Theory of Quantum Matter

Lecturer: Prof. Otfried Gühne (Mon 14:00, Fri 10:00, Room D120)
Exercises: Chau Nguyen (Fri 14:00, Room B030) **Sheet 6**

Hand in: Mon 26.11.2018 *(questions marked as ∗ are optional)*
Discussion date: Fri 30.11.2018

9. Effective mass and the density of state of electrons

(a) (5pts) Compute the effective mass for the 1D tight-binding model with the energy band given by $E(q) = -2t\cos(qd)$, where t is the hopping energy.

(b) (5pts) Compute the density of states for the 1D tight-binding model above. Where is the Fermi energy at half-filling?

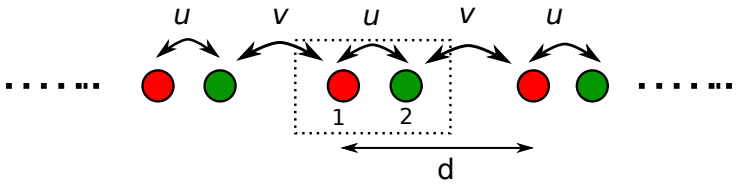
(c) (∗) Taking the tight-binding band structure for the triangular lattice in Problem 8b, compute the effective mass m^* for the electron at the bottom of the band.

Hint: Note that the lattice is highly symmetric, thus the effective mass is a scalar (not a tensor). You can exploit this fact in your calculation (proving is encouraged, but not required).

(d) (5pts) For low energy excitations, the band can be considered to be quadratic, $E(\vec{q}) \approx E_0 + \frac{\hbar^2 q^2}{2m^*}$. Compute the density of states of the electron in this quadratic approximation.

10. The topological insulating phases of the Su–Schrieffer–Heeger model

In this problem, we will formulate the tight-binding approximation when we have two atoms per unit cell. Consider a 1D chain of two sites per unit cell and periodicity d (see figure below).



Let $|m, \alpha\rangle$ denote the local state of electron at atom $\alpha = 1, 2$ in cell m (in the notation of the previous problems and lectures, this would be denoted by $|\phi_{m\alpha}\rangle$). The tight-binding ansatz assumes that the wavefunction of an electron in the chain is given by

$$|\psi\rangle = \sum_{m,\alpha} C_{m,\alpha} |m, \alpha\rangle . \tag{1}$$

For simplicity, we also assume that the local states are orthogonal, i.e., $\langle m, \alpha | n, \beta\rangle = \delta_{mn}\delta_{\alpha\beta}$ (orthogonality approximation). This is to say, *the localised states* $|m, \alpha\rangle$ *form an orthonormal basis to expand the state.* Also, we consider only nearest neighbour hoppings, which are of two types: $\langle n, 2| H |n, 1\rangle = \langle n, 1| H |n, 2\rangle = -u$ and $\langle n + 1, 1| H |n, 2\rangle = \langle n, 2| H |n + 1, 1\rangle = -v$ with $u, v > 0$; other further matrix elements are considered to be 0. We are to solve the Schrödinger equation $H |\psi\rangle = E |\psi\rangle$, which, in the local state basis is

$$\sum_{n\beta} H_{m\alpha,n\beta} C_{n\beta} = E C_{m\alpha}. \tag{2}$$

Now you can recall that this resembles exactly the problem of finding the dispersion relation for phonons in the previous lectures, and apply the techniques you have learned there to find the eigenvalues E. In particular, H can be organised as a block matrix with block $H(m,n)$ denoting the 2×2 matrix (elements indexed by α, β) acting between cells m and n. Equation (2) thus can be written as

$$\sum_n H(m,n)C_n = EC_m, \tag{3}$$

where each C_m is a column vector of 2 components, $C_m = (C_{m\alpha}, C_{m\beta})^t$. Recall that the lattice periodicity implies that $H(m,n) = H(m-l, n-l)$ for all l.

(a) (5pts) Show that the Bloch theorem imposes that one can choose $C_n = e^{iqnd}A$, with A being a column vector of 2 components.

Remark: For phonons, we took this as an ansatz. Now we know that it is in fact the implication of the Bloch theorem.

(b) (15pts) Using the ansatz for C_n above to simplify equation (3) to finding the eigenvalues of a 2×2 matrix,

$$K(q)A = E(q)A, \tag{4}$$

where $K(q) = \sum_n H(0,n)e^{iqnd}$. Compute $K(q)$ explicitly for our 1D chain. Diagonalise $K(q)$ to find the eigenvalues $E(q)$ and sketch them in the first Brillouin zone.

(c) (10pts bonus) Now we are very close to it, let us get a glimse of the concept of *topological insulating phases*, which has been a focus of condensed matter theory in recent years. Show that $K(q)$ can be written as

$$K(q) = \vec{d}(q)\cdot\vec{\sigma}, \tag{5}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ and the coefficients $\vec{d}(q) = (d_x(q), d_y(q))$ are for you to determine. Sketch the curve $\vec{d}(q)$ on the plane as q varies across the first Brillouin zone for the cases $u > v$ and $u < v$. A continuous deformation in u and v would deform the plotted curves a bit, but argue from the figure that: if the deformation does not close the energy gap in the band structure, one can not obtain a curve with $u > v$ from a curve with $u < v$. One says that the system has two distinct topological insulating phases.