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# Quantum Physics of Nanostructures - Problem Set 1

*Winter term 2014/2015*

**Due date:** The problem set will be discussed Wednesday, 22.10.2014.

**Internet:** Course information and problem sets are available online at
http://www.uni-leipzig.de/~stp/QP_of_Nanostructures_WS1415.html.

## 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 $i$th 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, $\epsilon_F$ is the Fermi energy, $\sum_{\mathbf{k}} \ldots$ 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 $i$th 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 $\xi_i$, $i = 1, \ldots, N$ 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. Thermal Transport *2+2+4 Points*

The Boltzmann equation for the distribution function $f(t, \mathbf{r}, \mathbf{p})$ with the collision term in the relaxation-time approximation reads

$$\frac{\partial}{\partial t} f(t, \mathbf{r}, \mathbf{p}) + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(t, \mathbf{r}, \mathbf{p}) + q\mathbf{E} \cdot \nabla_{\mathbf{p}} f(t, \mathbf{r}, \mathbf{p}) = -\frac{f - f_0}{\tau}.$$

In the following, restrict your computations to the stationary, field-free situation ($\partial_t f = 0$, $\mathbf{E} = 0$) with a finite temperature gradient $\nabla T$.

(a) Write $f = f_0 + f_1$ with the equilibrium distribution

$$f_0(\mathbf{r}, \mathbf{p}) = \frac{1}{e^{\beta(\mathbf{r})(\epsilon_{\mathbf{p}} - \mu)} + 1},$$

where $\mu$ and $\beta(\mathbf{r}) = 1/k_B T(\mathbf{r})$ denote the chemical potential and the local inverse temperature, respectively. Linearize the Boltzmann equation in $f_1$ and $\nabla T$.

(b) Determine the change $f_1$ in the distribution function due to the temperature gradient.

(c) Compute the heat current density $\mathbf{j}_Q$, defined as (the equilibrium part of $f$ does not yield a finite contribution)

$$\mathbf{j}_Q(\mathbf{r}) = 2 \int \frac{d^3k}{(2\pi)^3} \mathbf{v}\, (\epsilon_{\mathbf{p}} - \mu)\, f_1(\mathbf{r}, \mathbf{p}).$$

For vanishing electric field, the relation

$$\mathbf{j}_Q = -\kappa \nabla T$$

between heat current density and temperature gradient $\nabla T$ defines the electronic contribution to thermal conductivity, $\kappa$. Determine $\kappa$ and using the expression for $\sigma$ (take the result from the lecture) also determine the so-called *Lorenz number* $L_0 = \kappa/\sigma T$.

**Note:** Proceed for part (c) as done in the lecture for the computation of $\sigma$. The following remarks might prove useful:

- Express integrations over modulus of momentum $k = |\mathbf{k}|$ by integrations over the energy variable $\epsilon$ by employing the density of states $\rho(\epsilon)$.

- Assume the density of states $\rho(\epsilon) \simeq \rho(\mu)$ in an interval of width $k_B T$ around the Fermi energy.
- To evaluate energy integrals, make use of the Sommerfeld expansion

$$\int_0^{+\infty} d\epsilon \, \frac{H(\epsilon)}{e^{\beta(\epsilon-\mu)}+1} = \int_0^{\mu} d\epsilon \, H(\epsilon) + \frac{\pi^2}{6}(k_B T)^2 H'(\mu) + \mathcal{O}\left(\frac{1}{\beta\mu}\right)^4 .$$