Fachbereich C – Mathematik und Naturwissenschaften
– Physik –

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# Theoretical solid state physics, WS 08/09

## 3rd practice sheet

Closing date: 6.11.2008, at 12:00 into the PO Box

8. **One-dimensional potentials (10 points)**

   The Fourier coefficients $\psi_{\vec{k}-\vec{G}}$ of 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:

   $$\left(\frac{\hbar^2(\vec{k}-\vec{G})^2}{2m} - E\right)\psi_{\vec{k}-\vec{G}} + \sum_{\vec{G}'} V_{\vec{G}'-\vec{G}}\psi_{\vec{k}-\vec{G}'} = 0. \qquad (1)$$

   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 $V(x) = V_0 \cos(2\pi x/a)$ 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 $V(x) = -V_0 a \sum_{n\in\mathbb{Z}} \delta(x - na)$ (Kronig-Penney model). Draw the shape of energy bands.

9. **Kronig-Penney model (10 points)**

   Consider an electron with mass $m$ propagating in a one-dimensional periodic potential
   $V(x) = -V_0 a \sum_{n\in\mathbb{Z}} \delta(x - na)$, where $V_0 > 0$ is the strength of the potential and $a$ is the lattice parameter.

   (a) Define dimension-less units, so that the stationary Schrödinger equation becomes

   $$H\varphi(y) = \left[-\partial_y^2 - 2c \sum_{n=-\infty}^{\infty} \delta(y-n)\right]\varphi(y) = q^2\varphi(y). \qquad (2)$$

   How are $x$ and $y$, $V_0$ and $c$, $q^2$ and $E$ connected?

   (b) Justify the continuity condition $\varphi(0^+) = \varphi(0^-) =: \varphi(0)$ with symmetry arguments and show with the aid of the differential equation the jump of derivation $\varphi'(0^+) - \varphi'(0^-) = -2c\varphi(0)$.

   (c) Due to the periodicity of $V$ the Hamiltonian $H$ commutes with the translation operator $T$, defined by $T\varphi(y) = \varphi(y-1)$. So $H$ and $T$ have a common system of eigenfunctions:

   $$H\varphi(y) = q^2\varphi(y), \qquad (3)$$
   $$T\varphi(y) = e^{ik}\varphi(y). \qquad (4)$$

   Calculate solutions of these equations. Use the ansatz $\varphi(y) = Ae^{iqy} + Be^{-iqy}$ for $0 < y < 1$ and the conditions of part (b) to get an equation connecting $q$ and $k$.

   (d) Analyse the latter equation. Hint: $\varphi$ is bounded, so $k$ must be real. Therefore the eigenfunctions of $H$ and $T$ are limited to specific energy bands.