Physics 481: Condensed Matter Physics - Practice Exam

Problem 1: Fermi pancakes

Consider a thin layer of copper, 1 mm wide and 1 mm long along x and y. The layer is a few Å thick in z-direction. Treat the layer as a free electron gas, demanding the the wavefunction vanishes at the boundaries along the z direction (periodic boundary conditions in x and y directions). The electron density for copper is 8.49×10^{22} electrons/cm^3.

a) Solve the single-particle Schrödinger equation for the given geometry and write down the resulting single-particle wave functions as well as the energy eigenvalues. Specify the values that the quantum numbers can take.

b) Find the maximum thickness a of the layer for which only the perpendicular (z direction) ground state is occupied at zero temperature.

c) Calculate the Fermi wavevector in the $k_x - k_y$ plane for this thickness.

Problem 2: Hcp extinctions

a) The hexagonal Bravais lattice can be defined by the primitive vectors $(a, 0, 0), (a/2, a\sqrt{3}/2, 0)$ and $(0, 0, c)$. Prove that the reciprocal lattice is another hexagonal lattice rotated by 30° with respect to the original one and find primitive vectors for the reciprocal lattice.

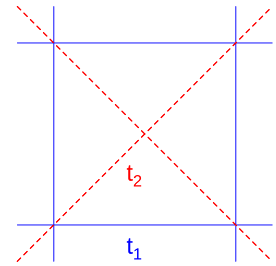
b) The hcp lattice is built upon the hexagonal Bravais lattice with basis $(0, 0, 0)$ and $(a/2, a/(2\sqrt{3}), c/2)$. Show that the modulation factor induced by the basis is

$$F_{\vec{q}} = \left|1 + e^{i(\pi/3)[2(n_1+n_2)+3n_3]}\right|^2$$

where n_1, n_2, n_3 are the coefficients of the momentum transfer in terms of the reciprocal primitive vectors.

c) Find all Bragg peaks of the hexagonal lattice for which scattering from the hcp lattice vanishes by extinction. Specifying the condition for the indices is sufficient.

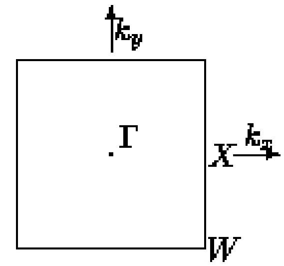
Problem 3: 2D tight-binding model



Consider a generalized tight-binding Hamiltonian on an (infinite) square lattice:

$$H = U \sum_{\mathbf{r}} |\mathbf{r}\rangle\langle\mathbf{r}| + t_1 \sum_{\langle \mathbf{r},\mathbf{r}'\rangle} \left(|\mathbf{r}\rangle\langle\mathbf{r}'| + |\mathbf{r}'\rangle\langle\mathbf{r}|\right) + t_2 \sum_{[\mathbf{r},\mathbf{r}']} \left(|\mathbf{r}\rangle\langle\mathbf{r}'| + |\mathbf{r}'\rangle\langle\mathbf{r}|\right)$$

where the second sum is over nearest-neighbor pairs and the third sum is over next-nearest neighbor pairs (along the diagonals of each square).



a) Find the energy eigenvalues $\epsilon(\mathbf{k})$ of this Hamiltonian, i.e., the band structure.

b) Sketch the band structure along the $\Gamma - X$ line for $U = 0$, $t_1 = t_2 = 1$.

c) Calculate the off-diagonal component $(M^{-1})_{xy}$ of the effective mass tensor.

d) Calculate the Fermi energy for two electrons per lattice site.

Problem 4: van-Hove singularities for phonons

a) In the linear harmonic chain with only nearest-neighbor interactions, the normal mode dispersion relation has the form $\omega(q) = \sqrt{4K/M}\,|\sin(qa/2)|$. Calculate the phonon density of states $D(\omega)$ and show that it takes the form

$$D(\omega) = \frac{2}{\pi a \sqrt{\omega_0^2 - \omega^2}}$$

where ω_0 is the maximum frequency (assumed when q is at the Brillouin zone boundary).

b) Discuss the singularity at $\omega = \omega_0$ (the van-Hove singularity) by expanding ω about this point.

c) Now consider phonons in three dimensions. Assume $\omega(\mathbf{q})$ has a simple quadratic maximum of ω_0 at $\mathbf{q}_0$. Show that the neighborhood of this maximum contributes a term to $D(\omega)$ that varies as $(\omega_0 - \omega)^{1/2}$.