Guía de Trabajos Prácticos Nro. 1(Jueves, Mayo 16)

1. The usual argument as to why the sky is blue involves scattering by a *single* atom: If the atoms are randomly located, then the total intensity in a given direction is the sum of the intensities scattered by each atom, that is, it is proportional to the number of atoms. Short wavelengths are favored because elastic (or Rayleigh)scattering is proportional to ω^4. However, this argument does not explain why scattering is not important in solids, which have a much larger density of scattering centers than for a gas, or why scattering is so much bigger for clouds (that's why we see them). To gain some insight into these questions, you are asked to calculate (numerically or analytically) the scattering intensity for a random distribution of scattering centers:

   (a) Consider a two-dimensional square lattice of parameter a_0. Using your favorite software, calculate the scattering intensity

   $$I(\mathbf{K}) = \left| \sum_{j=1}^{n} e^{i\mathbf{K}.\mathbf{d}_j} \right|^2$$

   as a function of $\mathbf{K}$ and n/N. Here n is the number of atoms, which are randomly distributed,N is the number of lattice sites and $\mathbf{d}_j$is the position of the jth atom.Consider wavevectors such that$|\mathbf{K}a_0| << 1$. How does $I(\mathbf{K})$depend on the magnitude and the direction of $\mathbf{K}$?

   (b) Show that the behavior of $I(\mathbf{K})$at long wavelengths in the high density limit, that is, $(N-n) << N$ is similar to that for $n << N$.

2. Divide the n atoms into square sets of $m\times m$ atoms ("drops"). Recalculate the scattering intensity for a random distribution of sets. Show that the scattering increases enormously when $\lambda \sim ma_0$. This is roughly what happens in clouds and milk.

Guía de Trabajos Prácticos Nro. 2(Martes, Mayo 21)

1. (a) Derive the Kramers-Krőnig relations using that

$$\int_0^\infty [\varepsilon_1(\omega)-1]\cos(\omega t)d\omega = \int_0^\infty \varepsilon_2(\omega)\sin(\omega t)d\omega$$

(b) If you had a course on complex variables, do the same using the analytical properties of the permittivity (dielectric constant) and Cauchy's theorem.

2. Explain in your own words why the imaginary parts of the permittivity, $\varepsilon_2(\omega)$ and the permeability, $\mu_2(\omega)$, are always positive. Hint: Using that

$$-\nabla.\mathbf{S} = \frac{1}{4\pi}\left(\mathbf{E}\cdot\frac{\partial \mathbf{D}}{\partial t} + \mathbf{H}\cdot\frac{\partial \mathbf{B}}{\partial t}\right)$$

where $\mathbf{S} = c\mathbf{E}\times\mathbf{H}/4\pi$ is the Poynting vector, show that the rate of heat dissipation per unit volume is $Q \equiv \omega\left(\varepsilon_2|\mathbf{E}|^2 + \mu_2|\mathbf{H}|^2\right)/8\pi$. The answer can be found in Landau and Lifshitz, *Electrodynamics of Continuous Media*(Section 80).

3. Show that in the absence of dissipation, that is, if $\varepsilon_2 = 0$, $\partial\varepsilon_1/\partial\omega > 0$. If, instead, $\varepsilon_2 \neq 0$, one can have *anomalous* dispersion, that is, $\partial\varepsilon_1/\partial\omega < 0$. Discuss these results in the context of the Lorentz model.

4. Single interface: Calculate the amplitude of the reflected electric and magnetic field for a plane wave impinging at an arbitrary angle of incidence.Discuss positive ($\varepsilon > 0$ and $\mu > 0$) and negative ($\varepsilon < 0$ and $\mu < 0$) refraction for a monochromatic field and for a wavepacket.

5. Graph the refractive index and the normal-incidence reflectivity as a function of frequency for a metal described by Drude's formula:

$$\sigma = \frac{Ne^2}{m(\gamma - i\omega)}$$

6. (a) Calculate transmission through a slab of thickness *d*and permittivity ε for an arbitrary angle of incidence(you should compare your results with the expressions given in Born and Wolf, *Principles of Optics*).(b) Use Drude formula to show that there is an absorption peak at the plasmon frequency for *p*- but not for *s*-polarized light.

Guía de Trabajos Prácticos Nro. 3(Jueves, Mayo 23)

1. Show (calculate the corresponding integral) that the behavior of the joint density of states near a two-dimensional Van Hove singularity of type M_1 is of the form $\ln|E_0\text{-}E|$.

2. Use the Kramers-Krőnig relations to obtain an expression for the real part of the permittivity in the vicinity of a three dimensional Van Hove singularity of type $M_0$for which $\varepsilon_2 \propto (E - E_0)^{1/2}$.

3. Using $\mathbf{k.p}$theory, one can show for a *non-degenerate* band that

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{mk^2} \sum_{n \neq 0} \frac{\left|\langle u_0 | \mathbf{k}.\hat{\mathbf{p}} | u_n \rangle\right|^2}{E_0 - E_n}$$

Here, m* is the effective mass of the non-degenerate band, m is the free electron mass, $\hat{\mathbf{p}} \equiv -i\hbar\vec{\nabla}$ is the momentum operator, and $\mathbf{k}$ is the Bloch wavevector. $u_n(\mathbf{r})$ is the solution to Schrődinger's equation of eigenenergy$E_n$at $\mathbf{k} = 0$; $E_0$and $u_0(\mathbf{r})$are the eigenenergy and eigenfunction of the non-degenerate band at $\mathbf{k} = 0$.

(a) Using measured values of the fundamental gap and the conduction effective mass **from the literature**, show that $P^2 = |\langle u_c | \hat{\mathbf{p}} | u_v \rangle|^2$ is approximately constant for III−V and II−VI semiconductors for which the *direct* fundamental gap involves *p*-like bonding and *s*-like anti-bonding states. What is the average value of $P^2/2m$(you should easily find values of the effective mass and gap for 20-30 compounds)?

(b) Do these arguments apply to group-IV silicon? To group-IV germanium?

Guía de Trabajos Prácticos Nro. 4(Martes, Mayo 28)

1. Ignoring spin degrees of freedom, the *p*–like Bloch states at the top of the valence band of a certain semiconductor are:

$$\begin{aligned} |X\rangle &= \sin k_0 x \cos k_0 y \cos k_0 z \\ |Y\rangle &= \cos k_0 x \sin k_0 y \cos k_0 z \\ |Z\rangle &= \cos k_0 x \cos k_0 y \sin k_0 z \end{aligned}$$

wherek_0=2π/a and a is the lattice parameter. These states have all the same energy, that is, with the origin of energy at thetopof the band $H_0|X\rangle = H_0|Y\rangle = H_0|Z\rangle$.

(a) Find the eigenstates and eigenvalues of $H_0 + H_{SO} + H_{Zeeman}$ where the spin-orbit coupling is

$$H_{SO} = \frac{\hbar}{4c^2m^2}(\nabla V \times \hat{\mathbf{p}}).\hat{\boldsymbol{\sigma}}$$

and the Zeeman coupling is

$$H_{Zeeman} = g^* \mu_0 \mathbf{B}.\hat{\boldsymbol{\sigma}} \qquad \left(\mu_0 = \frac{e\hbar}{2mc}\right)$$

V is the lattice potential, $\mathbf{B}$ is an external magnetic field, g^* is the band gyromagnetic factor, and $\hat{\sigma}$ is the electron spin operator. Assume that the spin-orbit splitting is much larger than the Zeeman energy (treat H_{Zeeman} as a perturbation).

(a) Considering a single *s*-like state at the bottom of the conduction band, discuss optical selection rules for valence-to-conduction band transitions.

(b) Show that this problem can be mapped exactly to that of atomic *p*–states.

(c) The behavior of the set of valence states under inversion, $\pi/2$-rotations and reflections is identical to that of the set (x,y,z), that is, *p*- states behave like a vector. Discuss how the problem would have been different if we would have chosen a different set of Bloch states with the same symmetry properties.

2. For a uniaxial stress of magnitude $\mathcal{F}$, parallel to the [001] axis, the pseudo-Hamiltonian describing the effect of strain on the valence band edge at $\mathbf{k} = 0$ for diamond or zinc-blende semiconductors can be written as

$$H_{\mathrm{STRAIN}} = -A_{\mathrm{v}}\left(\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz}\right) - eB_{\mathrm{v}}\left[\left(L_x^2-\mathbf{L}^2/3\right)\varepsilon_{xx}+\left(L_y^2-\mathbf{L}^2/3\right)\varepsilon_{yy}+\left(L_z^2-\mathbf{L}^2/3\right)\varepsilon_{zz}\right]$$

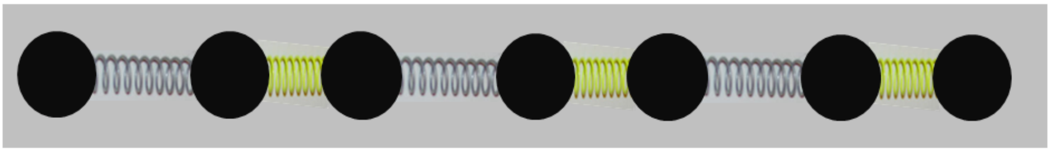
where ε_{ij} is the strain tensor, $\mathbf{L}$ is an effective angular-momentum operator and A_v and B_v are deformation potential constants. Using that the strain components are

$$\varepsilon_{zz} = S_{11}\mathcal{F}$$
$$\varepsilon_{xx} = \varepsilon_{yy} = S_{12}\mathcal{F}$$

show that the combination of stress and spin-orbit coupling completely lifts the orbital degeneracy of the valence band; S_{11} and S_{12} are elastic compliance constants. Discuss optical selection rules for valence-to-conduction transitions. **Note: The effect of uniaxial stress is very similar to that of quantum confinement. These results apply in particular to GaAs quantum wells.**

Guía de Trabajos Prácticos Nro. 5(Jueves, Mayo 30)

1. Consider the dimerized linear chain shown in the figure. The two atoms in the unit cell are the same, of mass equal to *M*, but the spring constant between nearest neighbors takes two values, k_1 and k_2.



   (a) Obtain analytical expressions for the phonon dispersion and plot Ω vs. q where q is the Bloch wavevector.

   (b) Calculate numerically the phonon density of states for the acoustic and optical branches.

   (c) Assuming that the optical mode has a non-zero Szigeti charge, sketch the absorption coefficient considering one-phonon and two-phonon overtone processes.

2. Consider a tetragonal (uniaxial) crystal which possesses two IR-active optical modes, one doubly degenerate -- call it *E*-- and another one that is singly degenerate -- call it *A*. The *E*-mode carries dipole moments oriented along *x* and *y*, while the atomic displacements for the *A*–mode are along the *z*-axis.

   (a) Show that the dielectric constants along the principal axes can be written as

$$\frac{\varepsilon_z}{\varepsilon_\infty} = \frac{\Omega^2_{\mathrm{ALO}} - \Omega^2}{\Omega^2_{\mathrm{ATO}} - \Omega^2}$$

$$\frac{\varepsilon_x}{\varepsilon_\infty} = \frac{\varepsilon_y}{\varepsilon_\infty} = \frac{\Omega^2_{\mathrm{ELO}} - \Omega^2}{\Omega^2_{\mathrm{ETO}} - \Omega^2}$$

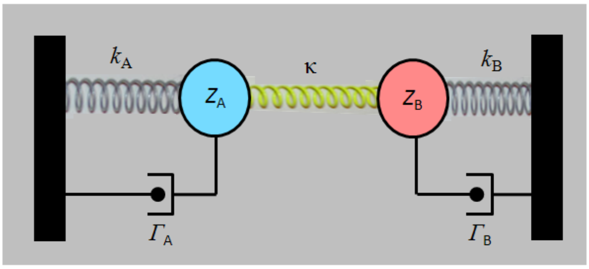
   (b) Plot the transverse and longitudinal solutions for Bloch wavevector $\mathbf{q}$ parallel to the *x*-axis and parallel to the *z*-axis.

   (c) Show that the dependence of the wavevector on the angle θ which $\mathbf{q}$ makes with the optical axis (the *z*–axis) is given by

$$\frac{\Omega^2}{q^2c^2}=\frac{\sin^2\theta}{\varepsilon_z(\Omega)}+\frac{\cos^2\theta}{\varepsilon_{x,y}(\Omega)}$$

Plot Ω vs. θ for $q\to\infty$. Discuss the significance of these results .

3. Consider two coupled oscillators *A* and *B*as in the figure. Γ and *k*represent the corresponding damping (dashpots) and restoring forces. The coupling energy is $U_C=\kappa(u_A-u_B)^2/2$ where, u_A and u_B are the corresponding displacements.



(a) Calculate the polarization $P=Z_Au_A+Z_Bu_B$ induced by an electric field of frequency ω and magnitude E. Find the real and imaginary part of the permittivity.

(b) By performing a linear unitary transformation, of the form

$$\begin{pmatrix}w_A\\w_B\end{pmatrix}=\begin{pmatrix}\cos\theta & \sin\theta\\-\sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}u_A\\u_B\end{pmatrix}\qquad \cot^2\theta+(k_A-k_B)\cot\theta/\kappa=1$$

show that the problem is equivalent to that of two coupled oscillators with interaction damping (*i.e.*, the spring of constant κ is replaced by a dashpot).

(c) If the two oscillators are oppositely charged, show that the imaginary part of the permittivity(the losses) *must* exhibit a minimum at a frequency intermediate between the two resonant frequencies. This effect is related in some sense to EIT (electromagnetically-induced transparency).

(d) Repeat for the case where one of the oscillators is strongly overdamped and the other one has no damping. This is the classical analog of Fano interference between a discrete level and the continuum in atomic systems.

Guía de Trabajos Prácticos Nro. 6(Martes, Junio 4)

1. *Rutherford Problem:* The effective-mass Hamiltonian describing a parabolic-band Wannier exciton is:

$$H = -\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{\hbar^2}{2m_h}\nabla_h^2 - \frac{e^2}{\varepsilon r}$$

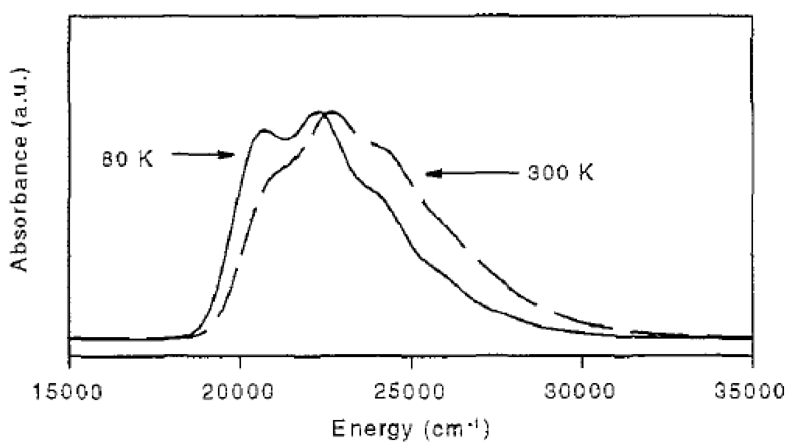
Where m_e and m_h are the effective masses of the electron and the hole, ε is the lattice permittivity and *r* is the relative electron-hole coordinate. Using this Hamiltonian, show that

$$|\phi|^2_{r=0} = \frac{\pi\alpha e^{\pi\alpha}}{V_C \sinh(\pi\alpha)} \quad ; \qquad \alpha^2 = \frac{m^* e^4}{2\hbar^2\varepsilon^2}\frac{1}{E} \quad .$$

Here $\phi(\mathbf{r})$ is the solution of Schrődinger's equation for the unbound (*scattering*) state of energy $E > 0$ and $m^* = m_e m_h/(m_e + m_h)$. Use this result to explain the fact that absorption near a band edge of type $M_0$is significantly larger than what one would expect for interband transitions in the absence of Coulomb interaction.**Hint:** The solution is given in some QM textbooks.

2. Using values of the relevant parametersfrom the literature, plot the exciton-polariton transverse and longitudinal branches for GaAs. Consider only the 1*s* state.

3. The figure shows the absorption spectrum of poly (p-phenylene vinylene) at two temperatures. The features in the data can be interpreted as due to a Frenkel exciton and its phonon sidebands (the phonon frequency is ~ 1700 cm^{-1}). Find the best fit to the experimental data using the Huang-Rhys model.



Guía de Trabajos Prácticos Nro. 7(Jueves, Junio 6)

1. What is wrong with the following argument?

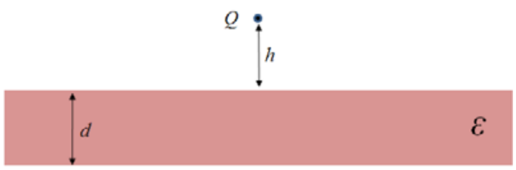
> "At large wavelengths, the permittivity of a metal is $\varepsilon(k) \approx 1 + k_0^2/k^2$ where k_0 is the Thomas-Fermi screening wavevector. Since $\varepsilon(k)$ does not vanish, there are no plasmons."

2. If one ignores retardation (*i.e.*, in the limit $c \to \infty$), plasmon frequencies are gained by solving Poisson's equation. Hence, they are purely *electrostatic* modes. Are there plasmons described by *magnetostatic* expressions? If not, why not?

3. Calculate the dispersion (ω vs. $\mathbf{q}$) of surface plasmons associated with infrared-active phonons. The permittivity is given by

$$\varepsilon = \varepsilon_\infty \frac{\omega_{LO}^2 - \omega^2}{\omega_{TO}^2 - \omega^2} \quad .$$

4. Find the electromagnetic resonances of a slab of thickness d and permittivity ε. Distinguish plasmons from waveguide modes. Repeat for the electrostatic approximation (plasmons only). Find the electric field due to a point charge Q at a distance h from one of the slab surfaces, as in the figure. Show that the field diverges when $\varepsilon = -1$.



5. Find the electromagnetic resonances of a spherical shell of permittivity ε with the parameters shown in the figure. Distinguish plasmons from waveguide modes. Repeat for the electrostatic approximation (plasmons only). Find the electric field due to a point charge at a the center of the sphere. Discuss divergences (if any).