

Theoretical Condensed Matter Physics Exercise 3

(Submission: 09.11.18, discussion: 12./14.11.18)

3.1 Band structure calculation: weak periodic potential (8 points)

In this exercise, we want to study the effect of a periodic potential $U(x)$ in one spatial dimension in the limit of vanishing potential strength. Let the period in position space be a , the “lattice constant”. We will see that this creates a band structure with energy gaps at the Brillouin-zone boundaries in k -space. We start our calculation with a free-electron system ($\varepsilon_k^0 = \frac{\hbar^2 k^2}{2m}$) and treat the periodic potential in 2nd-order perturbation theory.

- What are the reciprocal wave vectors (numbers) for this one-dimensional system? Express the potential and the electron wave function (Bloch theorem) as a Fourier series over all reciprocal lattice vectors, respectively. Write down the Schrödinger equation in k -space.
- Calculate the energy shift $\Delta E_k^{(1)}$ in 1st-order perturbation theory and show that it is a constant, which we then take to be zero.
- Continue with 2nd-order perturbation theory: Write down the 2nd-order correction $\Delta E_k^{(2)}$ to the dispersion and discuss in which k -regions it is negative or positive.
- Is there an energy degeneracy for some values of k ? Diagonalize the Hamiltonian in the degenerate Hilbert subspace and show that the potential creates an energy gap at the Brillouin-zone boundaries. Determine the size of this gap.
- Draw the dispersion relation ε_k in the presence of a weak periodic potential in the extended and in the reduced zone scheme.

3.2 Tight binding model (12 points)

We consider a d -dimensional cubic lattice ($d = 1, 2, 3$) with lattice constant a and a single atom on each lattice site \mathbf{R}_i . We will investigate the case of a strong periodic potential here. This leads to an enhancement of the electron probability density around the lattice sites \mathbf{R}_i . Taking the Wannier functions approximately as the atomic orbitals $\phi_i(\mathbf{r}) = \phi_0(\mathbf{r} - \mathbf{R}_i)$ centered around the lattice sites \mathbf{R}_i , and expanding the Bloch functions (of a given band) in terms of Wannier functions one obtains approximately,

$$\psi_{\mathbf{k}}(\mathbf{r}) \approx \sum_i e^{i\mathbf{k}\mathbf{R}_i} \phi_i(\mathbf{r}). \quad (1)$$

Since the interatomic overlap is assumed to be small, one can neglect all integrals containing atomic orbitals which are separated by more than a lattice constant, i.e., one obtains the matrix

elements of the Hamiltonian as (“tight-binding” Hamiltonian),

$$\langle \phi_i | H | \phi_j \rangle = \begin{cases} \varepsilon_0, & i = j \\ -t_{ij}, & i \text{ and } j \text{ nearest neighbors} \\ 0, & \text{else} \end{cases} \quad (2)$$

Here t_{ij} are the so called *hopping* matrix elements since they describe the transition or hopping of an electron from one lattice site to another. We assume isotropic atomic orbitals (*s*-waves) and set $t_{ij} = t$.

- (a) Calculate the band structure $\varepsilon(\mathbf{k})$ for $d = 1, 2, 3$ by diagonalizing the tight-binding Hamiltonian Eq. (2).
- (b) Sketch for the two-dimensional case the lines of constant energy $\varepsilon(\mathbf{k}) = \text{const.}$ in the 1st Brillouin zone. In particular, draw the constant energy lines in the band center, $\varepsilon(\mathbf{k}) = \varepsilon_0$.
- (c) Determine the positions of the van Hove singularities by calculating the group velocity $v_{\mathbf{k}}$ for $d = 1, 2$. Calculate the density of states $N(\varepsilon)$ for the one-dimensional case.
- (d) Show for $d = 2$ that the van Hove singularity at $\varepsilon = \varepsilon_0$ is logarithmically divergent.
Hint: Expand the group velocity around the saddle point $\kappa = (0, -\pi/a)$ up to second order. Afterwards evaluate $N(\varepsilon = \varepsilon_0 + \delta)$ for a small δ by approximating the corresponding curve of equal energy by a line, e.g. $k_x = k_y + \Delta k$.
- (e)* If you are interested, use a computer to calculate the integrals involved in $N(\varepsilon)$ and plot $N(\varepsilon)$ for $d = 2, 3$.

Hint: Use the formula

$$N(\varepsilon) = \sum_{\mathbf{k}} \delta(\varepsilon - \varepsilon(\mathbf{k}))$$

*Bonus question, does not count for the total number of points.