
Advanced Quantum Mechanics - Problem Set 4

Winter Term 2022/23

Due Date: Hand in solutions to problems marked with * to mailbox 39 with label “Advanced Quantum Mechanics” inside ITP room 105b before the lecture on **Friday, 11.11.2022, 09:15**. The problem set will be discussed in the tutorials on Monday 14.11.2022 and Wednesday 16.11.2022.

1. Eigenspinors

4+1 Points

Consider a spin 1/2 system in the presence of an external magnetic field $\mathbf{B} = B\hat{\mathbf{n}}$, where $\hat{\mathbf{n}}$ is a unit vector pointing in an arbitrary direction. The Hamiltonian of this system is given by

$$\hat{H} = -\frac{e}{mc}\hat{\mathbf{S}} \cdot \mathbf{B},$$

where $e < 0$ is the electron charge, m the electron mass, c the speed of light, and $\hat{\mathbf{S}}$ the vector of spin 1/2 operators.

- Calculate the eigenvalues and normalized eigenspinors of the Hamiltonian.
- Why does the direction of the eigenspinors only depend on $\hat{\mathbf{n}}$?

2. Time- and spin-reversal

2+3 Points

- Denote the wave function of a spinless particle corresponding to a plane wave in three dimensions by $\psi(\mathbf{x}, t)$. Show that $\psi^*(\mathbf{x}, -t)$ is the wave function for the plane wave if the momentum direction is reversed.
- Let $\chi(\hat{\mathbf{n}})$ be the eigenspinor you calculated in the previous problem, with eigenvalue +1. Using the explicit form of $\chi(\hat{\mathbf{n}})$ in terms of the polar and azimuthal angles which define $\hat{\mathbf{n}}$, verify that the eigenspinor with spin direction reversed is given by $-i\sigma_y\chi^*(\hat{\mathbf{n}})$.

*3. 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

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

where \mathbf{G} is a reciprocal lattice vector which satisfies $e^{i\mathbf{G}\cdot\mathbf{R}} = 1$, with \mathbf{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

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

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

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

can be written as

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

- (b) Perform the shift $\mathbf{q} = \mathbf{k} + \mathbf{K}$, where \mathbf{K} is a reciprocal lattice vector which ensures that we can always find a \mathbf{q} which lies in the first Brillouin zone¹, and show that the Schrödinger equation now gives

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

- (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 $q = \pi/a$?

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