Photonic theory : Green's functions, Scattering and Density of states

1. Electron wavelength Use the relativistic formula for a point particle to find the de Broglie wavelength of an electron whose kinetic energy is $K = 2$ eV. Give a numerical value (in metres and in nanometres).

Solution: The total (relativistic) energy of the electron is

$$E = \gamma m_0 c^2 = m_0 c^2 + K,$$

where m_0 is the electron rest mass, c the speed of light and K the kinetic energy. Using the energy–momentum relation

$$E^2 = (pc)^2 + (m_0 c^2)^2,$$

the relativistic momentum is

$$p = \frac{\sqrt{E^2 - (m_0 c^2)^2}}{c}.$$

The de Broglie wavelength is

$$\lambda = \frac{h}{p},$$

with Planck's constant h.

Substitute $E = m_0 c^2 + K$ to obtain

$$p = \frac{\sqrt{(mc^2 + K)^2 - (mc^2)^2}}{c} = \frac{\sqrt{2\,mc^2 K + K^2}}{c}.$$

Hence

$$\lambda = \frac{h\,c}{\sqrt{2\,mc^2 K + K^2}}.$$

Now plug in numerical values. We use

$$\begin{aligned} h &= 6.62607015 \times 10^{-34}\ \text{J s}, \\ c &= 2.99792458 \times 10^{8}\ \text{m/s}, \\ m &= 9.1093837015 \times 10^{-31}\ \text{kg}, \\ 1\ \text{eV} &= 1.602176634 \times 10^{-19}\ \text{J}, \\ K &= 2\ \text{eV} = 2 \times 1.602176634 \times 10^{-19}\ \text{J}. \end{aligned}$$

Compute the denominator:

$$\sqrt{2\,mc^2 K + K^2} \approx \sqrt{2\,(9.109 \times 10^{-31})(2.9979 \times 10^{8})^2\,(3.2043 \times 10^{-19}) + (3.2043 \times 10^{-19})^2}.$$

Evaluating numerically gives the momentum

$$p \approx 7.64065 \times 10^{-25}\ \text{kg m/s}.$$

Therefore

$$\lambda = \frac{h}{p} \approx \frac{6.62607015 \times 10^{-34}}{7.64065 \times 10^{-25}}\ \text{m} \approx 8.672 \times 10^{-10}\ \text{m}.$$

In more convenient units,

$$\lambda \approx 8.67 \times 10^{-10}\ \text{m} = 0.867\ \text{nm} = 8.67\ \text{Å}.$$

$$\boxed{\lambda \approx 8.67 \times 10^{-10}\ \text{m}\ (\approx 0.867\ \text{nm})}$$

Remark. At this low kinetic energy ($2\ \text{eV} \ll mc^2 \approx 511\ \text{keV}$) the non-relativistic expression $\lambda_{\text{nr}} = h/\sqrt{2mK}$ would give a value very close to the relativistic result; using the relativistic formula above ensures full correctness.

Why the energy $E = h\nu$ in non-relativistic quantum mechanics refers to kinetic energy

In non-relativistic quantum mechanics, the relation $E = h\nu$ connects the frequency ν of a particle's matter wave to its *mechanical* energy, that is, its kinetic (and possibly potential) energy rather than the total relativistic energy including the rest mass term mc^2.

Intuitive explanation. The rest energy mc^2 is an enormous constant that does not affect the particle's dynamics. Adding a constant to all energies merely multiplies the wavefunction by an overall phase factor,

$$\psi(t) = e^{-iE_{\text{tot}}t/\hbar} = e^{-i(mc^2 t/\hbar)}\, e^{-i(E_{\text{kin}}t/\hbar)}.$$

The first exponential, $e^{-imc^2 t/\hbar}$, corresponds to a uniform and unobservable phase rotation. Only the second term, containing E_{kin}, governs the observable time evolution of the wavefunction.

From relativity to Schrödinger. Starting from the relativistic relation

$$E^2 = p^2c^2 + m^2c^4,$$

one finds, for $p \ll mc$,

$$E = mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots.$$

When we insert this into a plane wave

$$\psi(\mathbf{r}, t) = e^{i(\mathbf{p}\cdot\mathbf{r} - Et)/\hbar} = e^{-imc^2 t/\hbar}\, e^{i(\mathbf{p}\cdot\mathbf{r} - \frac{p^2}{2m}t)/\hbar},$$

the first factor again produces only a global, unobservable phase. Discarding it leads directly to the Schrödinger equation, where $E = h\nu$ refers to the kinetic (and potential) energy.

In summary: in quantum mechanics, only *energy differences* affect physical observables. The rest energy mc^2 simply shifts all levels by a constant and can be ignored. Hence, in the non-relativistic limit, the E in $E = h\nu$ represents the kinetic energy of the particle.

Compton versus de Broglie wavelength

Two characteristic wavelengths can be associated with a massive particle, depending on which form of its energy is used in the relation $E = h\nu$.

1. Compton wavelength (rest-energy based):

$$\lambda_C = \frac{h}{mc}.$$

It corresponds to using the *total* relativistic energy $E = mc^2$ in $E = h\nu$. The associated frequency $\nu_C = mc^2/h$ describes the extremely rapid internal phase rotation of the particle's wavefunction:

$$\psi(t) \sim e^{-imc^2 t/\hbar}.$$

For an electron,

$$\lambda_C = 2.426 \times 10^{-12} \text{ m}.$$

The Compton wavelength marks the scale where relativistic and quantum effects (e.g. pair creation) become important; a particle cannot be localized to better than about λ_C without creating new particles.

2. de Broglie wavelength (momentum based):

$$\lambda_{\text{dB}} = \frac{h}{p}.$$

It follows from the *kinetic* energy or momentum of motion, and governs interference and diffraction phenomena. For a 2 eV electron,

$$\lambda_{\text{dB}} \approx 8.7 \times 10^{-10} \text{ m}.$$

In summary:

$$\boxed{\text{Compton: } E = mc^2 \Rightarrow \lambda_C = h/(mc)} \quad \text{vs.} \quad \boxed{\text{de Broglie: } p = h/\lambda_{\text{dB}}.}$$

The Compton wavelength is a fixed relativistic constant for a given particle, whereas the de Broglie wavelength depends on its velocity and describes its wave-like behavior in motion.

2. Calulate the wavelength of a 2eV photon. Compare this to the deBroglie wavelength of the electron.

Solution

For a photon, the energy–wavelength relation is

$$E = \frac{hc}{\lambda}, \qquad \lambda = \frac{hc}{E}.$$

With $hc \simeq 1240 \text{ eV} \cdot \text{nm}$ and $E = 2$ eV,

$$\lambda_{\text{photon}} = \frac{1240}{2} \simeq 620 \text{ nm}.$$

As we saw in the fist exercise, for an electron of kinetic energy $E = 2$ eV, the de Broglie wavelength is

$$\lambda_e = \frac{h}{\sqrt{2m_e K}} \simeq 0.87 \text{ nm}.$$

Conclusion: for the same energy, the photon wavelength is about 7×10^2 times larger than the electron de Broglie wavelength. This plays a major role in the "weakness" of the interaction of photons with the electrons in atoms and many of the difficulties in interfacing electronic circuits with photons.

3. Suppose we have a material medium that absorbs a single frequency so strongly that the imaginary of its complex susceptibility, $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$ can be approximated as a delta function :

$$\chi''(\omega) = K\delta(\omega - \omega_r) \tag{1}$$

where K is a real constant. This idealized model corresponds to an infinitely narrow absorption line and is therefore unphysical, but it illustrates clearly how dispersive features arise from absorption.

Use the Kramer's Krönig relations to determine the real part of the susceptibility, $\chi'(\omega)$

Solution : From the Kramer's Kronig relation :

$$\chi'(\omega) = \frac{2}{\pi}\mathcal{P}.\mathcal{V}.\int_0^\infty \frac{\omega'\chi''(\omega')}{\omega'^2 - \omega^2}d\omega' \tag{2}$$

gives us:

$$\chi'(\omega) = \frac{2}{\pi}\mathcal{P}.\mathcal{V}.\int_0^\infty \frac{\omega' K\delta(\omega' - \omega_r)}{\omega'^2 - \omega^2}d\omega' = \frac{2K}{\pi}\frac{\omega_r}{\omega_r^2 - \omega^2} \tag{3}$$

4. We consider small spherical scatterers composed of a noble metal (or another plasmonic material) with diameters below a few tens of nanometers, embedded in a homogeneous background medium with real constitutive parameters ε_b and μ_b. Assuming that the particles are much smaller than the in-medium wavelength λ of visible light, their electromagnetic response can be modeled by an induced electric dipole moment $\boldsymbol{p}(\omega)$.

If the particle response is linear and isotropic, the induced dipole moment is related to the incident electric field $\boldsymbol{E}_{\text{inc}}(\omega)$ through the polarizability $\alpha(\omega)$:

$$\boldsymbol{p}(\omega) = \epsilon_0\varepsilon_b\alpha(\omega)\boldsymbol{E}_{\text{inc}}(\omega)\ .$$

From considerations involving the Poynting vector and radiation flux, the extinction and scattering cross sections of an electric dipole scatterer can be expressed in terms of polarizability, $\alpha(\omega)$, as:

$$\sigma_{\text{ext}} = \kappa\Im m\{\alpha(\omega)\} \qquad \sigma_{\text{scat}} = \frac{\kappa^4}{6\pi}|\alpha(\omega)|^2\ . \tag{4}$$

where $\kappa = \frac{\omega}{c}\sqrt{\varepsilon_b\mu_b} \equiv \frac{2\pi}{\lambda}$ with λ the wavelength in the host (background) medium

Energy conservation in the scattering process imposes the inequality:

$$\frac{\kappa^3}{6\pi}|\alpha(\omega)|^2 \leq \Im m\{\alpha(\omega)\}\ . \tag{5}$$

(a) What are the physical dimensions of σ and α? Briefly justify why these dimensions are physically reasonable.

Solution : The cross section σ has the dimensions of an area (m^2), while the polarizability α has the dimensions of a volume (m^3). This is physically reasonable since σ characterizes an effective interaction area, whereas α measures the strength of an induced dipole moment and therefore scales with the particle volume.

(b) Express the inequality of eq.(5) in terms of the cross-sections given in eq.(4). The inequality becomes an equality in the case where scattering occurs in the absence of loss into material degrees of freedom. What does this imply for the relationship between the extinction, scattering, and absorption cross sections?

Solution : Substituting Eq.(4) into Eq.(5), yields:

$$\sigma_{\text{scat}} \leq \sigma_{\text{ext}} \ .$$

This expresses energy conservation: the scattered power cannot exceed the total extinguished power.

When $\sigma_{\text{scat}} = \sigma_{\text{ext}}$, there is no intrinsic material loss and the scattering is purely elastic. In general, the absorption cross section is given by

$$\sigma_{\text{abs}} = \sigma_{\text{ext}} - \sigma_{\text{scat}} \ , \tag{6}$$

which quantifies the power dissipated into internal degrees of freedom such as Joule heating.

(c) Write $\alpha(\omega) = \alpha'(\omega) + i\alpha''(\omega)$, with α' and α'' real.

i. Rewrite Eq. (5) in terms of α' and α''.
Solution : Writing $\alpha = \alpha' + i\alpha''$, Eq. (5) becomes

$$(\alpha')^2 + (\alpha'')^2 \leq \frac{6\pi}{\kappa^3}\,\alpha'', \tag{7}$$

which immediately implies $\alpha'' > 0$.

ii. Deduce the maximum allowed value of α''. *Hint:* The bound is saturated when $\alpha' = 0$.
Solution : The left-hand side is maximized when $\alpha' = 0$, corresponding to a purely imaginary polarizability. In this case,

$$\alpha'' \leq \frac{6\pi}{\kappa^3} \ .$$

The α is entirely imaginary corresponds to the fact that the strongest cross section occurs when the dipole is maximally out of phase with respect to the incident field. The amplitude is maximum response compatible with passivity (unitary limit).

Remark (explicit maximization). For completeness, one may verify the maximization explicitly by setting $x = \alpha'$, $y = \alpha''$, and $C = 6\pi/\kappa^3$, which leads to

$$x^2 + y^2 \leq Cy.$$

The maximum allowed value of y occurs when equality holds and $x = 0$, yielding $y = C$ and confirming the result above.

iii. Hence obtain an upper bound on σ_{ext}.

Solution :
Using $\sigma_{\text{ext}} = \kappa\,\alpha''$, one finds the bound

$$\sigma_{\text{ext}} \leq \frac{6\pi}{\kappa^2}.$$

(d) Recalling that the wavenumber is related to the wavelength in the external medium by, $\kappa = 2\pi/\lambda$, use the results of the previous question, and the approximation $\pi \simeq 3$ to find the often stated (but seldom derived) *unitary limit* for a dipole interaction cross section: $\sigma \leq \frac{\lambda^2}{2}$.
Solution. Using $\kappa = 2\pi/\lambda$, the previous bound gives

$$\sigma_{\text{ext}} \leq \frac{6\pi}{(2\pi/\lambda)^2} = \frac{6\pi\lambda^2}{4\pi^2} \approx \frac{\lambda^2}{2},$$

where we used $\pi \simeq 3$.

$$\boxed{\sigma_{\text{ext}} \lesssim \frac{\lambda^2}{2}}$$

Although often introduced via unitarity in quantum scattering theory, this bound follows directly from energy conservation and wave optics, and therefore applies to both classical and quantum descriptions of light-matter interactions.

5. The *quasi-static* expression for the electric dipolar polarizability of a sphere of volume, V, and dielectric permittivity ε_s, immersed in a background medium of dielectric permittivity, ε_b, can be written:

$$\alpha_{\text{qs}} \equiv \lim_{\omega\to 0} \alpha(\omega) = 3V\frac{\varepsilon_s - \varepsilon_b}{\varepsilon_s + 2\varepsilon_b}\,. \tag{8}$$

This expression is valid in the electrostatic (Rayleigh) limit, ($\kappa R \ll 1$), for non-magnetic, isotropic materials.

(a) If a peak in the cross sections is observed near $\lambda = 365\,\text{nm}$, what condition must be approximately satisfied by the real part of the metal permittivity ε_s relative to ε_b at this wavelength?
Solution : A peak in the extinction cross section corresponds to a peak in electric dipolar polarizability. From Eq. (8), we see that this occurs when the denominator is minimized, *i.e.* when:

$$\Re\{\varepsilon_s\} \simeq -2\varepsilon_b. \tag{9}$$

Thus the resonance peak in polarizability occurs at a frequency for which the real part of the metal's permittivity is negative satisfies the above condition. This can occur for "plasmonic" metals that have relatively low losses (*i.e.* permittivities with relatively small imaginary parts, ε'', at visible light frequencies.

(b) A commonly employed model for including 'radiative damping' to the quasi-static polarizability is given by:

$$\alpha(\omega) \simeq \frac{\alpha_{\text{qs}}}{1 - i\frac{\kappa^3}{6\pi}\alpha_{\text{qs}}}\,. \tag{10}$$

What is the limiting value of $\alpha(\omega)$ when $\alpha_{\text{qs}} \to \infty$? Comment on this result based on your results from question 4. Why is this model superior to simply using the quasi-static value for polarizability ?

Solution : This "radiative" corrected polarizability ensures that the dipolar form (and bounds) of the energy conservation relations in Eq. (5) are satisfied, something which the quasi-static polarizability of Eq.(8) is not required to do. A nice way of rewriting eq.(10) is

$$\alpha(\omega)^{-1} \simeq \alpha_{\rm qs}^{-1} - i\frac{\kappa^3}{6\pi} \ . \tag{11}$$

Thanks to the radiative correction, when $\alpha_{\rm qs} \to \infty$, the formulas of Eqs. (10) and (11) both correctly predict that the electric dipole polarizability remains finite and at best can obtain its unitary limited value of:

$$\alpha(\omega) \to i\,\frac{6\pi}{\kappa^3}.$$

(c) Even though the refinement proposed in Eq.(10) for including the radiative damping of the polarizability is crucial in many situations, it is often ignored by people modeling plasmonic particles with diameters less than 20nm. Explain why (hint: consider Eqs. (8) and (10)), and the real and imaginary parts of a typical Drude permittivity in the visible range as shown in Fig.(1).

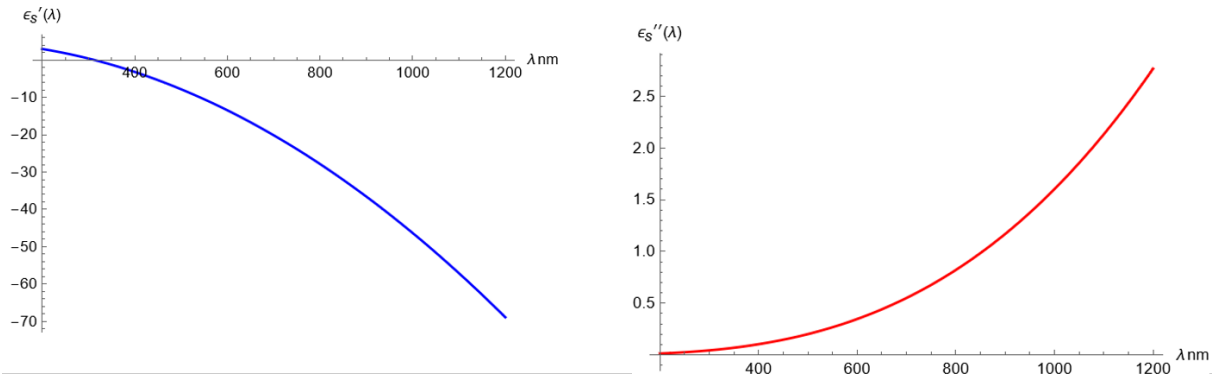

Figure 1: Real part of the permittivity (left: Re[ε_s]) and its imaginary part (right: Im[ε_s]) of an 'idealized' Drude permittity for a plasmonic conductor in the visible range.

Solution : The radiative damping of Eq.(10) can be very important when polarizability is real-valued (*i.e.* when ε_s and ε_b are real-valued). However, when ε_s has a non-negligible imaginary part, as seen in the Fig. 1, the radiative correction term scales as $\kappa^3\alpha_{\rm qs} \propto (R/\lambda)^3$ and is often quite small for particles with $R \ll \lambda$, and thereby negligible compared to the imaginary parts of the polarizability arising directly from the imaginary parts of ε_s. This often results in plasmonic resonant particles possessing relatively large absorption cross sections, but comparatively weak scattering cross sections. In such situations, the extinction and absorption cross sections are nearly equal, and one sometimes sees the formula for extinction cross section being used to calculate the absorption cross section.

Take-home message. Radiative damping enforces fundamental conservation laws and bounds on light–matter interaction, but is often masked by material absorption in deeply subwavelength plasmonic particles.

6. Free-space electromagnetic Green's function :

The electric-field free-space dyadic Green's function relates an oscillating electric dipole source to the the resulting electric field in the frequency domain :

$$\overleftrightarrow{\boldsymbol{g}}(\boldsymbol{r}) = \frac{e^{i\kappa r}}{4\pi\kappa^2 r^3}\mathcal{P}.\mathcal{V}.\left\{(1-i\kappa r)\left(3\boldsymbol{u}_r\boldsymbol{u}_r - \overleftrightarrow{\mathbb{I}}\right) + \kappa^2 r^2\left(\overleftrightarrow{\mathbb{I}} - \boldsymbol{u}_r\boldsymbol{u}_r\right)\right\} - \frac{\overleftrightarrow{\mathbb{I}}}{3\kappa^2}\delta^3(\boldsymbol{r}) \ , \tag{12}$$

where $\boldsymbol{u}_r \equiv \frac{\boldsymbol{r}}{r}$ is the unit vector in the radial direction, $\kappa \equiv \frac{\omega\sqrt{\varepsilon_b\mu_b}}{c} \equiv \frac{2\pi}{\lambda_b}$, is the wave-number in the external(background) medium, and finally $\mathcal{P}.\mathcal{V}.$ stands for principal value (associated with a 3D exclusion volume at the origin on account of the field being undefined when $r \to 0$. The Green's function $\overleftrightarrow{\boldsymbol{g}}$, allows one to directly obtain the time harmonic electric field of an oscillating dipole, $\boldsymbol{p}$, positioned at the coordinate system origin and oriented along a unit vector $\boldsymbol{n_p}$ (*i.e.* $\boldsymbol{p} = |\boldsymbol{p}|\boldsymbol{n}_p$). Since this field is produced by a source, (like a coaxial feed cable or induced by an "incident" field), we henceforth refer to it as the "scattered" field :

$$\begin{aligned}\boldsymbol{E}^{(\mathrm{s})}(\boldsymbol{r}) &= \frac{\omega^2}{\epsilon_0 c^2}\overleftrightarrow{\boldsymbol{g}}(\boldsymbol{r})\cdot\boldsymbol{p} \\ &= \mathcal{P}.\mathcal{V}.\left\{\frac{e^{i\kappa r}}{4\pi\epsilon_0\varepsilon_b r^3}\left[\kappa^2 r^2\left[\boldsymbol{p} - \boldsymbol{u}_r(\boldsymbol{u}_r\cdot\boldsymbol{p})\right] + (1-i\kappa r)(3(\boldsymbol{u}_r\cdot\boldsymbol{p})\boldsymbol{u}_r - \boldsymbol{p})\right]\right\} \\ &\quad - \frac{\boldsymbol{p}}{3\epsilon_0\varepsilon_b}\delta^3(\boldsymbol{r}) \ .\end{aligned} \tag{13}$$

a) Identify the **near-field** part of the scattered field, $\boldsymbol{E}^{(\mathrm{s})}$ and explain the physical relevance of the $-\frac{\boldsymbol{p}}{3\epsilon_0\varepsilon_b}\delta^3(\boldsymbol{r})$ term in eq.(13), including a discussion of why this term is directed in the direction opposite to the dipole, $\boldsymbol{p}$.

Solution :

$$\boldsymbol{E}^{(\mathrm{s})}_{\mathrm{n.f.}}(\boldsymbol{r}) = \mathcal{P}.\mathcal{V}.\left\{\frac{e^{i\kappa r}}{4\pi\epsilon_0\varepsilon_b r^3}\left[3(\boldsymbol{u}_r\cdot\boldsymbol{p})\boldsymbol{u}_r - \boldsymbol{p}\right]\right\} - \frac{\boldsymbol{p}}{3\epsilon_0\varepsilon_b}\delta^3(\boldsymbol{r}) \ .$$

The near field is so named because its field dominates when r is small (but are in turn negligible at large r). Therefore the "near field" are those contributions to that have a $1/r^3$ dependence. One can also include the delta function term as a near field in the sense that it only contributes at the position of the dipole's center, $\boldsymbol{r} = \boldsymbol{0}$. The delta function effectively describes the strong fields between the $\pm$ charges of the dipole when it is shrunk to a "point" dipole, thereby ensuring the correct self-interaction and is required for consistency with Maxwell's equations.

b) It is convenient to describe the dipole field mathematically by aligning the dipole moment along the z-axis so that the dipole moment is written $\boldsymbol{p} = |\boldsymbol{p}|\boldsymbol{n_p} \longrightarrow |\boldsymbol{p}|\boldsymbol{u}_z$, which can be induced by an electromagnetic plane wave propagating along the x-axis, *i.e.* $\boldsymbol{k}/|\boldsymbol{k}| = \boldsymbol{u}_x$. The scattered fields are in spherical coordinates are then:

$$\boldsymbol{E}^{(\mathrm{s})}(\boldsymbol{r}) = E_r^{(\mathrm{s})}(r,\theta)\boldsymbol{u}_r + E_\theta^{(\mathrm{s})}(r,\theta)\boldsymbol{u}_\theta + E_\phi^{(\mathrm{s})}(r,\theta)\boldsymbol{u}_\phi \tag{14}$$

We can obtain expressions for these components by using the relation,

$$\boldsymbol{u}_z = \cos\theta\boldsymbol{u}_r - \sin\theta\boldsymbol{u}_\theta \tag{15}$$

in Eq.(13). Determine the expressions for $E_r^{(\mathrm{s})}$, $E_\theta^{(\mathrm{s})}$, and $E_\phi^{(\mathrm{s})}$ that ignore the delta function contribution.

Solution : With the above substitutions we find:

$$E_r^{(\mathrm{s})}(r,\theta) = \frac{|\boldsymbol{p}|\cos\theta}{4\pi\epsilon_0\varepsilon_b}\frac{\exp(i\kappa r)}{r}\kappa^2\left[\frac{2}{\kappa^2 r^2} - \frac{2i}{\kappa r}\right] \tag{16a}$$

$$E_\theta^{(\mathrm{s})}(r,\theta) = \frac{|\boldsymbol{p}|\sin\theta}{4\pi\epsilon_0\varepsilon_b}\frac{\exp(i\kappa r)}{r}\kappa^2\left[\frac{1}{\kappa^2 r^2} - \frac{i}{\kappa r} - 1\right] \tag{16b}$$

$$E_\phi^{(\mathrm{s})} = 0 \tag{16c}$$

There are several interesting things to notice here: Only the "transverse" electric field, $E_\theta^{(\mathrm{s})}$, has radiating far-field components (*i.e.* a field that decrease as $1/r$ with distance), The radial oriented field, $E_r^{(\mathrm{s})}$ does not radiate, and therefore has no far-field components. That the $E_\phi^{(\mathrm{s})}$ is null, arrives directly from construction, but it is also a consequence of symmetry.

c) Since we know the scattered electric field, the scattered magnetic field is obtained from the Maxwell equation:

$$i\omega\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{E}\,, \tag{17}$$

the constitutive relation in the background medium, $\boldsymbol{H}_{\mathrm{S.I.}} = \frac{\boldsymbol{B}}{\mu_b\mu_0}$, and the curl in spherical coordinates:

$$\begin{aligned}\boldsymbol{\nabla}\times\boldsymbol{E}\,(r,\theta,\phi) = \frac{\boldsymbol{u}_r}{r\sin\theta}\left[\frac{\partial\left(E_\phi\sin\theta\right)}{\partial\theta} - \frac{\partial E_\theta}{\partial\phi}\right] + \frac{\boldsymbol{u}_\theta}{r}\left[\frac{1}{\sin\theta}\frac{\partial E_r}{\partial\phi} - \frac{\partial\left(rE_\phi\right)}{\partial r}\right] + \\ + \frac{\boldsymbol{u}_\phi}{r}\left[\frac{\partial\left(rE_\theta\right)}{\partial r} - \frac{\partial\left(E_r\right)}{\partial\theta}\right]\,.\end{aligned} \tag{18}$$

Find the expression for $\boldsymbol{H}^{(\mathrm{s})}(r,\theta,\phi)$. What do you remark about, $\boldsymbol{H}^{(\mathrm{s})}$, in the near and far fields respectively ?

Solution : Carrying out this somewhat tedious calculation, we find:

$$H_\phi^{(\mathrm{s})} = \frac{|\boldsymbol{p}|\sin\theta}{4\pi\epsilon_0\varepsilon_b}\frac{\exp(i\kappa r)}{r}\kappa^2\left[-\frac{i}{\kappa r} - 1\right]\sqrt{\frac{\epsilon_0\varepsilon_b}{\mu_0\mu_b}}\,, \tag{19}$$

The $\|\boldsymbol{H}^{(\mathrm{s})}\|$ field diverges in the near field, but its amplitude only diverges at the rate $\frac{1}{r^2}$ in the near field while we saw above that $\|\boldsymbol{E}^{(\mathrm{s})}\|$ diverges at a rate of $\frac{1}{r^3}$ in the near-field. Consequently, one often neglects the effect of $\boldsymbol{H}^{(\mathrm{s})}$ when $\lim_{r\to 0}$ despite its divergence in this limit.

In the far-field, we see that $\boldsymbol{H}^{(\mathrm{s})}$ is oriented perpendicular to $\boldsymbol{E}^{(\mathrm{s})}$, and the field amplitudes are related by:

$$\frac{H_\phi^{(\mathrm{s})}}{E_\theta^{(\mathrm{s})}} = \sqrt{\frac{\epsilon_0\varepsilon_b}{\mu_0\mu_b}} = \sqrt{\frac{\varepsilon_b}{\mu_b}}\eta_0 \tag{20}$$

where

$$\eta_0 \equiv \sqrt{\frac{\epsilon_0}{\mu_0}}\,, \tag{21}$$

is the famous "vacuum impedance" that is a unit-system consequence of S.I. unit conventions as we discussed in course. In other coordinate systems, like Gaussian units, where the electric and magnetic fields have the same units, one finds the electric and magnetic components of plane waves in free space have equal amplitudes. Such comparisons are more difficult in S.I. units.

d) A question of significant practical importance is to determine the total power radiated by the electric dipole field in eq.(13). At a fundamental level, this is done by determining the associated $\boldsymbol{H}^{(\mathrm{s})}$ field and then using the Poynting vector to calculate radiation flux leaving any closed volume surrounding the dipole. Such calculations can most easily be done in the far-field limit where the expressions for fields are the simplest. One can show that that in the far-field limit, the scattered, $\boldsymbol{H}^{(\mathrm{s})}$ field is related to the scattered $\boldsymbol{E}^{(\mathrm{s})}$ field via the relation :

$$\lim_{r\to\infty} \boldsymbol{H}^{(\mathrm{s})} \to \frac{\kappa}{\omega\mu_b\mu_0}\boldsymbol{u}_r \times \boldsymbol{E}^{(\mathrm{s})} = \sqrt{\frac{\varepsilon_b}{\mu_b}}\eta_0 \boldsymbol{u}_r \times \boldsymbol{E}^{(\mathrm{s})} \,. \tag{22}$$

Show that this relation is indeed consistent with the full expression for $\boldsymbol{H}^{(\mathrm{s})}$ found in the previous question.

e) Now we derive the radiated power of a dipole: The formula for the time averaged Poynting vector, in a time-harmonic formulation is:

$$\langle \boldsymbol{\Pi} \rangle_T = \frac{1}{2}\Re\left\{\boldsymbol{E}^{(\mathrm{s}),*} \times \boldsymbol{H}^{(\mathrm{s})}\right\} \tag{23}$$

Use this formula to calculate the time averaged Poynting vector in the far-field, and then integrate this over the surface of a sphere at infinity to determine the average power, $\langle P_{\mathrm{rad}} \rangle_T$, radiated by the oscillating electric dipole.

Solution : The Poynting vector in the far-field using eq.(23) is:

$$\lim_{r\to\infty} \langle \boldsymbol{\Pi}(r,\theta) \rangle_T = \frac{1}{2}\frac{|\boldsymbol{p}|^2 \sin^2\theta}{16\pi^2 r^2}\frac{\kappa^4}{\epsilon_0\varepsilon_b}\sqrt{\frac{1}{\epsilon_0\varepsilon_b\mu_0\mu_b}}\boldsymbol{u}_\theta \times \boldsymbol{u}_\phi = \frac{|\boldsymbol{p}|^2 \sin^2\theta}{32\pi^2 r^2}\frac{\kappa^3\omega}{\epsilon_0\varepsilon_b}\boldsymbol{u}_r \,. \tag{24}$$

Integrating the flux of the Poynting vector over the surface of a sphere of very large radius, we obtain that the power emitted by the dipole is:

$$\langle P_{\mathrm{rad}} \rangle_T = \oiint \lim_{r\to\infty} \langle \boldsymbol{\Pi}(r,\theta) \rangle_T \cdot d\boldsymbol{S} = \frac{|\boldsymbol{p}|^2}{32\pi^2}\frac{\kappa^3\omega}{\epsilon_0\varepsilon_b}\int_0^\pi \sin^3\theta d\theta \int_0^{2\pi} d\phi = \frac{|\boldsymbol{p}|^2}{12\pi}\frac{\kappa^3\omega}{\epsilon_0\varepsilon_b} \,, \tag{25}$$

where we used

$$\int_0^\pi \sin^3\theta d\theta \longrightarrow \int_{-1}^1 \left(1-\cos^2\theta\right) d(\cos\theta) = \frac{4}{3} \,. \tag{26}$$

f) From here on we connect Green's function to LDOS and radiated power. The component of the dipole's electric field parallel to $\boldsymbol{p}$ ($E_z(r,\theta) \equiv \boldsymbol{n_p} \cdot \boldsymbol{E}^{(\mathrm{s})}$) plays an important role in the quantum theory of spontaneous emission and in antenna theory. Use eq.(13) to demonstrate that:

$$\begin{aligned} E_z^{(\mathrm{s})}(r,\theta) &= \frac{|\boldsymbol{p}|}{4\pi\epsilon_0\varepsilon_b}\frac{\exp(i\kappa r)}{r}\mathcal{P}.\mathcal{V}.\left[\kappa^2\sin^2\theta - i\kappa\frac{3\cos^2\theta-1}{r} + \frac{3\cos^2\theta-1}{r^2}\right] \\ &= \kappa^3\frac{|\boldsymbol{p}|}{4\pi\epsilon_0\varepsilon_b}\frac{\exp(i\chi)}{\chi}\mathcal{P}.\mathcal{V}.\left[\sin^2\theta - i\frac{3\cos^2\theta-1}{\chi} + \frac{3\cos^2\theta-1}{\chi^2}\right] \,. \end{aligned} \tag{27}$$

where we defined $\chi \equiv \kappa r$.

g) Green function theory establishes that the local density of states (or local density of modes) is related to the *imaginary part* of $E_z^{(\mathrm{s})}(r,\theta)$ in eq.(27). This connection is workable since even though the real part of $E_z^{(\mathrm{s})}$ diverges as $r \to 0$, its imaginary

component, $\Im[E_z^{(s)}(r)]$ remains finite in this limit. To verify this behavior for small values of r, use the Taylor expansion of the exponential function for small arguments,

$$\exp(i\chi) = 1 + i\chi - \frac{\chi^2}{2} - i\frac{\chi^3}{6} + \dots \tag{28}$$

Approximating $\exp(i\chi)$ up to third order in χ is shown in eq.(28), find the imaginary part of $\lim_{r\to 0} E_z^{(s)}(r,\theta)$.

Solution : Given the presence of differing inverse powers of r inside the brackets of eq.(27), we have to include the expansion of $\exp(i\chi)$ up to third order in χ in order to obtain all the of the terms which diverge or remain finite when $r \to 0$. Carrying out each of these multiplications individually we find:.

$$\begin{aligned}
\Im\left\{1 \times \frac{1}{\chi}[\cdots]\right\} &= \frac{1}{\chi^2} - \frac{3\cos^2\theta}{\chi^2} \\
\Im\left\{i\chi \times \frac{1}{\chi}[\cdots]\right\} &= \frac{3\cos^2\theta}{\chi^2} + \sin^2\theta - \frac{1}{\chi^2} \\
\Im\left\{\frac{-\chi^2}{2} \times \frac{1}{\chi}[\cdots]\right\} &= \frac{3\cos^2\theta}{2} - \frac{1}{2} \\
\Im\left\{\frac{-i\chi^3}{6} \times \frac{1}{\chi}[\cdots]\right\} &= -\frac{\cos^2\theta}{2} + \frac{1}{6} - \frac{1}{6}\chi^2\sin^2\theta
\end{aligned} \tag{29}$$

Adding these terms together, we remark that all the terms that diverge when $r \to 0$, cancel amongst themselves. The cancellation of divergences is the key reason the LDOS remains finite. We don't need to include any higher orders since we can verify that all higher order contributions vanish in the $r \to 0$ limit. Retaining only the non-vanishing terms, we have:

$$\begin{aligned}
\lim_{r\to 0} \Im\left[E_z^{(s)}(r,\theta)\right] &= \frac{|\boldsymbol{p}|\kappa^3}{4\pi\epsilon_0\varepsilon_b}\mathcal{P}.\mathcal{V}.\frac{1}{3}\left[-1 + 3\cos^2\theta + 3\sin^2\theta + O(r^2)\right] \\
&= \frac{|\boldsymbol{p}|\kappa^3}{4\pi\epsilon_0\varepsilon_b}\frac{2}{3}\,.
\end{aligned} \tag{30}$$

h) The time averaged emitted power, $\langle P_e\rangle_T$ delivered by a time-harmonic *emitter*, located within a volume $\mathcal{V}$, is equal to the negative of the power carried out by the electric field, $\boldsymbol{E}$, acting on the time harmonic current $\boldsymbol{j}$, that produced the field:

$$\langle P_e\rangle_T = -\frac{1}{2}\iiint \Re\left\{\boldsymbol{E}^* \cdot \boldsymbol{j}\right\} d^3r\,. \tag{31}$$

The current created by an electric dipole placed at the origin is:

$$\boldsymbol{j} = -i\omega\boldsymbol{p}\delta^3(\boldsymbol{r})\,. \tag{32}$$

Use these expression to calculate the power emitted by the dipole source of the field, and discuss its relationship to the radiated power, $\langle P_{\text{rad}}\rangle$ calculated in part e).

Solution : Inserting the expressions of eq.(30) and (32) into eq.(31) one finds :

$$\langle P_e\rangle_T = \frac{|\boldsymbol{p}|^2\omega\kappa^3}{12\pi\epsilon_0\varepsilon_b}\,. \tag{33}$$

Given that $\langle P_e\rangle_T = \langle P_{\text{rad}}\rangle_T$ in free space, this is recognized as a statement of energy conservation, i.e. power emitted by the oscillating source is entirely radiated off to

infinity. Although, one might be tempted to see this results as simply providing two different ways of calculating the radiated power, the difference of their physical origins will become important when energy absorbing materials are placed in the dipole's environment. In such a case, emitted energy will be larger than the energy radiated off to infinity, and the difference between emitted and radiative powers can be used to deduce the rate of energy absorption into material degrees of freedom.

i) One can compare the imaginary part of the field at the origin, found in part g) with the expressions in eqs.(12) and (13) to demonstrate the important result for local density of states calculations that :

$$\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{g}}\left(\boldsymbol{0}\right)\cdot\boldsymbol{n_p}\right\}=\frac{\kappa}{6\pi}\,. \tag{34}$$

Expressing the Green's function in Fourier space using the same techniques as we saw in class for the scalar Helmholtz equation, one finds the formula for the Density Of States (DOS) in terms of the dyadic Green's function :

$$\rho_{\mathrm{DOS}}(\omega)=\frac{6\varepsilon_b\mu_b\omega}{\pi c^2}\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{g}}\left(\boldsymbol{r},\boldsymbol{r}\right)\cdot\boldsymbol{n_p}\right\}\,. \tag{35}$$

Question: Use the result of eq.(34) in eq.(35) to express the homogeneous medium density of states in terms of the speed of light in the background medium, $c_b\equiv\frac{c}{n_b}=\frac{c}{\sqrt{\varepsilon_b\mu_b}}$. How does this correspond to the expression arrived at by counting arguments in the calculation of black-body radiation ?

Solution :

$$\rho_{\mathrm{DOS}}(\omega)=\frac{\left(\varepsilon_b\mu_b\right)^{3/2}\omega^2}{\pi^2c^3}=\frac{\omega^2}{\pi^2c_b^3}\,.$$

This is the same as the electromagnetic density of states that we derived in the context of black-body radiation, except that we have replaced the speed of light in a vacuum with the speed of light in the background medium.

j) Express the emitted power, $\langle P_e\rangle_T$, determined in (i), in terms of the homogeneous medium density of states of the background medium, $\rho_{\mathrm{DOS}}(\omega)$, $|\boldsymbol{p}|^2$ and ω.

Solution :

$$\frac{\langle P_e\rangle_T}{\rho_{\mathrm{DOS}}}=\frac{|\boldsymbol{p}|^2\omega\kappa^3}{12\pi\epsilon_0\varepsilon_b}\frac{\pi^2c^3}{\left(\varepsilon_b\mu_b\right)^{3/2}\omega^2}=|\boldsymbol{p}|^2\frac{\pi\omega^2}{12\epsilon_0\varepsilon_b}\Longrightarrow\langle P_e\rangle_T=\rho_{\mathrm{DOS}}|\boldsymbol{p}|^2\frac{\pi\omega^2}{12\epsilon_0\varepsilon_b}\,. \tag{36}$$

This form anticipates Fermi's golden rule in quantum mechanics and quantum optics.

7. **Purcell factor and Local density of states:** Edward Mills Purcell was the first person to realize, in 1947, that an emitter's decay rate could be modified by its external environment.

Purcell initially formulated this concept in the context of a resonant cavities with a resonant frequency near a quantum mechanical transition frequency. He considered a high-Q resonance scenario where the decay rate enhancement would be largely independent of the emitter's position within the cavity. In this setting, he derived an expression, F_P for the enhancement of spontaneous decay as:

$$F_P=\frac{3}{4\pi^2}\left(\frac{\lambda}{n}\right)^3\frac{Q}{V} \tag{37}$$

where Q was the Quality factor of the resonance, and V the *mode volume* which was taken to be the physical volume of the cavity.

However, experiments later revealed that spontaneous decay rates could even be modified by open structures, like as a mirror, near the emitter. This discovery sparked decades-long debates about how the Purcell factor should be adapted to account for decay rate modifications in open systems. It is now generally accepted that as long as F_P is allowed to depend on the particle's position, $\boldsymbol{r}$, with respect to its local environment then it can be defined as:

$$F_P(\boldsymbol{r}) \equiv \frac{\tau_0}{\tau(\boldsymbol{r})} = \frac{\Gamma(\boldsymbol{r})}{\Gamma_0} \tag{38}$$

where Γ_0 is the spontaneous decay rate of the emitter measured in the vacuum, and $\Gamma(\boldsymbol{r})$ is its modified decay rate at a position $\boldsymbol{r}$, with the local environment typically structured at the wavelength scale in order produce significant deviations of F_P from 1.

Calculations of $F_P(\boldsymbol{r})$ tacitly assume that the emitter is sufficiently small with respect to the wavelength and the scale of the local environment, that the decay rates of an emitter at a given position is determined by the radiation reaction deduced from system's *total* Green function, $\boldsymbol{n}_p \cdot \overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r},\boldsymbol{r}) \cdot \boldsymbol{n_p}$, a quantity conventionally called the Local Density Of States (LDOS). For an emitter in a homogeneous medium, but which has nearby "scattering" materials, one can write:

$$\overleftrightarrow{\boldsymbol{G}} \equiv \overleftrightarrow{\boldsymbol{g}} + \overleftrightarrow{\boldsymbol{G}_s} \tag{39}$$

where $\overleftrightarrow{\boldsymbol{g}}$ is the homogeneous medium Green's function, and $\overleftrightarrow{\boldsymbol{G}_s}$ is the "scattering" Green's function that takes into account the scattering of the radiation emitted by the source. Given the definition, $F_P(\boldsymbol{r}) \equiv \frac{\Gamma(\boldsymbol{r})}{\Gamma_0}$, we deduce spontaneous decay rates should also be proportional to radiated power, such that :

$$F_P(\boldsymbol{r}) = \frac{P(\boldsymbol{r})}{P_{e,0}}. \tag{40}$$

which is a ratio of classical emitted powers rather than quantum transition rates. However, since F_P is defined as ration of radiation rates, F_P only depends on the density of state ratios that we will find here.

(a) Given your calculations of the previous exercise, one can deduce that the LDOS of a dipole emitter at a position, $\boldsymbol{r}$, operating at a frequency, ω, and oriented along the direction, $\boldsymbol{n_p}$ and placed in a "scattering" environment described by, $\overleftrightarrow{\boldsymbol{G}}$, is:

$$\rho_{\text{LDOS}}(\boldsymbol{r},\omega) = \frac{6\varepsilon_b\mu_b\omega}{\pi c^2}\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r},\boldsymbol{r})\cdot\boldsymbol{n_p}\right\}, \tag{41}$$

Furthermore, following part k) of the previous exercise, the power emitted by the dipole in a locally modified environment is:

$$\langle P_e(\boldsymbol{r},\omega)\rangle_T = \rho_{\text{LDOS}}(\boldsymbol{r},\omega)|\boldsymbol{p}|^2\frac{\pi\omega^2}{12\epsilon_0\varepsilon_b} \tag{42}$$

From the above formulas, give the expression for F_P directly in terms of the Green's functions, $\overleftrightarrow{\boldsymbol{G}}$ and $\overleftrightarrow{\boldsymbol{g}}$.

Solution :

$$F_P(\boldsymbol{r}) = \frac{P(\boldsymbol{r})}{P_{e,0}} = \frac{\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r},\boldsymbol{r})\cdot\boldsymbol{n_p}\right\}}{\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{g}}(\boldsymbol{r},\boldsymbol{r})\cdot\boldsymbol{n_p}\right\}} \tag{43}$$

(b) Take the expression derived in part a) above together with eq.(41) and the expression for $\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{g}}(\boldsymbol{r},\boldsymbol{r})\cdot\boldsymbol{n_p}\right\}$ that we obtained in eq.(34) in order to obtain an expression for F_P written entirely in terms of $\overleftrightarrow{\boldsymbol{G}}_s$:

Solution :

$$F_P(\boldsymbol{r}) = 1 + \frac{6\pi}{\kappa}\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{G}}_s(\boldsymbol{r},\boldsymbol{r})\cdot\boldsymbol{n_p}\right\} \tag{44}$$

(c) The utility of all these manipulations becomes clear once you realize that the expression that you derived in part b) gives you a concrete method for calculating F_P provided that you have a numerical solver capable of calculating the field resulting from a small dipole emitter in the desired structured environment. Describe briefly, how you would go about this.

Solution : You would place a dipole emitting at frequency ω at position, $\boldsymbol{r}$ and orientation $\boldsymbol{n_p}$ in the desired environment. You would then calculate the average of the imaginary part of the electric field over a small sphere around the emitter, being careful to subtract out the known imaginary part of the electric field of the emitter if the emitter was treated in isolation. The result you would obtain is allows you then to calculate $\Im\left\{\boldsymbol{n_p}\cdot\overleftrightarrow{\boldsymbol{G}}_s(\boldsymbol{r},\boldsymbol{r})\cdot\boldsymbol{n_p}\right\}$, and inserting this into eq.(44) would give you F_P. You would want to test this at several different small radii in order verify numerical stability. Of course, if you were able to formulate $\overleftrightarrow{\boldsymbol{G}}_s$ in a multipole framework like that discussed in class, the result would be more direct and precise, but this is typically beyond the scope of numerical solvers.