

1. Nearly free electrons part 1

- a) Consider a two-dimensional square lattice of lattice constant
- a
- and take

$$U(\vec{r}) = -4U_0 \cos \frac{2\pi x}{a} \cos \frac{2\pi y}{a}.$$

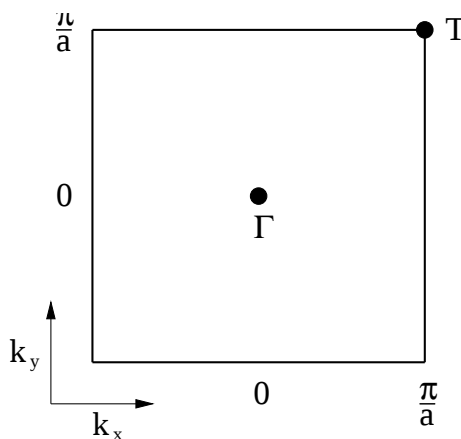
Find the Fourier transform $U_{\vec{q}}$.

- b) For $\vec{k}_1 = (\pi/a, \pi/a)$, $c_{\vec{k}_1}$ will couple strongly to three other components of ψ , $c_{\vec{k}_2} \dots c_{\vec{k}_4}$. What are $\vec{k}_2 \dots \vec{k}_4$? Identify the values of $\vec{K}$ that one must include when doing perturbation theory to find $c_{\vec{k}_1} \dots c_{\vec{k}_4}$ to first order in U_0 .
- c) Evaluate $U_{\vec{K}}$ for the necessary values of $\vec{K}$. Show that $U_{\vec{K}} = U_{-\vec{K}}$ is nonzero only for one value of $\vec{K}$. Therefore perturbation theory can be reduced to the subspace involving only $c_{\vec{k}_1}$ and, say, $c_{\vec{k}_2}$.

2. Nearly free electrons part 2

Continue analysing the previous problem.

- d) Write down Schrödinger's equation in the subspace involving only $c_{\vec{k}_1}$ and $c_{\vec{k}_2}$.
- e) Solve the resulting 2×2 system of equations and find the two allowed energies at Bloch index $\vec{k}_1$.



- f) Sketch $\mathcal{E}_{\vec{k}}$ for the lowest two bands along the line Γ -T, and indicate the size of the energy gap.

3. **Nearly free electron Fermi surface near a single Bragg plane**

To investigate the band structure close to a Bragg plane, it is convenient to measure the wave vector $\vec{k}$ with respect to the point $-\frac{1}{2}\vec{K}$ on the Bragg plane. Writing $\vec{k} = -\frac{1}{2}\vec{K} + \vec{q}$ and resolving $\vec{q}$ into its components parallel ($q_{\parallel}$) and perpendicular ($q_{\perp}$) to $-\vec{K}$, the effect of the weak periodic potential on the energies of the two free electron levels is

$$\mathcal{E} = \mathcal{E}_{\frac{1}{2}\vec{K}}^0 + \frac{\hbar^2}{2m}q^2 \pm \sqrt{4\mathcal{E}_{\frac{1}{2}\vec{K}}^0 \frac{\hbar^2}{2m}q_{\parallel}^2 + |U_{\vec{K}}|^2}.$$

It is also convenient to measure $\mathcal{E}_F$ with respect to the lowest value assumed by either of the bands in the Bragg plane, writing

$$\mathcal{E}_F = \mathcal{E}_{\frac{1}{2}\vec{K}}^0 - |U_{\vec{K}}| + \Delta,$$

so that when $\Delta < 0$, no Fermi surface intersects the Bragg plane.

- a) Let $0 < \Delta < 2|U_{\vec{K}}|$. Show that the Fermi surface lies entirely in the lower band and intersects the Bragg plane in a circle of radius $\sqrt{2m\Delta/\hbar^2}$.
- b) How do the Fermi surface and Bragg plane intersect when $\Delta > 2|U_{\vec{K}}|$?

4. **Reciprocal lattice and Brillouin zones**

- a) Consider a two-dimensional lattice with primitive vectors $a(1, 0)$ and $a(\frac{1}{2}, 1)$. Find the primitive vectors for the reciprocal lattice, and draw a picture of the first and second Brillouin zones.
- b) Find the areas of the first and second Brillouin zones.
- c) With 2 noninteracting electrons per site and a weak potential U , visualize the Fermi surface of the system.