h_\ell^{(1)}(kr)$. The two transverse families constructed above:

- TE: $\mathbf{M}_{\ell m}^{(q)}$ (tangential electric modes)
- TM: $\mathbf{N}_{\ell m}^{(q)}$ (tangential magnetic modes)

therefore, furnish a complete set for source-free Maxwell fields in a homogeneous spherical region.

4.1.6 Plane Wave Expansion and Mie Scattering Solution

A plane wave can be expanded on this basis. For definiteness, take propagation along $+\hat{\mathbf{z}}$ and polarization along $\hat{\mathbf{x}}$. Then (Bohren–Huffman convention):

$$\mathbf{E}_{\text{inc}} = E_0 \sum_{\ell=1}^{\infty} i^{\ell} \frac{2\ell+1}{\ell(\ell+1)} \Big(\mathbf{M}^{(1)}_{o1\ell}(k_m \mathbf{r}) - i\, \mathbf{N}^{(1)}_{e1\ell}(k_m \mathbf{r}) \Big),$$

with a corresponding $\mathbf{H}_{\text{inc}}$ related by the medium impedance $\eta_m = \sqrt{\mu_m/\varepsilon_m}$.

The scattered field in the host must be purely outgoing:

$$\mathbf{E}_{\text{sca}} = E_0 \sum_{\ell=1}^{\infty} i^{\ell} \frac{2\ell+1}{\ell(\ell+1)} \Big(a_\ell\, \mathbf{N}^{(3)}_{e1\ell}(k_m \mathbf{r}) + b_\ell\, \mathbf{M}^{(3)}_{o1\ell}(k_m \mathbf{r}) \Big),$$

and the internal field in the particle must be regular:

$$\mathbf{E}_{\text{int}} = E_0 \sum_{\ell=1}^{\infty} i^{\ell} \frac{2\ell+1}{\ell(\ell+1)} \Big(c_\ell\, \mathbf{N}^{(1)}_{e1\ell}(k_p \mathbf{r}) + d_\ell\, \mathbf{M}^{(1)}_{o1\ell}(k_p \mathbf{r}) \Big),$$

with $k_p = \omega\sqrt{\varepsilon_p \mu_p} = m k_m$.

The four sets of coefficients $\{a_\ell, b_\ell, c_\ell, d_\ell\}$ are fixed by electromagnetic boundary conditions at $r = a$.

4.2 Boundary conditions at the spherical interface (derivation and 2×2 systems)

We take the time dependence $e^{-i\omega t}$ and define

$$x \equiv k_m a, \qquad m \equiv \sqrt{\frac{\varepsilon_p \mu_p}{\varepsilon_m \mu_m}}, \qquad \psi_\ell(\rho) = \rho\, j_\ell(\rho), \quad \xi_\ell(\rho) = \rho\, h^{(1)}_\ell(\rho),$$

with prime $'$ denoting $d/d\rho$. The vector spherical wave functions (VSWFs) satisfy

$$\mathbf{M}^{(q)}_{\ell m} = z^{(q)}_\ell(kr)\, \sqrt{\ell(\ell+1)}\, \mathbf{X}_{\ell m}, \qquad \mathbf{N}^{(q)}_{\ell m} = \frac{\ell(\ell+1)}{kr}\, z^{(q)}_\ell(kr)\, Y_{\ell m}\, \hat{\mathbf{r}} + \frac{1}{r} \frac{d}{d(kr)} \big[(kr) z^{(q)}_\ell(kr)\big] \mathbf{W}_{\ell m},$$

so that on a sphere $r = a$ the tangential parts are proportional to $z_\ell(ka)$ for $\mathbf{M}$ and to $\frac{d}{d(ka)}[(ka)z_\ell(ka)]$ for $\mathbf{N}$. Outside (host, $r > a$) we write the field as the sum of incident (regular) and scattered (outgoing) parts; inside ($r < a$) the field is regular. For each fixed (ℓ, m) this yields two uncoupled 2×2 systems, one for TM (electric-type, $\mathbf{N}$) and one for TE (magnetic-type, $\mathbf{M}$), obtained by enforcing continuity of the tangential components of $\mathbf{E}$ and $\mathbf{H}$ and using $\mathbf{H} = (1/i\omega\mu)\nabla \times \mathbf{E}$ together with $\nabla \times \mathbf{M} = k\mathbf{N}$, $\nabla \times \mathbf{N} = k\mathbf{M}$.

TM (electric-type) block. Let c_ℓ and a_ℓ denote, respectively, the internal and scattered coefficients of the TM ($\mathbf{N}$) mode. Continuity of $\mathbf{E}_t$ and $\mathbf{H}_t$ at $r = a$ gives

$$\psi_\ell'(mx)\, c_\ell \;-\; \xi_\ell'(x)\, a_\ell = \psi_\ell'(x), \tag{4.1}$$

$$\frac{\psi_\ell(mx)}{\mu_p}\, c_\ell \;-\; \frac{\xi_\ell(x)}{\mu_m}\, a_\ell = \frac{\psi_\ell(x)}{\mu_m}. \tag{4.2}$$

Equations (4.1)–(4.2) form a 2×2 linear system for (c_ℓ, a_ℓ).

TE (magnetic-type) block. Let d_ℓ and b_ℓ denote, respectively, the internal and scattered coefficients of the TE ($\mathbf{M}$) mode. Continuity of $\mathbf{E}_t$ and $\mathbf{H}_t$ yields

$$\psi_\ell(mx)\, d_\ell \;-\; \xi_\ell(x)\, b_\ell = \psi_\ell(x), \tag{4.3}$$

$$\frac{\psi_\ell'(mx)}{\varepsilon_p}\, d_\ell \;-\; \frac{\xi_\ell'(x)}{\varepsilon_m}\, b_\ell = \frac{\psi_\ell'(x)}{\varepsilon_m}. \tag{4.4}$$

Equations (4.3)–(4.4) form a 2×2 linear system for (d_ℓ, b_ℓ).

Solution for the Mie coefficients. Solving the systems (e.g. by Cramer's rule) for a_ℓ and b_ℓ gives the magneto–dielectric Mie coefficients

$$a_\ell = \frac{\mu_p\, \psi_\ell(mx)\, \psi_\ell'(x) - \mu_m\, \psi_\ell(x)\, \psi_\ell'(mx)}{\mu_p\, \psi_\ell(mx)\, \xi_\ell'(x) - \mu_m\, \xi_\ell(x)\, \psi_\ell'(mx)}, \qquad b_\ell = \frac{\varepsilon_p\, \psi_\ell(mx)\, \psi_\ell'(x) - \varepsilon_m\, \psi_\ell(x)\, \psi_\ell'(mx)}{\varepsilon_p\, \psi_\ell(mx)\, \xi_\ell'(x) - \varepsilon_m\, \xi_\ell(x)\, \psi_\ell'(mx)}. \tag{4.5}$$

For nonmagnetic particles $\mu_p = \mu_m$ these reduce to the familiar textbook formulas in terms of the relative index m only.

Equivalent (m,z) form Introducing the impedance ratio $z \equiv \eta_p/\eta_m = \sqrt{(\mu_p\varepsilon_m)/(\mu_m\varepsilon_p)}$ and $m = \sqrt{(\varepsilon_p\mu_p)/(\varepsilon_m\mu_m)}$, (4.5) can be rearranged algebraically into the "(m,z)" representation

$$a_\ell = \frac{m\,\psi_\ell(mx)\,\psi_\ell'(x) - z\,\psi_\ell(x)\,\psi_\ell'(mx)}{m\,\psi_\ell(mx)\,\xi_\ell'(x) - z\,\xi_\ell(x)\,\psi_\ell'(mx)}, \qquad b_\ell = \frac{z\,\psi_\ell(mx)\,\psi_\ell'(x) - m\,\psi_\ell(x)\,\psi_\ell'(mx)}{z\,\psi_\ell(mx)\,\xi_\ell'(x) - m\,\xi_\ell(x)\,\psi_\ell'(mx)}.$$

4.2.1 From VSWFs to the angle–resolved amplitudes $S_1(\theta), S_2(\theta)$

1) Far-field ansatz and meaning of S_1, S_2. In the radiation zone ($k_m r \gg 1$) any outgoing spherical solution has the universal radial factor $e^{ik_m r}/r$ and is locally transverse with $\mathbf{H}_{\text{sca}} = \eta_m^{-1}\,\hat{\mathbf{r}} \times \mathbf{E}_{\text{sca}}$, where $\eta_m = \sqrt{\mu_m/\varepsilon_m}$. We therefore *define* the two scalar amplitude functions $S_1(\theta)$ and $S_2(\theta)$ by

$$\mathbf{E}_{\text{sca}}(r,\theta,\phi) = E_0\,\frac{e^{ik_m r}}{-ik_m r}\Big[S_2(\theta)\,\hat{\boldsymbol{\theta}} + S_1(\theta)\,\hat{\boldsymbol{\phi}}\Big], \qquad \mathbf{H}_{\text{sca}} = \frac{1}{\eta_m}\,\hat{\mathbf{r}} \times \mathbf{E}_{\text{sca}}.$$

The task is to compute S_1, S_2 from the Mie series.

2) Scattered-field expansion in outgoing VSWFs. For a $+\hat{\mathbf{z}}$ plane wave with $\hat{\mathbf{x}}$ polarization, only $m = 1$ terms enter. Using the "odd"/"even" parity VSWFs, the scattered field outside the sphere ($r > a$) is

$$\mathbf{E}_{\text{sca}}(r,\theta,\phi) = E_0 \sum_{\ell=1}^{\infty} i^\ell \frac{2\ell+1}{\ell(\ell+1)} \Big(a_\ell\,\mathbf{M}^{(3)}_{o1\ell}(k_m\mathbf{r}) - i\,b_\ell\,\mathbf{N}^{(3)}_{e1\ell}(k_m\mathbf{r})\Big),$$

with a_ℓ (electric/TM) and b_ℓ (magnetic/TE) fixed by the boundary conditions at $r = a$.

3) Far-field forms of $\mathbf{M}^{(3)}$ and $\mathbf{N}^{(3)}$. Write $\rho \equiv k_m r$. The outgoing radial dependence is carried by $h_\ell^{(1)}(\rho)$, whose large-argument asymptotic is

$$h_\ell^{(1)}(\rho) \sim (-i)^{\ell+1}\frac{e^{i\rho}}{\rho}, \qquad \frac{1}{\rho}\frac{d}{d\rho}\big[\rho\,h_\ell^{(1)}(\rho)\big] \sim i\,h_\ell^{(1)}(\rho) \qquad (\rho \to \infty).$$

Using the component forms of the VSWFs,

$$\mathbf{M}_{o1\ell}^{(3)} = \left[\frac{\cos\phi}{\sin\theta} P_\ell^1(\cos\theta)\, h_\ell^{(1)}(\rho)\right]\hat{\boldsymbol{\theta}} - \left[\sin\phi\, \frac{dP_\ell^1(\cos\theta)}{d\theta}\, h_\ell^{(1)}(\rho)\right]\hat{\boldsymbol{\phi}},$$

$$\mathbf{N}_{e1\ell}^{(3)} = \left[\cos\phi\, \frac{dP_\ell^1(\cos\theta)}{d\theta}\, \frac{1}{r}\frac{d}{d\rho}\big(\rho h_\ell^{(1)}(\rho)\big)\right]\hat{\boldsymbol{\theta}} - \left[\frac{\sin\phi}{\sin\theta} P_\ell^1(\cos\theta)\, \frac{1}{r}\frac{d}{d\rho}\big(\rho h_\ell^{(1)}(\rho)\big)\right]\hat{\boldsymbol{\phi}} + (\text{radial}),$$

and defining the standard Mie angular functions

$$\pi_\ell(\cos\theta) = \frac{P_\ell^1(\cos\theta)}{\sin\theta}, \qquad \tau_\ell(\cos\theta) = \frac{d}{d\theta} P_\ell^1(\cos\theta),$$

the radiation-zone (tangential) parts become

$$\mathbf{M}_{o1\ell}^{(3)} \xrightarrow{k_m r\to\infty} (-i)^{\ell+1}\frac{e^{ik_m r}}{k_m r}\left[\ \pi_\ell\ \cos\phi\ \hat{\boldsymbol{\theta}}\ -\ \tau_\ell\ \sin\phi\ \hat{\boldsymbol{\phi}}\ \right],$$

$$\mathbf{N}_{e1\ell}^{(3)} \xrightarrow{k_m r\to\infty} (-i)^{\ell+1}\frac{e^{ik_m r}}{k_m r}\, i\left[\ \tau_\ell\ \cos\phi\ \hat{\boldsymbol{\theta}}\ -\ \pi_\ell\ \sin\phi\ \hat{\boldsymbol{\phi}}\ \right].$$

When these are inserted into the series of Step 2, the ϕ-dependence cancels between the even/odd combinations appropriate to an x-polarized plane wave, leaving a purely θ-dependent pattern. Collecting the $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ components and matching to the far-field ansatz of Step 1 yields

$$S_1(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)}\Big(a_\ell\, \pi_\ell(\cos\theta) + b_\ell\, \tau_\ell(\cos\theta)\Big), \qquad S_2(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)}\Big(a_\ell\, \tau_\ell(\cos\theta) + b_\ell\, \pi_\ell(\cos\theta)\Big).$$

By construction,

$$\mathbf{E}_{\text{sca}}(r,\theta,\phi) = E_0\, \frac{e^{ik_m r}}{-ik_m r}\Big[S_2(\theta)\,\hat{\boldsymbol{\theta}} + S_1(\theta)\,\hat{\boldsymbol{\phi}}\Big], \qquad \mathbf{H}_{\text{sca}} = \frac{1}{\eta_m}\,\hat{\mathbf{r}}\times\mathbf{E}_{\text{sca}}.$$

4.2.2 From far field to differential and integrated cross-sections

Set–up and notation. We use the time convention $e^{-i\omega t}$ and the host wavenumber k_m. In the far field ($k_m r \gg 1$), the scattered field is purely transverse and we *define* the scalar amplitude functions $S_1(\theta), S_2(\theta)$ by

$$\mathbf{E}_{\text{sca}}(r,\theta,\phi) = E_0 \frac{e^{ik_m r}}{-i\,k_m r}\Big[S_2(\theta)\,\hat{\boldsymbol{\theta}} + S_1(\theta)\,\hat{\boldsymbol{\phi}}\Big], \qquad \mathbf{H}_{\text{sca}} = \frac{1}{\eta_m}\,\hat{\mathbf{r}}\times\mathbf{E}_{\text{sca}}, \tag{4.6}$$

with medium impedance $\eta_m = \sqrt{\mu_m/\varepsilon_m}$. For a $+\hat{\mathbf{z}}$ plane wave (polarized along $\hat{\mathbf{x}}$), only $m = 1$ contributes, and the amplitude functions are (Mie series)

$$S_1(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)}\Big(a_\ell\,\pi_\ell(\cos\theta) + b_\ell\,\tau_\ell(\cos\theta)\Big), \qquad S_2(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)}\Big(a_\ell\,\tau_\ell(\cos\theta) + b_\ell\,\pi_\ell(\cos\theta)\Big), \tag{4.7}$$

where

$$\pi_\ell(\cos\theta) = \frac{P_\ell^1(\cos\theta)}{\sin\theta}, \qquad \tau_\ell(\cos\theta) = \frac{d}{d\theta}P_\ell^1(\cos\theta).$$

Differential cross-section. The time-averaged Poynting vector of the scattered field in the radiation zone is

$$\langle\mathbf{S}\rangle = \frac{1}{2}\,\mathrm{Re}\{\mathbf{E}_{\text{sca}}\times\mathbf{H}^*_{\text{sca}}\} = \frac{1}{2\eta_m}\left|\mathbf{E}_{\text{sca}}\right|^2\hat{\mathbf{r}},$$

because $\mathbf{H}_{\text{sca}} = (1/\eta_m)\hat{\mathbf{r}}\times\mathbf{E}_{\text{sca}}$ and $\hat{\mathbf{r}}\cdot\mathbf{E}_{\text{sca}} = 0$. Using (4.6), the magnitude is

$$\left|\mathbf{E}_{\text{sca}}\right|^2 = |E_0|^2\,\frac{1}{(k_m r)^2}\Big(|S_1(\theta)|^2 + |S_2(\theta)|^2\Big).$$

Hence the scattered power per unit solid angle is

$$\frac{dP_{\text{sca}}}{d\Omega} = r^2\,\langle\mathbf{S}\rangle\cdot\hat{\mathbf{r}} = \frac{|E_0|^2}{2\eta_m}\,\frac{1}{k_m^2}\,\Big(|S_1|^2 + |S_2|^2\Big).$$

Dividing by the incident intensity $I_0 = |E_0|^2/(2\eta_m)$ gives the *differential* cross-section

$$\frac{dC_{\text{sca}}}{d\Omega} = \frac{1}{k_m^2}\,\Big(|S_1(\theta)|^2 + |S_2(\theta)|^2\Big). \tag{4.8}$$

Orthogonality ingredients. Insert (4.7) into (4.8), expand the modulus squares, and integrate over solid angle. Since $S_{1,2}$ depend only on θ, the ϕ–integration gives a factor 2π. For the

θ–integration, use the standard identities (with prime denoting a different multipole index)

$$\int_0^\pi \big[\pi_\ell \pi_{\ell'} + \tau_\ell \tau_{\ell'}\big] \sin\theta \, d\theta = \frac{2\,\ell(\ell+1)}{2\ell+1}\,\delta_{\ell\ell'}, \tag{4.9}$$

$$\int_0^\pi \big[\pi_\ell \tau_{\ell'} + \tau_\ell \pi_{\ell'}\big] \sin\theta \, d\theta = 0, \tag{4.10}$$

which ensure that all cross terms with $\ell \neq \ell'$ vanish and π–τ cross-terms cancel.

Integrated scattering cross-section. Let $c_\ell = (2\ell+1)/[\ell(\ell+1)]$. Then

$$\int_0^\pi |S_1|^2 \sin\theta \, d\theta = \sum_\ell c_\ell^2 \, \frac{2\,\ell(\ell+1)}{2\ell+1} \big(|a_\ell|^2 + |b_\ell|^2\big) = \sum_\ell \frac{2(2\ell+1)}{\ell(\ell+1)} \big(|a_\ell|^2 + |b_\ell|^2\big),$$

and the same result holds for $\int_0^\pi |S_2|^2 \sin\theta \, d\theta$. Therefore,

$$\int |S_1|^2 + |S_2|^2 \, d\Omega = 2\pi \cdot 2 \sum_\ell \frac{2\ell+1}{\ell(\ell+1)} \big(|a_\ell|^2 + |b_\ell|^2\big).$$

Finally, inserting into (4.8) yields

$$C_{\text{sca}} = \int \frac{dC_{\text{sca}}}{d\Omega} \, d\Omega = \frac{2\pi}{k_m^2} \sum_{\ell=1}^{\infty} (2\ell+1) \big(|a_\ell|^2 + |b_\ell|^2\big). \tag{4.11}$$

4.2.3 Optical theorem and extinction (derivation in our normalization)

Setup and definitions. Let the incident intensity be $I_0 = |E_0|^2/(2\eta_m)$ with time dependence $e^{-i\omega t}$. On a large sphere of radius r, the total time-averaged power flowing out is

$$P_{\text{tot}} = \oint_{S_r} \langle \mathbf{S} \rangle \cdot \hat{\mathbf{r}} \, dA = \frac{1}{2} \operatorname{Re} \oint_{S_r} \big(\mathbf{E}_{\text{inc}} + \mathbf{E}_{\text{sca}}\big) \times \big(\mathbf{H}_{\text{inc}} + \mathbf{H}_{\text{sca}}\big)^* \cdot \hat{\mathbf{r}} \, dA.$$

Decompose into the incident, scattered-only, and *interference* parts:

$$P_{\text{tot}} = P_{\text{inc}} + P_{\text{sca}} + P_{\text{int}}.$$

Define cross-sections by $P_{\text{sca}} = I_0\, C_{\text{sca}}$ and the *extinction*

$$P_{\text{ext}} = -P_{\text{int}} = I_0\, C_{\text{ext}}.$$

By energy balance in the far field, $C_{\text{abs}} = C_{\text{ext}} - C_{\text{sca}}$.

Interference term in the far field. Using $\mathbf{H}_{\text{sca}} = (1/\eta_m)\,\hat{\mathbf{r}} \times \mathbf{E}_{\text{sca}}$ and keeping the $1/r$ terms (radiation zone),

$$P_{\text{int}} = \frac{1}{2}\,\mathrm{Re} \oint_{S_r} \Big(\mathbf{E}_{\text{inc}} \times \mathbf{H}^*_{\text{sca}} + \mathbf{E}_{\text{sca}} \times \mathbf{H}^*_{\text{inc}} \Big) \cdot \hat{\mathbf{r}}\, dA.$$

Insert the far-field ansatz $\mathbf{E}_{\text{sca}} = E_0\, \dfrac{e^{ik_m r}}{-ik_m r}\, [S_2(\theta)\hat{\boldsymbol{\theta}} + S_1(\theta)\hat{\boldsymbol{\phi}}]$ and expand the tangential incident plane wave on the spherical surface in vector spherical harmonics. Using orthogonality on the unit sphere, the ϕ-integration eliminates cross-couplings, and the θ-integration reduces the interference integral to the *forward* direction. This yields the optical-theorem identity

$$C_{\text{ext}} = \frac{4\pi}{k_m^2}\, \mathrm{Re}\{S(0)\}, \qquad S(0) \equiv S_1(0) = S_2(0) \quad \text{(sphere)}.$$

Forward amplitude in terms of Mie coefficients. Recall the Mie angular functions $\pi_\ell(\mu) = P_\ell^1(\mu)/\sin\theta$, $\tau_\ell(\mu) = \dfrac{d}{d\theta} P_\ell^1(\mu)$ with $\mu = \cos\theta$, and

$$S_1(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \big(a_\ell\, \pi_\ell + b_\ell\, \tau_\ell \big), \qquad S_2(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \big(a_\ell\, \tau_\ell + b_\ell\, \pi_\ell \big).$$

Use $P_\ell^1(\mu) = -\sqrt{1-\mu^2}\, P_\ell'(\mu)$ to write

$$\pi_\ell(\mu) = \frac{P_\ell^1(\mu)}{\sin\theta} = -P_\ell'(\mu), \qquad \tau_\ell(\mu) = \frac{dP_\ell^1}{d\theta} = -\sin\theta\, \frac{dP_\ell^1}{d\mu}.$$

Taking $\theta \to 0$ ($\mu \to 1$) and using $P_\ell'(1) = \ell(\ell+1)/2$, one finds the standard limits

$$\pi_\ell(1) = \tau_\ell(1) = -\,\frac{\ell(\ell+1)}{2}.$$

Hence, in the forward direction,

$$S_1(0) = S_2(0) = \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\ell(\ell+1)} \Big(a_\ell \, \tfrac{-\ell(\ell+1)}{2} + b_\ell \, \tfrac{-\ell(\ell+1)}{2} \Big) = -\frac{1}{2} \sum_{\ell=1}^{\infty} (2\ell+1)\,(a_\ell + b_\ell).$$

Combining with the optical theorem then gives

$$C_{\text{ext}} = \frac{4\pi}{k_m^2} \,\text{Re}\{S(0)\} = \frac{4\pi}{k_m^2} \,\text{Re}\{-S_1(0)\} = \frac{2\pi}{k_m^2} \sum_{\ell=1}^{\infty} (2\ell+1) \,\text{Re}\{a_\ell + b_\ell\}.$$

Scattering and absorption. From the angle integration of the differential cross-section using the orthogonality of π_ℓ, τ_ℓ; one has

$$C_{\text{sca}} = \frac{2\pi}{k_m^2} \sum_{\ell=1}^{\infty} (2\ell+1) \big(|a_\ell|^2 + |b_\ell|^2 \big), \qquad C_{\text{abs}} = C_{\text{ext}} - C_{\text{sca}}.$$

Summary

$$\boxed{C_{\text{ext}} = \frac{2\pi}{k_m^2} \sum_{\ell=1}^{\infty} (2\ell+1) \,\text{Re}\{a_\ell + b_\ell\}, \quad C_{\text{sca}} = \frac{2\pi}{k_m^2} \sum_{\ell=1}^{\infty} (2\ell+1) \big(|a_\ell|^2 + |b_\ell|^2 \big), \quad C_{\text{abs}} = C_{\text{ext}} - C_{\text{sca}}.}$$

Rayleigh scaling check (nonmagnetic): detailed derivation. Let $x \equiv k_m a \ll 1$ and assume $\mu_p = \mu_m$ so the magnetic dipole term is higher order ($b_1 = O(x^5)$).

Keeping only the dipole term in C_{sca}:

$$C_{\text{sca}} = \frac{2\pi}{k_m^2} \sum_{\ell=1}^{\infty} (2\ell+1) \big(|a_\ell|^2 + |b_\ell|^2 \big) \xrightarrow[\text{keep } \ell=1]{} \frac{2\pi}{k_m^2} \, 3\,|a_1|^2 + O(x^8).$$

Small-x expansion of the dipole Mie coefficient:

i) Exact a_1 (nonmagnetic sphere). Let $x = k_m a$ and $m^2 = \varepsilon_p / \varepsilon_m$. With $\psi_\ell(\rho) = \rho j_\ell(\rho)$ and $\xi_\ell(\rho) = \rho h_\ell^{(1)}(\rho)$, the electric-type dipole coefficient is

$$a_1 = \frac{m\,\psi_1(mx)\,\psi_1'(x) \;-\; \psi_1(x)\,\psi_1'(mx)}{m\,\psi_1(mx)\,\xi_1'(x) \;-\; \xi_1(x)\,\psi_1'(mx)}. \tag{1}$$

ii) Small-argument series needed. From $j_1(z) = \dfrac{\sin z}{z^2} - \dfrac{\cos z}{z}$ and $y_1(z) = -\dfrac{\cos z}{z^2} - \dfrac{\sin z}{z}$, expand as $z \to 0$:

$$j_1(z) = \frac{z}{3} - \frac{z^3}{30} + O(z^5), \qquad y_1(z) = -\frac{1}{z^2} - \frac{1}{2} + \frac{z^2}{8} + O(z^4).$$

Hence, for the Riccati–Bessel functions

$$\psi_1(z) = z j_1(z) = \frac{z^2}{3} - \frac{z^4}{30} + O(z^6), \quad \psi_1'(z) = \frac{2z}{3} - \frac{2z^3}{15} + O(z^5),$$

and, using $\xi_1(z) = \psi_1(z) + i\, z y_1(z)$,

$$\xi_1(z) = -\frac{i}{z} - \frac{i}{2}z + \frac{z^2}{3} - \frac{i}{8}z^3 - \frac{z^4}{30} + O(z^5), \quad \xi_1'(z) = \frac{i}{z^2} + \frac{2z}{3} - \frac{i}{2} + O(z^2). \tag{2}$$

iii) Expand numerator and denominator of (1). Keep the lowest nonvanishing powers in x. Using (2),

$$\begin{aligned} \text{Num} &:= m\,\psi_1(mx)\,\psi_1'(x) - \psi_1(x)\,\psi_1'(mx) \\ &= m\Big(\tfrac{m^2x^2}{3}\Big)\Big(\tfrac{2x}{3}\Big) \;-\; \Big(\tfrac{x^2}{3}\Big)\Big(\tfrac{2mx}{3}\Big) \;+\; O(x^5) = \frac{2m}{9}(m^2-1)\,x^3 + O(x^5), \\ \text{Den} &:= m\,\psi_1(mx)\,\xi_1'(x) - \xi_1(x)\,\psi_1'(mx) \\ &= m\Big(\tfrac{m^2x^2}{3}\Big)\Big(\tfrac{i}{x^2}\Big) \;-\; \Big(-\tfrac{i}{x}\Big)\Big(\tfrac{2mx}{3}\Big) \;+\; O(x^2) = i\,\frac{m}{3}(m^2+2) \;+\; O(x^2). \end{aligned} \tag{3}$$

iv) Form the ratio. From (3),

$$a_1 = \frac{\text{Num}}{\text{Den}} = \frac{\frac{2m}{9}(m^2-1)x^3}{i\,\frac{m}{3}(m^2+2)} \;+\; O(x^5) = i\,\frac{2}{3}\,\frac{m^2-1}{m^2+2}\,x^3 \;+\; O(x^5). \tag{4}$$

Since $m^2 = \varepsilon_p/\varepsilon_m$ (nonmagnetic), this is

$$a_1 = i\,\frac{2}{3}\,\frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m}\,x^3 \;+\; O(x^5). \tag{5}$$

v) Magnitude. Taking the modulus of (5),

$$|a_1|^2 = \left|\tfrac{2}{3}\right|^2 \left|\frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m}\right|^2 x^6 \;+\; O(x^8). \tag{6}$$

Plug into C_{sca} and simplify powers of x:

$$\begin{aligned} C_{\text{sca}} &\simeq \frac{2\pi}{k_m^2}\, 3 \left(\tfrac{4}{9}\right) \left|\frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m}\right|^2 x^6 \\ &= \frac{8\pi}{3}\,\frac{x^6}{k_m^2} \left|\frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m}\right|^2 \;=\; \frac{8\pi}{3}\, k_m^4 a^6 \left|\frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m}\right|^2 . \end{aligned}$$

Neglecting dynamical corrections in the imaginary part in the strict Rayleigh limit,

$$C_{\text{ext}} \simeq \frac{k_m}{\varepsilon_m}\, \Im\{\alpha_e^{(0)}\} = \frac{k_m}{\varepsilon_m}\, \Im\left\{ 4\pi\varepsilon_m a^3 \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m} \right\} = \boxed{4\pi k_m a^3\, \Im\left\{ \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m} \right\}}.$$

Thus $C_{\text{abs}} = C_{\text{ext}} - C_{\text{sca}}$, and as $a \to 0$ one has $C_{\text{ext}} \propto a^3$ while $C_{\text{sca}} \propto a^6$, so absorption dominates for sufficiently small lossy particles.

Chapter 5

Appendix A

5.1 Derivation of black body radiation energy density per unit frequency formula in a system with harmonic interaction

To derive the blackbody radiation energy density per unit frequency, $u(\omega, T) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{e^{\hbar\omega/k_B T} - 1}$, we use fundamental principles of quantum statistical mechanics and electromagnetic theory. This expression represents the energy per unit volume per unit frequency for blackbody radiation at temperature T, where $\hbar$ is the reduced Planck constant, ω is the angular frequency, c is the speed of light, k_B is the Boltzmann constant, and T is the temperature.

5.1.1 Density of States for Photons

Blackbody radiation consists of electromagnetic waves in thermal equilibrium within a cavity. To find the energy density $u(\omega, T)$, we need the number of photon modes per unit volume per unit frequency, known as the density of states.

Consider a cubic cavity with volume $V = L^3$, where L is the side length. Electromagnetic waves in the cavity form standing waves with wave vectors $\mathbf{k} = (k_x, k_y, k_z)$, where each component is quantized due to boundary conditions. For periodic boundary conditions, the allowed wave vectors are:

$$k_x = \frac{2\pi n_x}{L}, \quad k_y = \frac{2\pi n_y}{L}, \quad k_z = \frac{2\pi n_z}{L}$$

where n_x, n_y, n_z are integers. The magnitude of the wave vector is $k = |\mathbf{k}| = \sqrt{k_x^2 + k_y^2 + k_z^2}$, and the angular frequency is related to k by the dispersion relation for photons, $\omega = ck$, where c is the speed of light.

To count the number of modes, we work in k-space. The number of states within a spherical shell in k-space between k and $k + dk$ corresponds to the number of modes with frequencies between ω and $\omega + d\omega$. The volume element in k-space for a single mode is:

$$\Delta k_x \Delta k_y \Delta k_z = \frac{(2\pi)^3}{L^3} = \frac{(2\pi)^3}{V}$$

In spherical coordinates, the number of states in a shell between k and $k + dk$ is found by integrating over the positive octant (since $k_x, k_y, k_z \geq 0$):

$$dN' = \frac{V}{(2\pi)^3} \cdot 4\pi k^2 dk \cdot \frac{1}{8}$$

Adding a factor of 2 for the two polarisation states of photons gives:

$$dN = 2 \cdot \frac{V}{(2\pi)^3} \cdot 4\pi k^2 dk = \frac{V k^2 dk}{\pi^2}$$

Since $\omega = ck$, we have $k = \frac{\omega}{c}$, and $dk = \frac{d\omega}{c}$. Substituting:

$$k^2 = \left(\frac{\omega}{c}\right)^2, \quad dk = \frac{d\omega}{c}$$

$$dN = \frac{V}{2\pi^2} \cdot \left(\frac{\omega}{c}\right)^2 \cdot \frac{d\omega}{c} = \frac{V\omega^2 d\omega}{\pi^2 c^3}$$

The density of states per unit volume, $g(\omega)$, is the number of modes per unit frequency per unit volume:

$$g(\omega)d\omega = \frac{dN}{V} = \frac{\omega^2 d\omega}{\pi^2 c^3}$$

This $g(\omega)$ gives the number of photon modes per unit volume per unit frequency.

5.1.2 Energy per Photon Mode

Photons are bosons, and in thermal equilibrium at temperature T, the average number of photons in a mode with frequency ω follows the Bose-Einstein distribution:

$$\langle n(\omega) \rangle = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

Each photon in a mode with frequency ω has energy $\hbar\omega$. The average energy per mode is:

$$E(\omega) = \langle n(\omega) \rangle \cdot \hbar\omega = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

5.1.3 Energy Density

The energy density per unit frequency, $u(\omega, T)$, is the energy per mode multiplied by the number of modes per unit volume per unit frequency:

$$u(\omega, T) = g(\omega) \cdot E(\omega) = \left(\frac{\omega^2}{\pi^2 c^3}\right) \cdot \left(\frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}\right)$$

$$u(\omega, T) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

5.1.4 Notes

1. The factor $\frac{1}{\pi^2 c^3}$ arises from the density of states in three dimensions, accounting for the two polarization states of photons.

2. The Bose-Einstein distribution $\frac{1}{e^{\hbar\omega/k_B T} - 1}$ reflects the quantum statistical nature of photons, excluding the zero-point energy (which does not contribute to thermal radiation).

3. This derivation assumes an isotropic, equilibrium distribution of radiation, as is standard for blackbody radiation in a cavity.

   The derived expression matches the one provided, confirming its correctness as used in Chang et al.'s paper for calculating the absorption of blackbody radiation by a nanosphere.

Chapter 6

Appendix B

6.1 Derivation of the Time-Domain Poynting Theorem

We start from Maxwell's curl equations:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{6.1}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \tag{6.2}$$

First, we take the dot product of Eq. (6.1) with $\mathbf{H}$:

$$\mathbf{H} \cdot (\nabla \times \mathbf{E}) = -\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} \tag{6.3}$$

Next, we take the dot product of Eq. (6.2) with $\mathbf{E}$:

$$\mathbf{E} \cdot (\nabla \times \mathbf{H}) = \mathbf{E} \cdot \mathbf{J} + \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} \tag{6.4}$$

Now, we subtract Eq. (6.4) from Eq. (6.3):

$$\mathbf{H} \cdot (\nabla \times \mathbf{E}) - \mathbf{E} \cdot (\nabla \times \mathbf{H}) = -\left(\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} + \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t}\right) - \mathbf{E} \cdot \mathbf{J} \tag{6.5}$$

We use the vector identity $\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B})$. Applying this to the left-hand side (LHS) of Eq. (6.5) gives:

$$\nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\left(\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} + \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t}\right) - \mathbf{J} \cdot \mathbf{E} \tag{6.6}$$

Rearranging the terms to bring the time derivatives to the LHS, we get:

$$\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} + \mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\mathbf{J} \cdot \mathbf{E} \tag{6.7}$$

This answers the question: **before substituting the constitutive relations, the left-hand side is $\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} + \mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{E} \times \mathbf{H})$.**

Finally, we introduce the constitutive relations for a linear, isotropic medium: $\mathbf{D} = \varepsilon \mathbf{E}$ and $\mathbf{B} = \mu \mathbf{H}$. The time-derivative terms can be rewritten as:

$$\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} = \mathbf{E} \cdot \frac{\partial (\varepsilon \mathbf{E})}{\partial t} = \varepsilon \mathbf{E} \cdot \frac{\partial \mathbf{E}}{\partial t} = \frac{\partial}{\partial t}\left(\frac{1}{2}\varepsilon |\mathbf{E}|^2\right) \tag{6.8}$$

$$\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} = \mathbf{H} \cdot \frac{\partial (\mu \mathbf{H})}{\partial t} = \mu \mathbf{H} \cdot \frac{\partial \mathbf{H}}{\partial t} = \frac{\partial}{\partial t}\left(\frac{1}{2}\mu |\mathbf{H}|^2\right) \tag{6.9}$$

Here, we used the identity $\mathbf{v} \cdot \frac{d\mathbf{v}}{dt} = \frac{1}{2}\frac{d}{dt}(\mathbf{v} \cdot \mathbf{v}) = \frac{1}{2}\frac{d}{dt}(|\mathbf{v}|^2)$.

Substituting these back into Eq. (6.7) gives the final target equation, the differential form of Poynting's theorem:

$$\frac{\partial}{\partial t}\left[\frac{1}{2}(\varepsilon |\mathbf{E}|^2 + \mu |\mathbf{H}|^2)\right] + \nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\mathbf{J} \cdot \mathbf{E} \tag{6.10}$$

6.2 Time-Averaged Poynting Theorem and Ohmic Loss

In the time-domain Poynting theorem, $\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{S} = -\mathbf{J} \cdot \mathbf{E}$, the current density $\mathbf{J}$ represents only the **free (conduction) current**. Bound (polarization) currents are already accounted for within the $\partial \mathbf{D}/\partial t$ term, which becomes part of the stored energy density u.

For a lossy dielectric, we can model the loss as Ohmic, where $\mathbf{J} = \sigma \mathbf{E}$ for a conductivity $\sigma \geq 0$. This is equivalent to using a complex permittivity $\tilde{\varepsilon} = \varepsilon' + i\varepsilon''$ with $\varepsilon'' = \sigma/\omega$. Let's verify this equivalence for the power dissipation.

6.2.1 Phasor Time-Average Calculation

We express the fields in phasor form, assuming an $e^{-i\omega t}$ time-dependence:

$$\mathbf{E}(\mathbf{r}, t) = \mathrm{Re}\{\mathbf{E}(\mathbf{r})e^{-i\omega t}\} \tag{6.11}$$

$$\mathbf{J}(\mathbf{r}, t) = \mathrm{Re}\{\sigma\, \mathbf{E}(\mathbf{r})\, e^{-i\omega t}\} \tag{6.12}$$

The instantaneous power density dissipated is $\mathbf{J} \cdot \mathbf{E}$. We time-average this quantity over one period $T = 2\pi/\omega$. Using the identity for the time-average of two harmonic quantities, $\langle \mathrm{Re}\{Ae^{-i\omega t}\}\, \mathrm{Re}\{Be^{-i\omega t}\}\rangle = \frac{1}{2}\,\mathrm{Re}\{A \cdot B^*\}$, we get:

$$\begin{aligned}\langle \mathbf{J} \cdot \mathbf{E}\rangle &= \frac{1}{2}\,\mathrm{Re}\{\mathbf{E} \cdot (\sigma\mathbf{E})^*\} \\ &= \frac{1}{2}\,\mathrm{Re}\{\sigma\,\mathbf{E} \cdot \mathbf{E}^*\} \quad \text{(since } \sigma \text{ is real)} \\ &= \frac{1}{2}\sigma\, |\mathbf{E}|^2 \end{aligned} \tag{6.13}$$

We substitute $\sigma = \omega\varepsilon''$ into our result:

$$\langle \mathbf{J} \cdot \mathbf{E}\rangle = \frac{1}{2}(\omega\varepsilon'')\, |\mathbf{E}|^2 = \frac{\omega}{2}\varepsilon''\, |\mathbf{E}|^2 \tag{6.14}$$

This confirms that modeling Ohmic loss with conductivity σ is equivalent to using a complex permittivity with imaginary part $\varepsilon'' = \sigma/\omega$ for calculating time-averaged power dissipation.

In a steady harmonic regime, the time-average of the stored energy is constant, so $\partial\langle u\rangle/\partial t = 0$. The averaged Poynting theorem becomes (assuming magnetic losses are zero, $\mu'' = 0$):

$$\langle \nabla \cdot \mathbf{S}\rangle = -\frac{\omega}{2}\varepsilon''\, |\mathbf{E}|^2 \tag{6.15}$$

Integrating over a volume V enclosing the absorbing particle and applying the divergence theorem gives the total absorbed power, P_{abs}:

$$\oint_{\partial V} \langle \mathbf{S} \rangle \cdot \hat{\mathbf{n}} \, dA = -\frac{\omega}{2} \int_{V_{\text{particle}}} \varepsilon'' |\mathbf{E}|^2 \, dV \equiv -P_{\text{abs}} \tag{6.16}$$

The net power flux into the volume equals the power absorbed inside.

6.2.2 Derivation of Complex Permittivity in Phasor Form

The equivalence between Ohmic current and complex permittivity arises directly from Maxwell's equations in the frequency domain. We start with Ampere's law in the time domain, including the constitutive relations for a simple lossy dielectric:

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}, \qquad \mathbf{D} = \varepsilon' \mathbf{E}, \quad \mathbf{J} = \sigma \mathbf{E} \tag{6.17}$$

Transforming to the phasor domain, the time derivative $\partial/\partial t$ becomes a multiplication by $-i\omega$:

$$\begin{aligned} \nabla \times \mathbf{H} &= \sigma \mathbf{E} - i\omega\varepsilon' \mathbf{E} \\ &= (\sigma - i\omega\varepsilon')\mathbf{E} \\ &= -i\omega \left(\varepsilon' + i\frac{\sigma}{\omega} \right) \mathbf{E} \end{aligned} \tag{6.18}$$

This has the same form as the lossless Ampere's law, $\nabla \times \mathbf{H} = -i\omega\tilde{\varepsilon}\mathbf{E}$, if we define the complex permittivity $\tilde{\varepsilon}$ as:

$$\tilde{\varepsilon} = \varepsilon' + i\frac{\sigma}{\omega} = \varepsilon' + i\varepsilon'' \tag{6.19}$$

Note: Some texts use an $e^{+i\omega t}$ convention, which results in $\tilde{\varepsilon} = \varepsilon' - i\sigma/\omega$. Regardless of convention, for a passive (lossy) medium, the time-averaged dissipated power density, $\langle p_{\text{diss}} \rangle$, must be positive. This requires the imaginary part of the permittivity to have the correct sign to represent loss. For our $e^{-i\omega t}$ convention, this means $\varepsilon'' > 0$.

6.3 Proof of zero divergence for the incident Poynting vector

6.3.1 Convention

We consider time-harmonic fields with an assumed time dependence of $e^{-i\omega t}$. The exterior medium is homogeneous, lossless, and source-free, characterized by real permittivity ε_m and permeability μ_0. The incident fields $(\mathbf{E}_{\text{inc}}, \mathbf{H}_{\text{inc}})$ are solutions to the source-free Maxwell's equations in this medium. The time-averaged Poynting vector is defined as $\mathbf{S}_{\text{inc}} := \frac{1}{2}\operatorname{Re}(\mathbf{E}_{\text{inc}} \times \mathbf{H}^*_{\text{inc}})$.

Our goal is to show that $\langle \nabla \cdot \mathbf{S}_{\text{inc}} \rangle = 0$.

6.3.2 Derivation

Vector Identity for the Divergence of a Cross Product

We begin with the standard vector identity for the divergence of the cross product of two complex vector fields, $\mathbf{A}$ and $\mathbf{B}$:

$$\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B}) \tag{6.20}$$

We apply this identity by setting $\mathbf{A} = \mathbf{E}_{\text{inc}}$ and $\mathbf{B} = \mathbf{H}^*_{\text{inc}}$:

$$\nabla \cdot (\mathbf{E}_{\text{inc}} \times \mathbf{H}^*_{\text{inc}}) = \mathbf{H}^*_{\text{inc}} \cdot (\nabla \times \mathbf{E}_{\text{inc}}) - \mathbf{E}_{\text{inc}} \cdot (\nabla \times \mathbf{H}^*_{\text{inc}}) \tag{6.21}$$

Time average of phasors

$$\text{Let } A, B \in \mathbb{C} \text{ be phasors and } T = \frac{2\pi}{\omega}.$$

Use $\operatorname{Re} z = \frac{1}{2}(z + z^*)$:

$$\operatorname{Re}\{Ae^{-i\omega t}\} = \frac{1}{2}\big(Ae^{-i\omega t} + A^* e^{i\omega t}\big), \quad \operatorname{Re}\{Be^{-i\omega t}\} = \frac{1}{2}\big(Be^{-i\omega t} + B^* e^{i\omega t}\big).$$

Multiply:

$$\mathrm{Re}\{Ae^{-i\omega t}\}\ \mathrm{Re}\{Be^{-i\omega t}\} = \frac{1}{4}\Big[AB\,e^{-i2\omega t} + AB^* + A^*B + A^*B^*e^{i2\omega t}\Big].$$

Average over one period:

$$\Big\langle \mathrm{Re}\{Ae^{-i\omega t}\}\ \mathrm{Re}\{Be^{-i\omega t}\}\Big\rangle = \frac{1}{T}\int_0^T \frac{1}{4}\Big[AB\,e^{-i2\omega t} + AB^* + A^*B + A^*B^*e^{i2\omega t}\Big]\,dt$$

$$= \frac{1}{4}\Big[0 + AB^* + A^*B + 0\Big] = \frac{1}{2}\ \mathrm{Re}\{AB^*\}.$$

This proves

$$\boxed{\Big\langle \mathrm{Re}\{Ae^{-i\omega t}\}\ \mathrm{Re}\{Be^{-i\omega t}\}\Big\rangle = \frac{1}{2}\ \mathrm{Re}\{AB^*\}}.$$

$$\Big\langle \mathrm{Re}\{\mathbf{A}e^{-i\omega t}\}\cdot \mathrm{Re}\{\mathbf{B}e^{-i\omega t}\}\Big\rangle = \frac{1}{2}\ \mathrm{Re}\{\mathbf{A}\cdot\mathbf{B}^*\}, \qquad \Big\langle \mathrm{Re}\{\mathbf{A}e^{-i\omega t}\}\times \mathrm{Re}\{\mathbf{B}e^{-i\omega t}\}\Big\rangle = \frac{1}{2}\ \mathrm{Re}\{\mathbf{A}\times\mathbf{B}^*\}.$$

To find the divergence of the Poynting vector, we take the real part of this expression and divide by 2:

$$\langle \nabla\cdot\mathbf{S}_{\mathrm{inc}}\rangle = \frac{1}{2}\,\mathrm{Re}\left\{\mathbf{H}^*_{\mathrm{inc}}\cdot(\nabla\times\mathbf{E}_{\mathrm{inc}}) - \mathbf{E}_{\mathrm{inc}}\cdot(\nabla\times\mathbf{H}^*_{\mathrm{inc}})\right\} \tag{6.22}$$

Maxwell's Curl Equations (Phasor Form)

In the source-free, homogeneous exterior, the incident fields satisfy Maxwell's curl equations in phasor form:

$$\nabla\times\mathbf{E}_{\mathrm{inc}} = i\omega\mu_0\mathbf{H}_{\mathrm{inc}} \tag{6.23}$$

$$\nabla\times\mathbf{H}_{\mathrm{inc}} = -i\omega\varepsilon_m\mathbf{E}_{\mathrm{inc}} \tag{6.24}$$

We take the complex conjugate of the second equation (6.24). Since ε_m is real, this gives:

$$\nabla \times \mathbf{H}_{\text{inc}}^* = +i\omega\varepsilon_m \mathbf{E}_{\text{inc}}^* \tag{6.25}$$

Now, we substitute equations (6.23) and (6.25) into our result from above (6.22):

$$\langle \nabla \cdot \mathbf{S}_{\text{inc}} \rangle = \frac{1}{2} \operatorname{Re} \left\{ \mathbf{H}_{\text{inc}}^* \cdot (i\omega\mu_0 \mathbf{H}_{\text{inc}}) - \mathbf{E}_{\text{inc}} \cdot (i\omega\varepsilon_m \mathbf{E}_{\text{inc}}^*) \right\} \tag{6.26}$$

Simplifying and expanding the Pyonting vector

We can simplify the dot products inside the curly braces using the identities $\mathbf{H}_{\text{inc}}^* \cdot \mathbf{H}_{\text{inc}} = |\mathbf{H}_{\text{inc}}|^2$ and $\mathbf{E}_{\text{inc}} \cdot \mathbf{E}_{\text{inc}}^* = |\mathbf{E}_{\text{inc}}|^2$. These squared magnitudes are real, non-negative quantities.

$$\begin{aligned} \langle \nabla \cdot \mathbf{S}_{\text{inc}} \rangle &= \frac{1}{2} \operatorname{Re} \left\{ i\omega\mu_0 |\mathbf{H}_{\text{inc}}|^2 - i\omega\varepsilon_m |\mathbf{E}_{\text{inc}}|^2 \right\} && (6.27) \\ &= \frac{1}{2} \operatorname{Re} \left\{ i\omega \left(\mu_0 |\mathbf{H}_{\text{inc}}|^2 - \varepsilon_m |\mathbf{E}_{\text{inc}}|^2 \right) \right\} && (6.28) \end{aligned}$$

The term inside the curly braces is a purely imaginary number (the imaginary unit i times a real number). The real part of any purely imaginary number is zero. Therefore,

$$\langle \nabla \cdot \mathbf{S}_{\text{inc}} \rangle = 0 \tag{6.29}$$

Zero Net Flux for Any Closed Surface

By the divergence theorem, the net flux of $\langle \mathbf{S}_{\text{inc}} \rangle$ through any closed surface ∂V bounding a volume V in the lossless exterior must be zero:

$$\oint_{\partial V} \langle \mathbf{S}_{\text{inc}} \cdot \mathbf{n} \rangle \, dA = \int_V \langle \nabla \cdot \mathbf{S}_{\text{inc}} \rangle \, dV = \int_V 0 \, dV = 0 \tag{6.30}$$

This result is general and holds for any source-free field configuration in a lossless medium, such as plane waves, spherical waves, or focused beams (e.g., a Debye-Wolf beam), because the derivation relied only on Maxwell's equations.

6.4 Free-space Helmholtz Green's function and Sommerfeld condition

6.4.1 Setup

We consider a scalar wave field u in a homogeneous, lossless medium, governed by the Helmholtz equation. The wave is generated by sources or scattering objects confined to a finite region $|\mathbf{r}| \leq R_0$. Outside this region, the field u satisfies the source-free equation:

$$(\nabla^2 + k^2)u = 0, \quad \text{for } |\mathbf{r}| > R_0$$

We assume a time-harmonic dependence of $e^{-i\omega t}$. Our goal is to derive the mathematical condition that ensures our solution corresponds to a physically realistic wave radiating outwards to infinity.

Goal: $\boxed{\lim_{r\to\infty} r\big(\partial_r u - ik\,u\big) = 0}$ (Sommerfeld Radiation Condition)

6.4.2 Green's function method

Find $G(\mathbf{r}, \mathbf{r}')$ such that

$$(\nabla^2 + k^2)G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \qquad k > 0,$$

in a homogeneous, lossless medium with the time convention $e^{-i\omega t}$. By translation invariance let $\mathbf{R} := \mathbf{r} - \mathbf{r}'$ and $G(\mathbf{r}, \mathbf{r}') = G(R)$, $R = |\mathbf{R}|$.

6.4.3 Fourier transform and retarded prescription

Define the spatial Fourier transform $\widehat{G}(\mathbf{q}) = \int_{\mathbb{R}^3} G(\mathbf{R})\, e^{-i\mathbf{q}\cdot\mathbf{R}}\, d^3R$. Transforming the PDE gives

$$(-|\mathbf{q}|^2 + k^2)\,\widehat{G}(\mathbf{q}) = -1 \quad \Rightarrow \quad \widehat{G}(\mathbf{q}) = \frac{1}{k^2 - |\mathbf{q}|^2}\,.$$

To select the *outgoing* (retarded) solution under the $e^{-i\omega t}$ convention, use the *limiting-absorption* prescription

$$\boxed{\widehat{G}(\mathbf{q}) = \frac{1}{k^2 - |\mathbf{q}|^2 - i0}} \qquad \text{(vanishingly small loss } k \to k + i0 \Rightarrow -i0 \text{ here).}$$

6.4.4 Inverse transform reducing to one oscillatory integral)

Using spherical $\mathbf{q}$-coordinates with polar axis along $\mathbf{R}$,

$$\int_{\mathbb{S}^2} e^{i\mathbf{q}\cdot\mathbf{R}}\, d\Omega_q = 4\pi \frac{\sin(qR)}{qR},$$

so

$$G(R) = \frac{1}{(2\pi)^3} \frac{4\pi}{R} I(R), \qquad I(R) := \int_0^\infty \frac{q\, \sin(qR)}{k^2 - q^2 - i0}\, dq.$$

6.4.5 Evaluating scalar Helmholtz Equation Green's function by Sokhotski-Plemelj

Using,

$$\frac{1}{k^2 - q^2 - i0} = \mathrm{PV}\frac{1}{k^2 - q^2} + i\pi\, \delta(k^2 - q^2).$$

Hence

$$I(R) = \underbrace{\mathrm{PV}\int_0^\infty \frac{q \sin(qR)}{k^2 - q^2}\, dq}_{\text{principal value}} + i\pi \int_0^\infty q \sin(qR)\, \delta(k^2 - q^2)\, dq.$$

The delta term is elementary since $\delta(k^2 - q^2) = \frac{1}{2k}\, \delta(q - k)$ on $[0, \infty)$:

$$\int_0^\infty q \sin(qR)\, \delta(k^2 - q^2)\, dq = \frac{1}{2} \sin(kR).$$

For the PV integral, we use the standard sine-transform identity (proved by differentiating a known cosine PV integral):

For $a > 0$ and $b > 0$,

$$\boxed{\mathrm{PV}\int_0^\infty \frac{x\,\sin(ax)}{b^2 - x^2}\,dx = -\,\frac{\pi}{2}\cos(ab)}\,.$$

Define

$$K(a) := \mathrm{PV}\int_0^\infty \frac{\cos(ax)}{b^2 - x^2}\,dx, \qquad a > 0.$$

Extend to the full line using evenness and write

$$2K(a) = \mathrm{PV}\int_{-\infty}^\infty \frac{\cos(ax)}{b^2 - x^2}\,dx = \mathrm{Re}\left\{\mathrm{PV}\int_{-\infty}^\infty \frac{e^{iax}}{b^2 - x^2}\,dx\right\}.$$

Compute the PV integral by residues: for $a > 0$ close in the upper half–plane and take half–residues at the real poles $x = \pm b$ (the PV prescription). Since

$$\mathrm{Res}\left(\frac{e^{iax}}{b^2 - x^2}, x = \pm b\right) = \mp\frac{e^{\pm iab}}{2b},$$

their sum is $-\frac{i}{b}\sin(ab)$, hence

$$\mathrm{PV}\int_{-\infty}^\infty \frac{e^{iax}}{b^2 - x^2}\,dx = i\pi\left(-\frac{i}{b}\sin(ab)\right) = \frac{\pi}{b}\sin(ab).$$

Taking the real part and halving,

$$K(a) = \frac{\pi}{2b}\sin(ab).$$

Differentiate under the (principal–value) integral sign (justified since the integrand decays and the PV removes the pole):

$$K'(a) = \mathrm{PV}\int_0^\infty \frac{-x\sin(ax)}{b^2 - x^2}\,dx.$$

But from the closed form, $K'(a) = \frac{\pi}{2}\cos(ab)$. Therefore

$$\mathrm{PV}\int_0^\infty \frac{x\sin(ax)}{b^2 - x^2}\,dx = -\,K'(a) = -\,\frac{\pi}{2}\cos(ab),$$

as claimed.

Applying this with $a = R$, $b = k$ yields

$$I(R) = \frac{\pi}{2}\cos(kR) \; + \; i\,\frac{\pi}{2}\sin(kR) = \frac{\pi}{2}\,e^{ikR}.$$

$$\boxed{G(R) = \frac{1}{(2\pi)^3}\,\frac{4\pi}{R}\,\frac{\pi}{2}\,e^{ikR} = \frac{e^{ikR}}{4\pi R}}. \tag{6.31}$$

6.4.6 Sommerfeld radiation condition

Differentiate:

$$(\partial_R - ik)\,G(R) = \Big(\frac{ik}{4\pi R} - \frac{1}{4\pi R^2} - \frac{ik}{4\pi R}\Big)e^{ikR} = -\frac{e^{ikR}}{4\pi R^2}.$$

Hence

$$\boxed{\lim_{R\to\infty} R\big(\partial_R - ik\big)G(R) = 0} \qquad \text{(Sommerfeld condition).} \tag{6.32}$$

Remark on sign conventions. With $e^{-i\omega t}$, the *retarded/outgoing* prescription is $k^2 - |\mathbf{q}|^2 - i0$ and yields $e^{+ikR}/(4\pi R)$. If one instead used $+\,i0$, the result would be $e^{-ikR}/(4\pi R)$, i.e. the *incoming* (advanced) solution under this time convention.

6.5 Dyadic Green's function from the scalar Helmholtz Green's function

6.5.1 Setting and notation

Let $k > 0$ be the (free-space) wavenumber. The scalar Green's function $G : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{C}$ is

$$G(\mathbf{r}, \mathbf{r}') = \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|},$$

and solves, in the distributional sense,

$$(\nabla^2 + k^2)G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'). \tag{6.33}$$

Here ∇ acts on $\mathbf{r}$ and ∇' acts on $\mathbf{r}'$. We also use

$$\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} \quad \text{for any smooth vector field } \mathbf{A}.$$

Claim

Define the dyadic (tensor) field

$$\mathbf{\Gamma}(\mathbf{r}, \mathbf{r}') \ := \ \left(\mathbf{I} - \frac{1}{k^2} \nabla\nabla'\right) G(\mathbf{r}, \mathbf{r}'). \tag{6.34}$$

Then

$$\nabla \times \nabla \times \mathbf{\Gamma}(\mathbf{r}, \mathbf{r}') - k^2\, \mathbf{\Gamma}(\mathbf{r}, \mathbf{r}') = \mathbf{I}\, \delta(\mathbf{r} - \mathbf{r}'), \tag{6.35}$$

and the reciprocity/symmetry relation

$$\tilde{\mathbf{\Gamma}}(\mathbf{r}', \mathbf{r}) = \mathbf{\Gamma}(\mathbf{r}, \mathbf{r}') \tag{6.36}$$

holds (where $\tilde{\cdot}$ denotes transpose).

6.5.2 Proof of (6.35)

We act with the operator $\mathcal{L} := \nabla \times \nabla \times -k^2\mathbf{I}$ on $\mathbf{\Gamma}$ and show that $\mathcal{L}\mathbf{\Gamma} = \mathbf{I}\, \delta$.

Divergence of $\mathbf{\Gamma}$. Compute $\nabla \cdot \mathbf{\Gamma}$. Using (6.34) and the fact that ∇ and ∇' commute on G,

$$\nabla \cdot \mathbf{\Gamma} = \nabla G - \frac{1}{k^2} \nabla \cdot \left(\nabla\nabla' G\right) = \nabla G - \frac{1}{k^2} \nabla \left(\nabla^2 G\right)',$$

where $(\cdot)'$ indicates that the derivative inside is with respect to $\mathbf{r}'$. Since $G = G(\mathbf{r} - \mathbf{r}')$, we have the standard identity $\nabla G = -\nabla' G$. Using (6.33), $\nabla^2 G = -k^2 G - \delta$, hence

$$\nabla \cdot \boldsymbol{\Gamma} = \nabla G - \frac{1}{k^2}\nabla\big(-k^2 G - \delta\big)' = \nabla G + \nabla' G + \frac{1}{k^2}\nabla'\delta = \frac{1}{k^2}\nabla'\delta,$$

because $\nabla G + \nabla' G = 0$. Therefore

$$k^2\,\nabla \cdot \boldsymbol{\Gamma}(\mathbf{r}, \mathbf{r}') = \nabla'\delta(\mathbf{r} - \mathbf{r}'). \tag{6.37}$$

Apply $\mathcal{L}$ to the two pieces in (6.34). Write $\boldsymbol{\Gamma} = \mathbf{I}\,G - \frac{1}{k^2}\nabla\nabla' G$ and use linearity.

(i) First term: $\mathcal{L}(\mathbf{I}\,G)$. Using $\nabla \times \nabla \times (\mathbf{I}\,G) = \nabla(\nabla G) - \nabla^2(\mathbf{I}\,G)$,

$$\mathcal{L}(\mathbf{I}\,G) = \nabla\nabla G - \mathbf{I}\,\nabla^2 G - k^2\,\mathbf{I}\,G.$$

By (6.33), $-\nabla^2 G - k^2 G = \delta$, hence

$$\mathcal{L}(\mathbf{I}\,G) = \mathbf{I}\,\delta + \nabla\nabla G. \tag{6.38}$$

(ii) Second term: $\mathcal{L}\big(-\frac{1}{k^2}\nabla\nabla' G\big)$. Consider any column of the dyadic $\nabla\nabla' G$, say $\nabla(\partial_j' G)$. Since the curl of a gradient vanishes,

$$\nabla \times \nabla \times \big(\nabla(\partial_j' G)\big) = \nabla\big(\nabla^2(\partial_j' G)\big) - \nabla^2\big(\nabla(\partial_j' G)\big) = \mathbf{0},$$

because Laplacian and gradient commute on scalars. Therefore

$$\mathcal{L}\big(\nabla(\partial_j' G)\big) = -k^2\,\nabla(\partial_j' G),$$

and, columnwise,

$$\mathcal{L}\big(\nabla\nabla' G\big) = -k^2\,\nabla\nabla' G. \tag{6.39}$$

Hence

$$\mathcal{L}\left(-\frac{1}{k^2}\nabla\nabla' G\right) = +\nabla\nabla' G. \tag{6.40}$$

Combining term From (6.38) and (6.40) we get

$$\mathcal{L}\boldsymbol{\Gamma} = \big(\mathbf{I}\,\delta + \nabla\nabla G\big) + \nabla\nabla' G.$$

Using $\nabla G = -\nabla' G$ again, we have $\nabla\nabla G = -\,\nabla\nabla' G$, so the last two terms cancel:

$$\mathcal{L}\boldsymbol{\Gamma} = \mathbf{I}\,\delta,$$

which is (6.35). □

6.5.3 Proof of reciprocity (6.36)

Since $G(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}', \mathbf{r})$ and ∇ (on $\mathbf{r}$) and ∇' (on $\mathbf{r}'$) commute on G,

$$\tilde{\boldsymbol{\Gamma}}(\mathbf{r}', \mathbf{r}) = \left(\mathbf{I} - \frac{1}{k^2}\nabla'\nabla\right) G(\mathbf{r}', \mathbf{r}) = \left(\mathbf{I} - \frac{1}{k^2}\nabla\nabla'\right) G(\mathbf{r}, \mathbf{r}') = \boldsymbol{\Gamma}(\mathbf{r}, \mathbf{r}'),$$

which proves (6.36). □

6.5.4 Remarks

(i) Eq. (6.37) is the divergence relation used in the Levine–Schwinger method: $k^2\,\nabla\cdot\boldsymbol{\Gamma} = -\nabla\delta = \nabla'\delta$, since $\nabla\delta(\mathbf{r}-\mathbf{r}') = -\nabla'\delta(\mathbf{r}-\mathbf{r}')$.

(ii) The outgoing radiation condition is inherited from G; hence the dyadic $\boldsymbol{\Gamma}$ defined in (6.34) is the outgoing Green dyadic for the vector Helmholtz operator.