1. Cyclotron Frequency

If the magnetic field is applied in the z direction, the cyclotron effective mass is defined as:

$$m^* = \left(\frac{det|\bar{\bar{m}}|}{m_{zz}}\right)^{1/2}$$

Where $\bar{\bar{m}}$ is the effective mass tensor defined as $\bar{\bar{m}}_{ij} = \left(\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}\right)^{-1}$.

Calculate the cyclotron frequency for electrons at the Fermi surface in a nearly empty tight-binding band, described by:

$$E = -\left(E_1 cosk_x a + E_2 cosk_y b + E_3 cosk_z c\right),$$

And show that the result indeed corresponds to the cyclotron frequency of free electrons of mass m^*.

2. de Haas-van Alphen effect

a) Show that for the density of states $D(E)$ of the free electron gas in a cubic crystal with edge length L in a magnetic field B the following relation holds:

$$D(E) = \frac{L^3}{(2\pi)^2} \cdot \left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} \cdot (\hbar\omega_c^*) \sum_{n=0}^{n_{max}} \frac{1}{\sqrt{E - \left(n + \frac{1}{2}\right)\hbar\omega_c^*}}$$

$\omega_c^* = \frac{eB}{m^*}$ is the cyclotron frequency and n_{max} is the number of Landau cylinders with states of the energies less than E.

b) For $E_F \gg \hbar\omega_c^*$ (E_F is being the Fermi energy in zero field), show that $D(E_F)$ as a function of $1/B$ has periodic discontinuities.

c) Calculate the period $\Delta(1/B)$, which can be expected for the de Haas-van Alphen effect in Potassium following the free electron model. Note that potassium crystallizes in a body centered cubic unit cell with lattice constant $a = 5.225\,\text{Å}$.

3. Dirac Cone in Graphene and photoemission

Graphene is a two-dimensional material that consists of a monoatomic layer of Carbon atoms arranged in a 2D honeycomb lattice (cf. Pb 2 in tutorial #1). Lattice constant a is 2,4 Å.

It can be shown that the dispersion relation for the $2p_z$-derived band in graphene has the following dispersion relation (E_F is set to 0 here):

$$E_{\mathbf{k}} = \pm t_{pp} \sqrt{1 + 4\cos\left(\frac{3ak_x}{2}\right)\cos\left(\frac{\sqrt{3}ak_y}{2}\right) + 4\cos^2\left(\frac{\sqrt{3}ak_y}{2}\right)}.$$

1) Represent the real space unit cell and first Brillouin zone for Graphene. How does the Fermi surface look like?
2) Show that for wave vector k = k0 + q, where k0 is a corner of the Brillouin zone, (also referred to as K-point) we can write:

$$E_{\mathbf{k}} = \pm t_{pp} \frac{3a}{2}|q|$$

Sketch the dispersion.

3) For a photon energy of 100 eV, evaluate the polar and azimuthal angles θ and ϕ which are needed to determine the wave vectors for 6 different states around one of the K points (use the high symmetry directions) which have a constant binding energy E_B = 1eV (knowing that the Fermi velocity is $8x10^5$ m/s) and that the work function into the spectrometer is $\Phi = 4.5\ eV$.

4. ARPES spectra for interacting electrons

For simplicity we work here in 1D ($\boldsymbol{k} \rightarrow k$). For electrons photo-emitted from a many-body state of energy ε and momentum k, the ARPES intensity is given by :

$I(\varepsilon,k)=I_0 \times A(\varepsilon,k) \times f(\varepsilon,T)$

where I_0 is the "dipole matrix element", that we will consider henceforth constant and equal to 1 (in reality, I_0 can depend on electron momentum and photon energy and polarization!), f(ε,T) is the Fermi-Dirac distribution at temperature T, and A(ε,k) is the many-body spectral function, given by :

$$A(\varepsilon,k) = \frac{1}{\pi}\frac{\Sigma_2(\varepsilon,k)}{[\varepsilon - \varepsilon_0(k) - \Sigma_1(\varepsilon,k)]^2 + \Sigma_2(\varepsilon,k)^2}$$

Where $\varepsilon_0(k)$ is the bare electron dispersion (i.e. Bloch band of a free independent electron in the ionic periodic lattice) and $\Sigma_1(\varepsilon, k)$ and $\Sigma_2(\varepsilon, k)$ are the real and imaginary parts of the electron self-energy which contain all the information regarding the electron´s interactions. $\Sigma_1(\varepsilon, k)$ and $\Sigma_2(\varepsilon, k)$ are

Hilbert transforms of each other. We assume that the carriers are electrons, and their density is small, so that $\varepsilon_0(k) \approx -E_0 + (\hbar^2/2m_e)k^2$ (i.e., the periodic variation of the energy is neglected), with $(-E_0) < 0$ the energy of the bottom of the band. Additionally, we assume that the self- energy is k-independent: $\Sigma(\varepsilon, k) = \Sigma(\varepsilon)$.

1) The imaginary part of the self-energy corresponds to the scattering rate of the electrons. Assume this scattering rate is constant (e.g. case of impurity scattering): $\Sigma_2(\varepsilon) = \Gamma_0$. Represent $A(\varepsilon)$. How does it look like in the $\Gamma_0 \to 0$ limit?
2) The interaction of an electron with a single phonon (Einstein mode) at energy $\hbar\Omega_0 > 0$ is characterized by

$$\Sigma_2{}^{EP}(\varepsilon) = \begin{cases} 0 \; if \; -\hbar\Omega_0 < \varepsilon < \hbar\Omega_0 \\ \dfrac{\pi}{2} g\hbar\Omega_0 \; otherwise \end{cases}$$

Where g is a dimensionless electron-phonon coupling constant. The total imaginary part is now: $\Sigma_2(\varepsilon) = \Gamma_0 + \Sigma_2{}^{EP}(\varepsilon)$. Calculate $\Sigma_1(\varepsilon)$. Use your favorite plotting software to represent $A(\varepsilon)$ using realistic energy scales: $\Gamma_0 = 0{,}02\ eV$, $\hbar\Omega_0 = 5\ meV$, g =1. Plot I(ε) for 10K and 300K.

3) Bonus: For a 3D Fermi liquid of band-bottom $-E_0$ (hence "Fermi energy E_0"), the imaginary part of the self-energy is:

$$\Sigma_2{}^{FL}(\varepsilon) = A\frac{\varepsilon^2 + (\pi k_B T)^2}{1 + e^{-\varepsilon/k_B T}}$$

Set A to 1, evaluate numerically $\Sigma_1{}^{FL}(\varepsilon)$ and plot I(ε) for different temperatures.