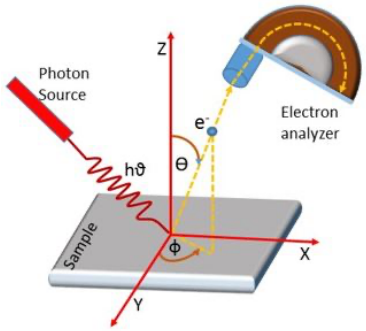
12. Dirac Cone in Graphene and photoemission

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):

$$E(k_x, k_y) = \pm t_{pp} \sqrt{1 + 4cos\left(\frac{3ak_x}{2}\right) cos\left(\frac{\sqrt{3}ak_y}{2}\right) + 4cos^2\left(\frac{\sqrt{3}ak_y}{2}\right)}$$

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 $k = k_0 + q$, where k_0 is a corner of the Brillouin zone, (also referred to as K-point) we can write: $E(k_x, k_y) = \pm t_{pp} \frac{3a}{2} |q|$. Sketch the dispersion.
3) For a photon energy of 100 eV, evaluate the polar and azimuthal angles θ and ϕ (see figure below) 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 8×10^5 m/s) and that the work function into the spectrometer is $\Phi = 4.5\ eV$.



13. ARPES spectra for interacting electrons

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

$$I(E, k) = I_0 \times \mathrm{A(E, k)} \times \mathrm{f(E, T)}$$

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

$$A(E,k) = \frac{1}{\pi}\frac{\Sigma_2(E,k)}{[E - E_0(k) - \Sigma_1(E,k)]^2 + \Sigma_2(E,k)^2}$$

where $E(k)$ is the bare electron dispersion (i.e. Bloch wave of independent electron in the ionic periodic lattice) and $\Sigma_1(E,k)$ and $\Sigma_2(E,k)$ are the real and imaginary parts of the electron self-energy which contain all the information regarding the electron´s interactions. $\Sigma_1(E,k)$ and $\Sigma_2(E,k)$ are Hilbert transforms of each other. We assume that the carriers are electrons, and their density is small, so that $E_0(k) \sim -E_0 + \frac{\hbar^2 k^2}{2m}$ (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: $\Sigma(E, k) = \Sigma(E)$.

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): $\Sigma_2(E) = \Gamma_0$. Represent $A(E)$. 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

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

Where g is a dimensionless electron-phonon coupling constant. The total imaginary part is now: $\Sigma_2(E) = \Gamma_0 + \Sigma_2{}^{EP}(E)$. Calculate $\Sigma_1(E)$. Use your favorite plotting software to represent $A(E)$ using realistic energy scales: $\Gamma_0 = 0.02\ eV$, $\hbar\Omega_0 = 5\ meV$, g =1. Plot I(E) 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:

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

Set A to 1, evaluate numerically $\Sigma_1{}^{FL}(E)$ and plot I(E) for a few temperatures.

14. Arrott-plot Method

Landau theory of a ferromagnet in a magnetic field B states that the free energy is given by

$$F(M) = F_0 + a(T - T_c)M^2 + bM^4 - MB$$

Where a and b positive constants.

a) Show that we can write $M^2 = u + v\frac{B}{M}$, where u and v are constants.

b) Explain how this can be used to determine the critical temperature T_c by plotting M^2 vs $\frac{B}{M}$ for temperature above, below and right at T_c. This method is known as the Arrott-plot method.

c) A ferromagnetic transition has been detected in the heavy-electron compound URu2Si2 doped with Re or Tc. Use the Arrott-plot method to determine the transition temperature T_c based on the data shown in the figure below (taken from Phys. Rev. B 39, 2423 (1989)) for two of these compounds.

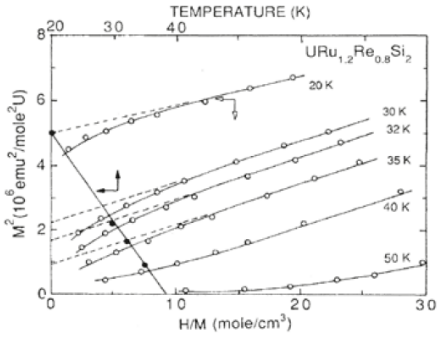


FIG. 4. Isotherms of M^2 vs H/M, where M is the magnetization and H is the applied magnetic field, for $URu_{1.2}Re_{0.8}Si_2$ for $20\ K \leq T \leq 50\ K$. Zero-field values of M^2, obtained by linear extrapolation of the high-field M^2 vs H/M data to $H=0$ (dashed lines), are plotted vs T. The Curie temperature Θ_C is defined as the temperature corresponding to $M^2=0$. Solid lines are guides to the eye.

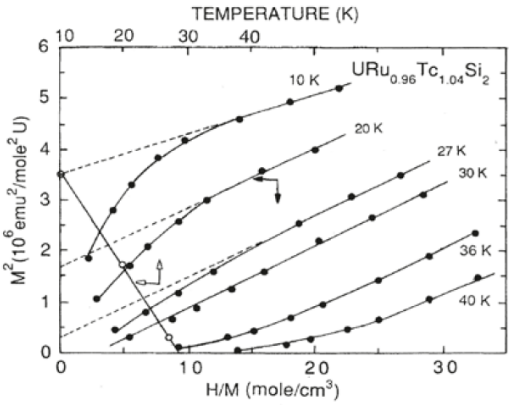


FIG. 5. Isotherms of M^2 vs H/M, where M is the magnetization and H is the applied magnetic field, for $URu_{0.96}Tc_{1.04}Si_2$ for $10\ K \leq T \leq 40\ K$. Zero-field values of M^2, obtained by linear extrapolation of the high-field M^2 vs H/M data to $H=0$ (dashed lines), are plotted vs T. The Curie temperature Θ_C is defined as the temperature corresponding to $M^2=0$. Solid lines are guides to the eye.