8.231 Physics of Solids I — Fall 2017
Problem Set 2

Posted: Tuesday, Sep 12, 2017
***Due:* Tuesday, Sep 19, 2017**

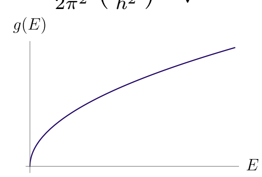
Readings (Optional)

- Simon, Steven H. *The Oxford Solid State Basics*, Chapter 2-6.
- K. S. Novoselov, A. K. Geim, et al. "Electric Field Effect in Atomically Thin Carbon Films". *Science*, **306**, 666 (2004).

Problem 1

Electronic Density of States

Compute and sketch the density of states per unit volume $g(E)$ in a metal under the following conditions. $g(E)$ for quadratic dispersion in 3D is already given as an example.

	1D	2D	3D
Quadratic dispersion $E(\mathbf{k}) = \frac{(\hbar\mathbf{k})^2}{2m}$	One should expect a divergence at $E = 0$, called a van-Hove singularity — if interested, see Wikipedia for more details.		$\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}$ 
Linear dispersion $E(\mathbf{k}) = \hbar v\lvert\mathbf{k}\rvert$		This occurs in graphene.	This occurs in Dirac semimetals, discovered only four years ago in Na_3Bi and Cd_3As_2.

Problem 2

A Phenomenology Model for Optical Property of Solids

In this problem, we will derive a simple phenomenology model to study the optical property of a wide range of solids. This model, historically known as Lorentz model, is classical and is very crude. Nevertheless, it characterizes the optical property of many solids qualitatively well.

We will come back to this topic later in this course with a quantum mechanical theory.

Part I: Driven Damped Harmonic Oscillators Solids are composed of atoms, which are further composed of nuclei and electrons.

- Assume there is only one electron of charge $-q$ associated with each nucleus of charge q. In other words, this model should work best for solids with one valence electron.
- Since nucleus is much heavier than the electron, we can set its mass to infinity. The electron has mass m.
- The force between nuclei and electrons is spring-like. Suppose the displacement of the electron with respect to the equilibrium is $\delta\mathbf{x}$, the restoring force is then $\mathbf{F}_{\text{restoring}} = -k\delta\mathbf{x}$.
- The internal collisions between electrons and nuclei are taken into account by a damping force linearly proportional to the velocity of the electron $\mathbf{F}_{\text{damping}} = -m\gamma\mathbf{v}$, where γ is the damping constant.

(a) According to Newton's second law, write down the equation of motion when the electron is in an external electric field $\mathbf{E} = E_0 e^{-i\omega t}\hat{\mathbf{z}}$.

(b) Solve the equation of motion with the ansatz $\delta\mathbf{x}(\omega, t) = \tilde{x}(\omega)e^{-i\omega t}\hat{\mathbf{z}}$. Express $\tilde{x}(\omega)$ (which is a complex number) with m, γ, k, q, ω and E_0.

Part II: Electromagnetic Waves in Dielectrics The previous part is the microscopic description of the solid. In this part, we explore how electromagnetic waves propagate in such solids.

(a) The nucleus-electron pair is an electric dipole. Suppose the dipole moment is zero at the equilibrium position. Write down the dipole moment $\mathbf{p}$ as a function of the displacement of electron $\delta\mathbf{x}$.

(b) Microscopically, many such electric dipoles constitute the dielectrics. The polarization vector of the dielectrics is just $\mathbf{P} = N\mathbf{p}$, where N is the dipole density. For linear dielectric materials (which is the case here), $\mathbf{P} = \varepsilon_0\chi_e\mathbf{E}$, where χ_e is the electric susceptibility. Combine the result in Part I, write down the expression of χ_e. It should be in the following form:

$$\chi_e = \frac{\omega_p^2}{(\omega_0^2 - \omega^2) - i\gamma\omega}. \tag{1}$$

Identify what are ω_0 and ω_p. In the following, you can express everything with ω_0, ω_p and γ. ω_p is called the "plasma frequency". You will see the reason for this name at the end of the problem.

(c) The Maxwell's equations of electromagnetic wave in dielectrics when there are no free charges or currents are

$$\nabla \cdot \mathbf{D} = 0, \tag{2}$$

$$\nabla \cdot \mathbf{B} = 0, \tag{3}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{4}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}, \tag{5}$$

where $\mathbf{D} = \varepsilon_0\mathbf{E} + \mathbf{P} = \varepsilon\mathbf{E}$ and $\mathbf{H} = \mathbf{B}/\mu$. Derive the wave equation for the electric field $\mathbf{E}$ and the dispersion $\omega(k)$ of a plane wave in the infinity space.

(d) The complex refractive index $\tilde{n}$ is defined as $\tilde{n} = \sqrt{(\varepsilon\mu)/(\varepsilon_0\mu_0)}$. Suppose the material is non-magnetic, i.e. the magnetic permittivity is $\mu = \mu_0$. Express the real and imaginary part of $\tilde{n} = n + i\kappa$ using the real and imaginary part of complex electric permittivity $\tilde{\varepsilon}/\varepsilon_0 = \varepsilon_r + i\varepsilon_i$.

(e) Assume the electromagnetic plane wave propagates along z direction. Denote the intensity of the wave as $I(z)$. The Beer-Lambert law of light absorption is

$$I(z) = I(0)e^{-\alpha z}, \tag{6}$$

where α is the absorption coefficient. Express α with κ, ω and c.

(Hint: The intensity of the light is proportional to the square of the wave amplitude $|\mathbf{E}|^2$.)

(f) Combine your results in (b) and (d) and express ε_r and ε_i as functions of ω. You should obtain a Lorentzian line shape for ε_i. Assume $\omega_0 < \omega_p$. Sketch ε_r and ε_i as well as n and κ as functions of ω. You should find κ is maximal around ω_0, with a peak width of approximately γ. What is the physical significance ω_0? Is this result within your expectation?

(Hint: You should find the answer in Part I.)

(g) Suppose the electromagnetic wave is incident normally to the dielectric from vacuum. The coefficient of the reflection is given by (you do not have to derive this)

$$R = \frac{(1-n)^2 + \kappa^2}{(1+n)^2 + \kappa^2}. \tag{7}$$

Sketch R as a function of ω.

Part III: Optical Property of Insulators, Metals and Plasmas

(a) This model characterizes the optical property of insulators when $0 < \omega_0 < \omega_p$. Fill in the following table according to your sketches before.

Light frequency ω	Reflection (strong/weak)	Absorption (strong/weak)	Net effect (transmissive/absorptive/reflective)
$[0, \omega_0 - \gamma)$			
$[\omega_0 - \gamma, \omega_0 + \gamma)$			
$[\omega_0 + \gamma, \omega_p)$			
$[\omega_p, +\infty)$			

(b) In the metal, the electrons are delocalized and form the "electron sea". This corresponds to the limit of $\omega_0 = 0$ in this model, i.e., the vanishing of the restoring force. Again, sketch n, κ and R as functions of ω, and fill in the following table.

Light frequency ω	Reflection (strong/weak)	Absorption (strong/weak)	Net effect (transmissive/absorptive/reflective)
$[0, \gamma)$			
$[\gamma, \omega_p)$			
$[\omega_p, +\infty)$			

For metals like copper or silver, typically the electron density is $N = 10^{23}\,\text{cm}^{-3}$. Estimate the plasma frequency ω_p. What should these metals look like under visible lights? Compare your results with the following experimental results in Figure 1.

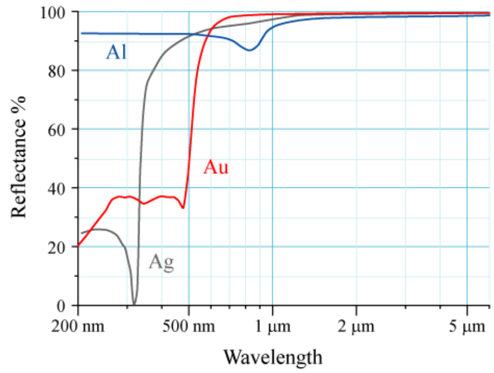


Figure 1: Reflection coefficient R of aluminum, gold and silver metal mirrors at normal incidence.

(c) In Problem Set 1 we derived the electric permittivity $\tilde{\varepsilon}$ for Drude theory. Compare the results above with those of Drude theory. What is scattering time τ in Drude theory now in the phenomenological model? In Problem Set 1, we solved the Maxwell's equations with a free current:

$$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t}, \tag{8}$$

by assuming Ohm's law $\mathbf{J}_f(\omega) = \sigma(\omega)\mathbf{E}(\omega)$. However, in Eq. (5) we assume there is no free current. Why can we obtain the same result from two totally different models? How do you reconcile this paradox?

(d) In the plasma, the electrons are so far away from the nuclei so that there is even no internal collision. In this case, $\omega_0 = \gamma = 0$. What is the optical property of plasmas?

Ionosphere, from about 60 km to 1,000 km altitude, are composed of plasmas ionized from air molecules by the ultraviolet sun light. The typical electron density in ionosphere is $N = 10^{12}\ \mathrm{m}^{-3}$. Estimate the plasma frequency ω_p. If we want to communicate with a satellite in space by radio wave, what frequency range would you suggest? If we want to communicate with a radio station beyond the horizon, what frequency range would you suggest?

(e) What do you think is wrong about this phenomenological model? You can think of it either based on theory assumptions or based on real life experiences that are not consistent with the results you obtained above. It is even better you also think up a way to remedy the problem you just raised.

(This is an open problem and it is fine you do not answer it.)