Solid State Spectroscopy – Problem Set 6

Due date: June 15th, 2015

Problem 5.1 Brillouin Scattering

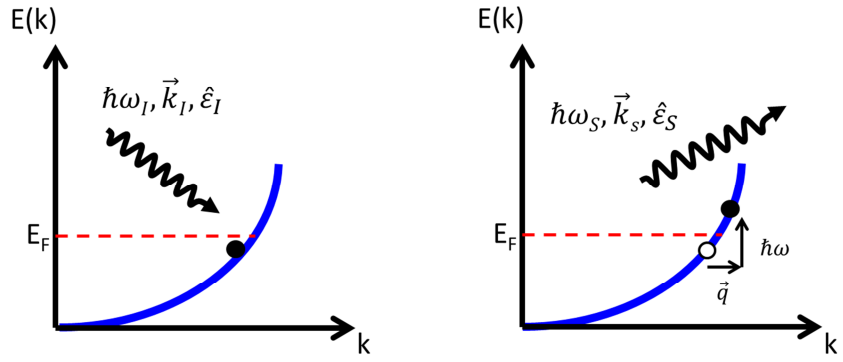
In contrast to reflection spectroscopy, inelastic light scattering allows the observation of acoustic phonons, whose dispersion relation at low frequencies can be written as $\omega_s = c_s q$. Show that the scattering angle θ (that is, the angle between the wave vectors of incident and scattered photons) is given by

$$\omega_s = \frac{\omega_i c_s}{c}\sqrt{\left(n_i - n_f\right)^2 + 4n_i n_f sin^2\left(\frac{\theta}{2}\right)}$$

where ω_i is the incident photon frequency, c is the velocity of light, n_i and n_f are the refractive indices of the medium at the incoming and outgoing photon frequencies. (Remember that $c_s << c$.)

Problem 5.2 Electronic Raman Scattering

In class we have studied the inelastic scattering of light by lattice vibrations.
In metals or semi-conductors, light can also be inelasticity scattered by free charge carriers.



a) Evaluate the energy up to which can scattering from free carriers be expected (linearize the electronic dispersion close to the Fermi level). Numerical estimate: what would be that energy in a semi-conductor with carrier concentration $n=10^{18}$ cm^{-3}, if the excitation is performed with a green laser.

b) Draw the simplest Feynman diagram for electronic Raman scattering

c) Consider the Hamiltonian of free electrons in an electro-magnetic field ($\boldsymbol{p} \rightarrow \boldsymbol{p} - e\boldsymbol{A}$) and apply perturbation theory to express the transition rate. Which term should be considered? to which perturbation order?

d) Electronic Raman scattering probes the dynamics of charges carriers. It can be shown that the electronic Raman response is proportional to a density-density correlation function $\int dt\, e^{i\omega t}\langle\tilde{\rho}(-\boldsymbol{q}, t)\tilde{\rho}(\boldsymbol{q}, 0)\rangle$, in which the usual density operator (in the second

quantization language) $\rho(\boldsymbol{q}) = \sum_{\boldsymbol{k},\sigma} c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma}$ is replaced by an 'effective' density $\tilde{\rho}_{IS}(\boldsymbol{q}) = \sum_{\boldsymbol{k},\sigma} \gamma_{IS}(\boldsymbol{k},\boldsymbol{q}) c^{\dagger}_{\boldsymbol{k}+\boldsymbol{q},\sigma} c_{\boldsymbol{k},\sigma}$.
$\gamma_{IS}(\boldsymbol{k},\boldsymbol{q})$ is known as the Raman vertex, and depends on the incident (I) and scattered (S) light polarizations.

$$\gamma_{IS}(\boldsymbol{k},\boldsymbol{q}) = \hat{\varepsilon_S}.\gamma(\boldsymbol{k},\boldsymbol{q}).\hat{\varepsilon_I} = \sum_{\alpha,\beta} \hat{\varepsilon}_S^{\beta}.\gamma_{\alpha\beta}(\boldsymbol{k},\boldsymbol{q}).\hat{\varepsilon}_I^{\alpha}$$

where indices α and β stand for x,y or z. In the limit where q→0 and away from resonance conditions, $\gamma_{\alpha\beta}$ can simply be expressed from the electronic band structure:

$$\gamma_{\alpha\beta}(\boldsymbol{k}, q \to 0) = \frac{1}{\hbar^2}\frac{\partial^2 E(\boldsymbol{k})}{\partial k_\alpha \partial k_\beta}$$

This expression is known as the effective mass approximation. Why?

The following expression is a good approximation for the electronic dispersion of the CuO_2 plane of superconducting cuprates.

$$E(\boldsymbol{k}) = -2t\big(\cos(k_x a) + \cos\big(k_y a\big)\big) + 4t' \cos(k_x a)\cos\big(k_y a\big) - E_F$$

d1) Sketch $E(\boldsymbol{k})$ along the (1,0) and (1,1) directions of the reciprocal space (use t'=0.4t and E_F=0 for simplicity). Plot the Fermi Surface (Consider first the case where t'=0).

d2) Evaluate $\gamma(\boldsymbol{k}, q \to 0)$ for this band structure in the effective mass approximation.

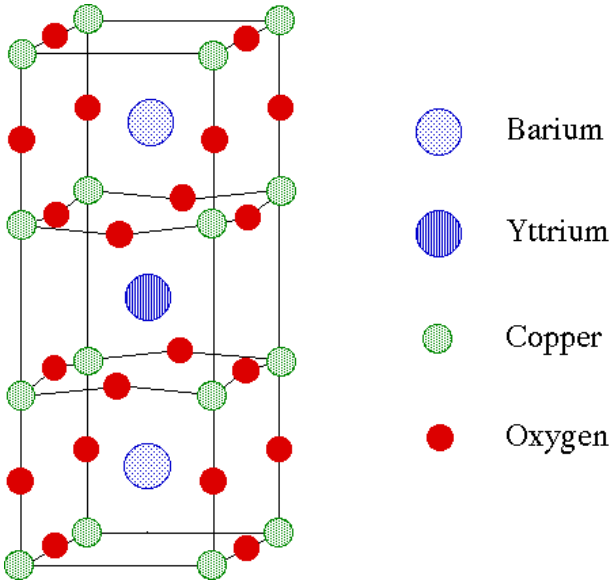
d3) Sketch $|\gamma_{IS}(\boldsymbol{k}, q \to 0)|$ for the following polarization settings and discuss the role of the Raman vertex in an electronic Raman scattering experiment.

$$\hat{\varepsilon_I} = \begin{pmatrix}1\\0\end{pmatrix}, \hat{\varepsilon_S} = \begin{pmatrix}0\\1\end{pmatrix}$$

$$\hat{\varepsilon_I} = \begin{pmatrix}1\\1\end{pmatrix}, \hat{\varepsilon_S} = \begin{pmatrix}1\\-1\end{pmatrix}$$

Problem 5.3 Selection Rules

1) $YBa_2Cu_3O_7$ is a prototypical high temperature superconductor. The unit cell is represented below. How many optical phonons do we expect for this compound? At first glance, which atom will not give any Raman active vibration?



2) YBCO has formally an orthorhombic structure, but given the relatively small amplitude of the orthorhombic distortion (~1%), the Raman tensors are often expressed in the tetragonal notation

$$A_{1g} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{pmatrix}, B_{1g} = \begin{pmatrix} c & 0 & 0 \\ 0 & -c & 0 \\ 0 & 0 & 0 \end{pmatrix}, B_{2g} = \begin{pmatrix} 0 & d & 0 \\ d & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$E_g = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & f \\ 0 & f & 0 \end{pmatrix} and \begin{pmatrix} 0 & 0 & f \\ 0 & 0 & 0 \\ f & 0 & 0 \end{pmatrix}$$

For which polarization settings phonons with the B_{1g} symmetry can be observed? Same question for the A_{1g} phonons.