Department of Physics, NTNU

Homework 2
TFY4210/FY8302 Quantum theory of solids
Spring 2021.

Problem 1

Consider a tightbinding Hamiltonian with nearest-neighbor hopping on a general two dimensional Bravais lattice with N lattice points, in contact with a particle reservoir. The chemical potential of the system is denoted μ. The nearest-neighbor hopping element is given by t. The Hamiltonian is given by

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}$$

Here, $(c^\dagger_{i,\sigma}, c_{i,\sigma})$ create and destroy particles in spin-state σ on site i. Introduce Fourier-transformed operators

$$\begin{aligned} c^\dagger_{\mathbf{k},\sigma} &= \frac{1}{\sqrt{N}} \sum_i c^\dagger_{i,\sigma} \ e^{-i\mathbf{k}\cdot\mathbf{r}_i} \\ c_{\mathbf{k},\sigma} &= \frac{1}{\sqrt{N}} \sum_i c_{i,\sigma} \ e^{i\mathbf{k}\cdot\mathbf{r}_i} \end{aligned}$$

where $\mathbf{r}_i$ is the position at lattice site i.

a) Show that Hamiltonian may be written on form

$$H = \sum_{\mathbf{k},\sigma} E_\mathbf{k} \ c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

and give an expression for $E_\mathbf{k}$ for a general two-dimensional Bravais lattice.

c) Imagine that we now consider a model on a *honeycomb* lattice, see Figure 1. Explain what the *principal* difference between this lattice and the square lattice is.

d) Write down a tight-binding model for this system, conidering only nearets neighbor interactions, and find $E_{\mathbf{k}}$. (Hint: You need to introduce two distinct types of fermions, one type for the red atoms and one type for the blue atoms).

Problem 2

Consider a tight-binding model in a uniform external magnetic field h directed along the z-direction. The Hamiltonian is given by

$$H = -t \sum_{\langle i,j \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} c^{\dagger}_{i,\sigma} c_{i,\sigma} - h \sum_{i,\sigma} \sigma c^{\dagger}_{i\sigma} c_{i\sigma}$$

in the same notation as in Problem 1. The last term is the second-quantized version of the Zeeman-term $-\mathbf{h} \cdot \mathbf{S} = -h \sum_i S_{iz} = -h \sum_i \left[c^{\dagger}_{i,\uparrow} c_{j,\uparrow} - c^{\dagger}_{i,\downarrow} c_{j,\downarrow} \right] = -h \sum_{i,\sigma} \sigma c^{\dagger}_{i\sigma} c_{i\sigma}$.

a) Introduce the same Fourier-transform as in Problem 1, and show that the Hamiltonian may be written on the form

$$H = \sum_{\mathbf{k},\sigma} E_{\mathbf{k},\sigma} \; c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

and give an expression for $E_{\mathbf{k},\sigma}$ for a general two-dimensional Bravais lattice.

b) Consider instead another variant of the tight-binding model, now in the absence of a magnetic field, but with a spin-dependent hopping matrix element. (In lectures Week 4, we discuss what the origin of such spin-dependent hopping could be). The Hamiltonian is given by, with a general spin-dependent hopping matrix element $t^{\sigma\sigma'}_{ij}$

$$H = - \sum_{\langle i,j \rangle, \sigma, \sigma'} t^{\sigma\sigma'}_{ij} c^{\dagger}_{i,\sigma'} c_{j,\sigma} - \mu \sum_{i,\sigma} c^{\dagger}_{i,\sigma} c_{i,\sigma}$$

Consider a special case $t^{\sigma\sigma'}_{ij} = t^{\sigma\sigma}_{ij} \delta_{\sigma,\sigma'}$, with $t^{\uparrow\uparrow}_{ij} \neq t^{\downarrow\downarrow}_{ij}$. Introduce the same Fourier-transform as in Problem 1, and show that the Hamiltonian may be written on the form

$$H = \sum_{\mathbf{k},\sigma} E_{\mathbf{k},\sigma} \; c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

and give an expression for $E_{\mathbf{k},\sigma}$ for a general two-dimensional Bravais lattice.

c) Compare with the results in Problem 2 **a)**, and show that this sort of spin-dependent hopping may be interpreted as particles moving in a $\mathbf{k}$-dependent external magnetic field along the z-axis.