Institut für Theoretische Physik
Universität Leipzig

Prof. Dr. B. Rosenow
Dr. C. Drukier
Dr. T. Hyart

Quantum Mechanics 2 - Problem Set 3

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Abgabe: The problem set will be discussed in the tutorials on **Thursday, 02.11.2017, 11:00** (German) and **Friday, 03.11.2017, 13:30** (English).

8. Eigenspinors

4+1 Punkte

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

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

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

9. Time- and spin-reversal

2+3 Punkte

(a) Denote the wavefunction 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 wavefunction for the plane wave if the momentum direction is reversed.

(b) Let $\chi(\hat{\mathbf{n}})$ be the eigenspinor calculated in the previous problem for eigenvalue $-e\hbar B/(2mc)$. 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 $-i\sigma_y\chi^*(\hat{\mathbf{n}})$.

10. Nearly free electron model

3+2+2+3 Punkte

Consider a particle in a periodic potential with lattice vectors $\mathbf{R}_i$ i.e. $U(\mathbf{x} + \mathbf{R}_i) = U(\mathbf{x})$. For such problems it is useful to write the periodic potential as a Fourier series

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

where $\mathbf{G}$ are reciprocal lattice vectors satisfying $e^{i\mathbf{G}\cdot\mathbf{R_i}} = 1$. We expand the wavefunctions 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

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

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 zone[1] , 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 $k = \pi/a$ the Schrödinger equation reduces to

$$\begin{pmatrix} \frac{\hbar^2}{2m}\left(k - \frac{2\pi}{a}\right)^2 - E & U_0 \\ U_0 & \frac{\hbar^2 k^2}{2m} - E \end{pmatrix} \begin{pmatrix} c_{k-2\pi/a} \\ c_k \end{pmatrix} = 0.$$

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

[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 $\mathbf{R_1} = a\hat{\mathbf{x}}$, $\mathbf{R_2} = a\hat{\mathbf{y}}$, and $\mathbf{R_3} = a\hat{\mathbf{z}}$. In reciprocal space the basis vectors become $\mathbf{b_1} = \frac{2\pi}{a}\hat{\mathbf{x}}$, $\mathbf{b_2} = \frac{2\pi}{a}\hat{\mathbf{y}}$, and $\mathbf{b_3} = \frac{2\pi}{a}\hat{\mathbf{z}}$. In this case the first Brillouin zone is the region $-\pi/a \leq k_i \leq \pi/a$ $(i = x, y, z)$. The reciprocal lattice vectors can be written as $\mathbf{K} = \sum_i n_i \mathbf{b_i}$ $(n_i \in \mathbb{Z})$. 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.