Fachbereich C – Mathematik und Naturwissenschaften
– Physik –

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Theoretical solid state physics, WS 08/09

2nd practice sheet

Closing date: 30.10.2008, at 12:00 into the PO Box

5. **Bases of reciprocal lattices (4 points)**

   Consider bases of the following lattice types:

   (a) simple cubic,
   (b) body-centered cubic,
   (c) face-centered cubic.

   Calculate bases of the corresponding reciprocal lattices and compare the results.

6. **The cubic point group (6 points)**

   Let G be a group. Two elements g_1, g_2 of G are called equivalent, $g_1 \simeq g_2$, if there exist an element g in G such that $g_1 = g g_2 g^{-1}$. This equivalence relation induces a decomposition of G in equivalence classes $\bar{a} := \{b \in G | b \simeq a\}$.

   (a) Show that the point group of the simple cubic lattice consists of 24 elements and decomposes in 5 equivlance classes. Hint: The equivalence classes are characterized by rotation axes and angles

   (b) Consider an electron in a potential with cubic symmetry. The Hamiltonian is invariant under symmetry transformations of the discrete point group. In subspaces of the Hilbert space, where irreducible representations are realized, the energies of the electron are the same. It can be shown that

   $$\#\,\text{irreducible representations} = \#\,\text{equivalence classes} =: s \tag{1}$$

   Let n_ν $(\nu = 1, \ldots, s)$ be the dimensions of the different irreducible representations. Then

   $$\sum_{\nu=1}^{s} n_\nu^2 = \#\,G. \tag{2}$$

   Show that only elcetron energies with multiplicities 1, 2 and 3 are possible.

7. **Bloch's theorem (6 points)**

   Consider an electron in an effective lattice potential with spin-orbit coupling. Then the Hamiltonian is given by

   $$H = \frac{p^2}{2m} + V(\vec{r}) + \frac{1}{4m^2c^2}(\vec{\sigma} \times \vec{\nabla} V(\vec{r})) \cdot \vec{P}, \tag{3}$$

   where the potential V is periodic respect to the lattice symmetry, i.e. $V(\vec{r} + \vec{R}) = V(\vec{r})$ for all lattice vectors $\vec{R}$.

   (a) Show that the translation operator $T_{\vec{R}}$, defined by $T_{\vec{R}}\Psi(\vec{r}) = \Psi(\vec{r} - \vec{R})$, fulfils the relations

   $$[H, T_{\vec{R}}] = 0 \qquad \text{and} \qquad [T_{\vec{R}}, T_{\vec{R}'}] = 0. \tag{4}$$

(b) It follows that H and $T_{\vec{R}}$ have a common system of eigenfunctions $\{\Psi_{\varepsilon,\vec{k}}\}$, i.e.

$$H\Psi_{\varepsilon,\vec{k}} = \varepsilon\Psi_{\varepsilon,\vec{k}} \qquad \text{and} \qquad T_{\vec{R}}\Psi_{\varepsilon,\vec{k}} = c(\vec{R})\Psi_{\varepsilon,\vec{k}}. \tag{5}$$

Show that $c(\vec{R}) = e^{i\vec{k}\vec{R}}$. Use the properties $T_{\vec{R}}T_{\vec{R}'} = T_{\vec{R}+\vec{R}'}$ and $\|T_{\vec{R}}\Psi(\vec{r})\| = 1$.