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# Advanced Quantum Mechanics - Problem Set 4

*Winter Term 2021/22*

**Due Date:** Hand in solutions to problems marked with * before **Monday, 15.11.2021, 12:00**. Because of the holiday on Wednesday, 17.11.2021, we will have one tutorial to discuss the problem set for both groups on Friday, 19.11.2021

## *1. Nearly free electron model

*3+2+2+3 Points*

Often it is sufficient to treat the periodic potential on a lattice as a small perturbation. For such problems it is useful to expand the periodic potential in a plane wave expansion which only contains waves with the periodicity of the reciprocal lattice, such that

$$U(\boldsymbol{x}) = \sum_{\boldsymbol{G}} U_{\boldsymbol{G}} e^{i\boldsymbol{G}\cdot\boldsymbol{x}},$$

where $\boldsymbol{G}$ is a reciprocal lattice vector which satisfies $e^{i\boldsymbol{G}\cdot\boldsymbol{R}} = 1$, with $\boldsymbol{R}$ denoting a point on the lattice. We moreover expand the wave functions in terms of a set of plane waves which satisfy the periodic boundary conditions of the problem

$$\psi(\boldsymbol{x}) = \sum_{\boldsymbol{k}} c_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}.$$

(a) Using the expansions above, show that the Schrödinger equation

$$\left[\frac{-\hbar^2\nabla^2}{2m} + U(\boldsymbol{x})\right]\psi(\boldsymbol{x}) = E\psi(\boldsymbol{x}),$$

can be written as

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) c_{\boldsymbol{k}} + \sum_{\boldsymbol{G}} U_{\boldsymbol{G}} c_{\boldsymbol{k}-\boldsymbol{G}} = 0.$$

(b) Perform the shift $\boldsymbol{q} = \boldsymbol{k} + \boldsymbol{K}$, where $\boldsymbol{K}$ is a reciprocal lattice vector which ensures that we can always find a $\boldsymbol{q}$ which lies in the first Brillouin zone[1], and show that the Schrödinger equation now gives

$$\left(\frac{\hbar^2}{2m}(\boldsymbol{q} - \boldsymbol{K})^2 - E\right) c_{\boldsymbol{q}-\boldsymbol{K}} + \sum_{\boldsymbol{G}} U_{\boldsymbol{G}-\boldsymbol{K}} c_{\boldsymbol{q}-\boldsymbol{G}} = 0.$$

[1] As an example of a Brillouin zone consider the simple cubic lattice with sides of length $a$. The lattice vectors can be written as $\boldsymbol{R}_1 = a\hat{\boldsymbol{x}}$, $\boldsymbol{R}_2 = a\hat{\boldsymbol{y}}$, and $\boldsymbol{R}_3 = a\hat{\boldsymbol{z}}$. In reciprocal space the basis vectors become $\boldsymbol{b_1} = \frac{2\pi}{a}\hat{\boldsymbol{x}}$, $\boldsymbol{b_2} = \frac{2\pi}{a}\hat{\boldsymbol{y}}$, and $\boldsymbol{b_3} = \frac{2\pi}{a}\hat{\boldsymbol{z}}$. In this case the first Brillouin zone is the region $-\pi/a \leq k_i < \pi/a$ (where $i = x, y, z$). The reziprocal lattice vectors can be written as $\boldsymbol{K} = \sum_i n_i \boldsymbol{b}_i$ (where $n_i \in \mathbb{Z}$). Therefore, for arbitrary $\boldsymbol{k}$ it is possible to find $\boldsymbol{q} = \boldsymbol{k} + \boldsymbol{K}$ so that $\boldsymbol{q}$ lies in the first Brilloin zone.

(c) Consider for concreteness a one-dimensional chain, but in the simple case where only the leading Fourier component contributes to the potential

$$U(x) = 2U_0 \cos\frac{2\pi x}{a}.$$

Explain how your result in (b) can be used to calculate the energy of the system.

(d) Suppose now that $U_0$ is very small. Near $q = \pi/a$ the Schrödinger equation reduces to

$$\begin{pmatrix} \frac{\hbar^2}{2m}\left(q - \frac{2\pi}{a}\right)^2 - E & U_0 \\ U_0 & \frac{\hbar^2 q^2}{2m} - E \end{pmatrix} \begin{pmatrix} c_1 \\ c_0 \end{pmatrix} = 0.$$

Calculate and plot the energy eigenvalues. What happens at $q = \pi/a$?

## 2. Spin 1 system

*3+2 Points*

The Hamiltonian for a spin 1 system is given by

$$\hat{H} = A\hat{S}_z^2 + B(\hat{S}_x^2 - \hat{S}_y^2),$$

where the $\hat{S}_i$ are spin operators and $A, B$ are real constants.

(a) Find the normalized energy eigenstates and eigenvalues.

(b) Is the Hamiltonian invariant under time reversal? How do the normalized eigenstates you calculated in part (a) transform under time reversal?