INSTITUTE FOR THEORETICAL CONDENSED MATTER PHYSICS

(10 + 5 + 5 = 20 points)

Condensed Matter Theory I WS 2022/2023

Prof. Dr. A. Shnirman	Sheet 2
Dr. D. Shapiro, H. Perrin	Tutorial: 10.11.2020

Category A

1. Rotation symmetry

The proof of the Bloch theorem was based on the commutation of the Hamiltonian with the translation operators $T_{\mathbf{R}}$. In fact, any unitary symmetry can be expressed similarly. As an example, consider particles in a two-dimensional lattice potential which has C_n symmetry, i.e. it has an *n*-fold rotation symmetry ($n \in \{2, 3, 4, 6\}$).

- (a) Assuming spinless particles, express the C_n symmetry in terms of a group of unitary operators (in a specific representation) that commute with the Hamiltonian.
- (b) Now repeat the task with spin- $\frac{1}{2}$ particles.
- (c) Can you label the eigenstates of the Hamiltonian with a rotation eigenvalue c_n and the crystal momentum **k** at the same time?

Category B

2. Bloch wavefunctions

$$(10+5+10+5=30 \text{ points})$$

Consider an infinitely extended one-dimensional system of electrons in a potential of periodically occurring delta functions. The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U \sum_{n=-\infty}^{\infty} \delta(x+na)$$
(1)

with a constant U. This is a simple version of the Kronig-Penney model. It allows us to study the properties of Bloch states ψ_k exactly.

- (a) Let U > 0. Derive the Bloch wavefunctions and an implicit form of the dispersion relation E(k) by solving the Schrödinger equation. Start with one unit cell, then use the Bloch theorem.
- (b) Show explicitly that the group velocity in this system is zero at the zone boundaries in reciprocal space.
- (c) Use the dispersion relation from (a) to state a condition for which energies are allowed in this system. In between these bands, energy gaps occur. Derive the approximate size of the gap between the energetically lowest bands for both the limit of very weak U and the limit of very strong U.
- (d) Now let U < 0. Obtain the (implicit) dispersion relation for states with E < 0.