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Quantum Physics of Nanostructures - Problem Set 1

Winter term 2022/2023

Due date: The problem set will be discussed Wednesday, 26.10.2022, 15:15-16:45, Room 114.

1. Electronic Density of States

2+2+4 Points

Consider a system of free electrons in d spatial dimensions confined to a cubic volume $\Omega = L^d$. The single-particle wave functions $\psi_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}/\sqrt{\Omega}$ are eigenfunctions of the single-particle Hamiltonian $\hat{H} = \hat{\mathbf{p}}^2/2m$ with corresponding energy eigenvalues $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$. Assume periodic boundary conditions, i.e., $\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r} + L\mathbf{e}_i)$ for $i = 1, \ldots, d$ with $\mathbf{e}_i$ the ith unit vector and L the side length of the cube.

(a) Derive the quantization condition $k_i = 2\pi n_i/L$, $n_i \in \mathbb{Z}$ for the components k_i of the wave vectors $\mathbf{k} \in \mathbb{R}^d$ from the requirement of periodic boundary conditions in each of the d spatial directions. Which volume $(\Delta k)^d$ can be assigned to a quantum state with fixed $\mathbf{k}$ in $\mathbf{k}$-space?

(b) The number of electrons in the system can be computed from

$$N = 2 \sum_{\mathbf{k}} \Theta(\epsilon_F - \epsilon_{\mathbf{k}}).$$

Here, ϵ_F is the Fermi energy, $\sum_{\mathbf{k}} \cdots$ denotes the sum over discrete wave vectors, $\Theta(x)$ is the Heaviside function, and the factor of 2 is due to spin degeneracy. In the thermodynamic limit $N \to \infty$, $\Omega \to \infty$ with $n = N/\Omega = \text{const.}$ the sum can be replaced by integration over continuous wave vectors. Perform this limit an find an expression for the particle density n. Show that the particle density can also be represented as

$$n = \int_0^{\epsilon_F} d\epsilon \, \rho(\epsilon),$$

with the *density of states* per volume

$$\rho(\epsilon) = 2 \, \frac{1}{\Omega} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}),$$

and find the corresponding expression in the thermodynamic limit. The factor of 2 again takes into account the spin degree of freedom.

(c) Compute the function $\rho(\epsilon)$ in the cases $d = 1, 2, 3$.

2. Random Walk in one Dimension *4 Points*

Consider a particle in one spatial dimension, whose position at time $t = 0$ is given by x_0. The dynamics of the particle takes place in discrete time steps. After the ith time step, the particle's current position has changed by $\xi_i = +\Delta x$ with probability $P_+ = 1/2$, and by $\xi_i = -\Delta x$ with probability $P_- = 1/2$, where $\Delta x > 0$. For a total of N time steps, the position of the particle can be described by

$$x_N = \sum_{i=1}^{N} \xi_i + x_0.$$

Compute $\langle x_N \rangle$ and $\left\langle (x_N - \langle x_N \rangle)^2 \right\rangle$. The random variables ξ_i, $i = 1, \ldots, N$ are assumed to be independent and identically distributed. That is, they are mutually independent for $i \neq j$ and are all distributed according to $\{P_+, P_-\}$. How does $\left\langle (x_N - \langle x_N \rangle)^2 \right\rangle$ behave with increasing N? Specify how the limit $\Delta t \to 0$, $\Delta x \to 0$ has to be understood, in order to obtain a finite result.

3. Unitarity and Time-Reversal Symmetry I *3+3+3 Points*

In the following, consider the single-channel scattering matrix S that maps the amplitudes of incoming states (i_L, i_R, where L: left, R: right) to amplitudes of outgoing states (o_L, o_R) of some scattering region,

$$\begin{pmatrix} o_L \\ o_R \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} i_L \\ i_R \end{pmatrix}, \quad \text{where } S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}.$$

In the absence of magnetic fields or magnetic impurities, the Hamiltonian entering the Schrödinger equation obeys *time-reversal symmetry* (TRS): this tells us, that under $t \to -t$, for every solution ψ of the Schrödinger equation, ψ^* is a solution to the time-reversed equation (for simplicity, the spin degree of freedom is not considered here). In the scattering-matrix formalism, besides complex-conjugating amplitudes, incoming states become outgoing ones under time reversal and vice versa, while scattering is described by the same S, i.e., the following relation holds:

$$\begin{pmatrix} i_L^* \\ i_R^* \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} o_L^* \\ o_R^* \end{pmatrix}.$$

(a) From unitarity ($S^\dagger S = \mathbb{1}$) of the scattering matrix, derive the relations

$$T + R' = 1,\ T' + R = 1,\ T + R = 1 \text{ and } \frac{r}{t'} = -\left(\frac{r'}{t}\right)^*,$$

where $|r|^2 = R$, $|t|^2 = T$ and $|r'|^2 = R'$, $|t'|^2 = T'$.

(b) Show, that TRS implies $S = S^T$, where S^T denotes the transpose of S.

(c) Additionally assuming TRS, derive the following relation for amplitudes:

$$\frac{r}{t} = -\left(\frac{r'}{t}\right)^*.$$