Exercise 5 for Theoretical Solid State Physics in Summer 2021

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Submission: 14.05.2021, 12:00 in the P.O. Box Giesen on D.10 or by e-mail
Discussion: 17.05.2021, 14:15

1. **One-dimensional potentials (10 points)**
   The Fourier coefficients $\psi_{\vec{k}-\vec{G}}$ of the energy eigenfunctions $\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} \psi_{\vec{k}-\vec{G}} e^{i(\vec{k}-\vec{G})\vec{r}}$ are related among each other by the lattice potential $V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\vec{r}}$ due to the Schrödinger equation in Fourier space. In the lecture the following system of equations was derived:
   $$\left(\frac{\hbar^2 \left(\vec{k}-\vec{G}\right)^2}{2m} - E \right) \psi_{\vec{k}-\vec{G}} + \sum_{\vec{G}'} V_{\vec{G}'-\vec{G}} \psi_{\vec{k}-\vec{G}'} = 0$$
   Consider now cases of one-dimensional periodic lattices with lattice parameter a.
   (a) Calculate the energy bands of the "empty lattice", i.e. $V_{\vec{G}} \to 0$ for all $\vec{G}$. Draw a picture of the band structure in the first Brillouin zone.
   (b) For the periodic potential $V(x) = V_0 \cos \frac{2\pi x}{a}$ only two coefficients V_G do not vanish. Calculate all energy gaps in first order pertubation theory. Where are they located in Fourier space? Draw a picture of the band structure and compare it with the "empty lattice".
   (c) Calculate the coefficients V_G and all gaps in first order pertubation theory (V_0 small) for the potential $V(x) = -aV_0 \sum_{n\in\mathbb{Z}} \delta(x-an)$ (Kronig-Penney model). Draw the shape of energy bands.

2. **Dynamics of band electrons (4 points)**
   The Hamiltonian of an electron in energy band n exposed to an electro-magnetic field is given by
   $$H_n = E_n\left(\vec{p} - \frac{e}{c}\vec{A}\right) + e\phi(\vec{r}).$$

Show the relations

$$\dot{\vec{r}} = \vec{\nabla}_{\vec{k}} E_n\left(\vec{k}\right),$$
$$\dot{\vec{k}} = \frac{e}{c}\dot{\vec{r}} \times \vec{B} + e\vec{E}.$$

Hint: Prove first that $[k_\alpha, k_\beta] = i\frac{e}{c}\epsilon_{\alpha\beta\gamma}B_\gamma$.

3. **Landau quantization (6 points)**

   Consider a free electron with mass m and charge e in a magnetic field $\vec{B} = B\vec{e}_z$. The Hamiltonian H is given by

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2.$$

   The Landau gauge $\vec{A} = Bx\vec{e}_y$ fulfills $\vec{B} = B\vec{e}_z$ and $\vec{p}\vec{A} = \vec{A}\vec{p}$.

   (a) Show that the energy eigenvalues are given by

$$E_{n,k_y,k_z} = \hbar\omega_0\left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m},$$

   where $\omega_0 = \frac{|e|B}{mc}$ is called the cyclotron frequency.
   Hint: Show that the Hamiltonian transforms into

$$H = \frac{p_x^2}{2m} + \frac{m\omega_0^2}{2}\left(x - \frac{p_y}{m\omega_0}\right)^2 + \frac{p_z^2}{2m}$$

   and that the ansatz $\psi\left(\vec{r}\right) = \phi\left(x\right)e^{ik_y y}e^{ik_z z}$ leads to the Schrödinger equation for the one-dimensional harmonic oscillator. How does the solution depend on the wavenumber k_y?

   (b) Determine the degree of degeneracy. Assume periodic boundary conditions in y-direction, $k_y = \frac{2\pi l_y}{L_y}$, $l_y \in \mathbb{N}$ and use the condition, that the midpoint of the oscillator x_0 is resricted to $0 \leq x_0 \leq L_x$.