Karlsruhe Institute of Technology | Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Sheet 4
Tutorial: 23.11.2022

Category A

1. Van Hove singularity on a square lattice ($3 + 5 + 2 + 10 = 20$ points)

(a) Determine the tight-binding hamiltonian of the square lattice where we consider only nearest neighbour hopping, one orbital per atom and isotropic coupling.

(b) Find the band structure (dispersion relation) $\epsilon(\vec{k})$ of this Hamiltonian.

(c) Determine the iso-energy $E = 0$ in the Brillouin zone and plot a sketch of it.

(d) Show that the density of states $\rho(E) = \frac{1}{(2\pi)^2} \int_{1\ B.Z} \mathrm{d}\vec{k}\ \delta(E - \epsilon(\vec{k}))$ at the energy $E = 0$ diverges. What are the points in the Brillouin zone which cause this divergence? Expand the dispersion relation around one of these points and show that the divergence is logarithmic. Compute the group velocity at these peculiar points.

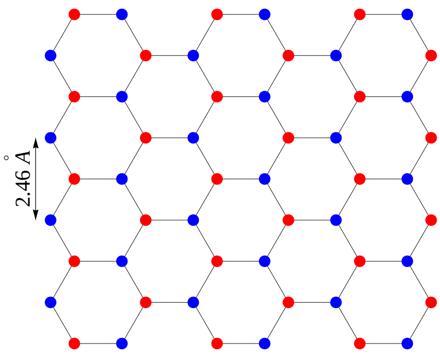
2. Bloch oscillations (10 points)

Consider the semiclassical dynamics of electrons in one one-dimensional lattice in the tight-binding approach (with the nearest neighbors hopping amplitude γ and one state per unit cell). Find the energy spectrum ϵ_k. Then consider the effect of a homogeneous electric field E solving the Bloch's equation of motion, $\frac{d}{dt}k = -eE$. Show that the location of an electron oscillates. Find the period and amplitude of the oscillations. *Hint:* use that the velocity, $v \equiv \frac{dr}{dt}$, satisfies the relation $v = \frac{\partial \epsilon_k}{\partial k}$.

Category B

3. Band structure of graphene ($7 + 8 + 5 = 20$ points)

Graphene is a two-dimensional material consisting of a honeycomb lattice of carbon atoms. We will study some of its fundamental electronic properties within the tight-binding approximation, where we restrict the model to nearest-neighbor hopping and a single orbital per atom with isotropic couplings. The honeycomb lattice is not a Bravais lattice. Note that each unit cell contains two atoms – let us denote them as site A and site B. These are shown in different colors in the sketch (although all atoms are carbon atoms). It turns out that all nearest neighbors of atoms at A-sites are located at B-sites, and vice versa. A lattice with this property is also called a *bipartite* lattice.



(a) Determine the tight-binding Hamiltonian of graphene. Find the Bloch states and express the Hamiltonian in reciprocal space in the basis of the Bloch states.
Hint: You will be able to write the Hamiltonian as a 2×2 *matrix.*

(b) Now use the Hamiltonian which you found in (a) to calculate the band structure. Show that there are special points in the Brillouin zone where the band gap vanishes. Show that the spectrum is approximately linear in proximity to these points.

(c) Include next-nearest neighbors in the model and recalculate the band structure. Expand the eigenenergies to second order for momenta close to one of the gap-closing points found in (b).