Quantum Mechanics 2 - Problem Set 5

Wintersemester 2017/2018

Abgabe: The problem set will be discussed in the tutorials on Thursday, 16.11.2017, 11:00 (German) and Friday, 17.11.2017, 13:30 (English).

15. Rashba wire

4+4+4 Punkte

In this problem we consider a quantum wire in the presence of a magnetic field. The Hamiltonian is given by

$$\hat{H} = \frac{p^2}{2m} + \alpha p \sigma^y + B_z \sigma^z,$$

where α is a constant, B_z denotes the magnetic field in the z-direction, and σ_i are the usual Pauli matrices.

- (a) First consider the case where $B_z = 0$. Calculate the eigenvalues and eigenstates of the Hamiltonian. Plot the eigenvalues as a function of momentum and indicate the Kramers pairs in your plot. What is the total degeneracy?
- (b) Repeat the calculation in (a) but with $B_z \neq 0$.
- (c) Let now \hat{V} denote an operator which is even under time-reversal, that is $\hat{T}\hat{V}\hat{T}^{-1} = \hat{V}$. Let $|k,\sigma\rangle$ and $|-k,-\sigma\rangle$ denote the wave functions for the Kramer's pairs obtained in (a). Show that $\langle -k,-\sigma|\hat{V}|k,\sigma\rangle=0$.

Remark: A matrix element like the one in part (c) appears, for example, when trying to calculate the rate of backscattering of electrons. The life-time τ of the electrons is then given by Fermi's golden rule as

$$\frac{1}{\tau} = \frac{2\pi}{\hbar} \rho_F |\langle -k, -\sigma | \hat{V} | k, \sigma \rangle|^2,$$

with ρ_F denoting the density of states at the Fermi level.

16. Graphene

(a) Consider a tight-binding Hamiltonian for graphene

$$\hat{H} = -\sum_{\langle \mathbf{R}', \mathbf{R} \rangle} t_{\mathbf{R}, \mathbf{R}'} |\mathbf{R}' \rangle \langle \mathbf{R}| + \text{h.c.}$$

where the summation is over the pairs of nearest-neighbour lattice sites and the tunnel couplings $t_{\mathbf{R},\mathbf{R}'}$ are t_1 , t_2 and t_3 for the bonds along the nearest-neighbor vectors $\vec{\delta}_1$, $\vec{\delta}_2$ and $\vec{\delta}_3$, respectively. Assume that the lattice sites corresponding to sublattice A are given as $\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2$ ($n_1, n_2 \in \mathbb{Z}$) and the lattice sites corresponding to sublattice B are $\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + \vec{\delta}_1$ ($n_1, n_2 \in \mathbb{Z}$) similarly as in the lectures.

Use the basis transformation

$$|\mathbf{k}, A\rangle = \frac{1}{N} \sum_{n_1, n_2 = 1}^{N} e^{i(n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2) \cdot \mathbf{k}} |n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2\rangle,$$

$$|\mathbf{k}, B\rangle = \frac{1}{N} \sum_{n_1, n_2 = 1}^{N} e^{i(n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + \vec{\delta}_1) \cdot \mathbf{k}} |n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + \vec{\delta}_1\rangle$$

to show that the Hamiltonian can be written as

$$\hat{H} = \sum_{\mathbf{k}} (|\mathbf{k},A\rangle,|\mathbf{k},B\rangle) \begin{pmatrix} 0 & -\sum_{i=1}^3 t_i e^{i\mathbf{k}\cdot\vec{\delta}_i} \\ -\sum_{i=1}^3 t_i e^{-i\mathbf{k}\cdot\vec{\delta}_i} & 0 \end{pmatrix} \begin{pmatrix} \langle \mathbf{k},A| \\ \langle \mathbf{k},B| \end{pmatrix}.$$

(b) Now consider next-nearest neighbour hoppings. The corresponding Hamiltonian is

$$\hat{H}_2 = -t' \sum_{\langle \langle \mathbf{R}', \mathbf{R} \rangle \rangle} |\mathbf{R}' \rangle \langle \mathbf{R}| + \text{h.c.}$$

where the summation is now over pairs of second-nearest-neighbour lattice sites. Show that with the help of the basis transformation given above this Hamiltonian can be written as

$$\hat{H}_2 = \sum_{\mathbf{k}} (|\mathbf{k}, A\rangle, |\mathbf{k}, B\rangle) \begin{pmatrix} -t'f(\mathbf{k}) & 0 \\ 0 & -t'f(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \langle \mathbf{k}, A| \\ \langle \mathbf{k}, B| \end{pmatrix}.$$

where

$$f(\mathbf{k}) = 2\cos\left(\sqrt{3}k_ya\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_ya\right)\cos\left(\frac{3}{2}k_xa\right).$$