Institut für Theoretische Physik
Universität Leipzig

Prof. Dr. B. Rosenow
M. Thamm

Advanced Quantum Mechanics - Problem Set 3

Winter Term 2019/20

Due Date: Hand in solutions to problems marked with * before the lecture on **Friday, 08.11.2019, 09:15**. The problem set will be discussed in the tutorials on Wednesday, 13.11.2019, and Friday, 15.11.2019

7. Eigenspinors

4+1 Points

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

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

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

(a) Calculate the eigenvalues and normalized eigenspinors of the Hamiltonian.

(b) Why does the direction of the eigenspinors only depend on $\hat{\boldsymbol{n}}$?

8. Time- and spin-reversal

2+3 Points

(a) Denote the wave function of a spinless particle corresponding to a plane wave in three dimensions by $\psi(\boldsymbol{x}, t)$. Show that $\psi^*(\boldsymbol{x}, -t)$ is the wave function for the plane wave if the momentum direction is reversed.

(b) Let $\chi(\hat{\boldsymbol{n}})$ be the eigenspinor you calculated in the previous problem, with eigenvalue +1. Using the explicit form of $\chi(\hat{\boldsymbol{n}})$ in terms of the polar and azimuthal angles which define $\hat{\boldsymbol{n}}$, verify that the eigenspinor with spin direction reversed is given by $-i\sigma_y\chi^*(\hat{\boldsymbol{n}})$.

*9. 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

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

(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 $q = \pi/a$?

[1] As an example of a Brillouin zone consider the simple cubic lattice with sides of length a. Any point on the lattice can be written in terms of $\boldsymbol{a_1} = a\hat{\boldsymbol{x}}$, $\boldsymbol{a_2} = a\hat{\boldsymbol{y}}$, and $\boldsymbol{a_3} = a\hat{\boldsymbol{z}}$. 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 $\boldsymbol{b_3} = \frac{2\pi}{a}\hat{\boldsymbol{z}}$. The boundaries of the first Brillouin zone are then the planes normal to the six vectors $\pm\boldsymbol{b_1}$, $\pm\boldsymbol{b_2}$, and $\pm\boldsymbol{b_3}$. The length of each side is $2\pi/a$.