Exercise 3 for Theoretical Solid State Physics in Summer 2021

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Submission: 30.04.2021, 12:00 in the P.O. Box Giesen on D.10 or by e-mail
Discussion: 03.05.2021, 14:15

1. **Face centered tetragonal structure (2 Points)**

   The tetragonal face-centered structure do not appear explicitly in the list of the 14 Bravais lattices. Why? How can you describe these lattices as one of the 14 Bravais lattices?

   Hint: Look at the orthorhombic crystal system D_{2h} splitting into 4 different Bravais classes and having a conventional unit cell with three 90° angles and three pairwise different edge lengths a, b, c. Now set $a = b$ and you obtain the tetragonal crystal system D_{4h}. Two of the four Bravais classes of the orthorhombic crystal system seem to "disappear". More reasonably: Do pairs of the Bravais classes of the orthorhombic crystal system degenerate into just one Bravais class of the tetragonal crystal system?

   `https://en.wikipedia.org/wiki/Bravais_lattice`

2. **Symmetries of unit cells (3 Points)**

   Find all symmetry axes and planes of the simple cubic lattice and the hexagonal Bravais lattice.

   What is the order of these symmetry groups (= number of group elements)?

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

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

   (a) Show that the point group (without reflections) of the simple cubic lattice consists of 24 elements and decomposes in 5 conjugacy classes.
   Hint: The conjugacy 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

$$\#\text{ irreducible representations} = \#\text{ conjugacy classes} =: s.$$

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

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

Show that due to symmetry, multiplicities of spectral levels may be 1, 2 or 3 only.

4. **The point groups C_n (3 points)**
Similar to problem 3, but much simpler. Show that the point group C_n consists of n elements. Is it an Abelian group? How many conjugacy classes exist? What are the dimensions of the irreducible representations?

Comment: The "simpler" a group, the lesser its usefulness.