Technische Universität Berlin
Institut für Theoretische Physik
Prof. Dr. Matthias Scheffler
Dr. Volker Blum, Dr. Clive Emary
Dipl. Phys. Philipp Zedler

May 13, 2008

http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/

Theoretical Material Science: exercise sheet 5

Return: Monday, May 26 in the exercise

Exercise 12 (4 points): *Hellmann-Feynman-Theorem*
The Hellmann-Feynman theorem states that the forces on atoms, i.e. the total energy derivative with respect to atomic positions, are due to pure classical electrostatics. Thus, all explicit quantum mechanical terms vanish exactly, and only the electrostatic interaction between the nuclei (the external potential $v(\mathbf{r})$), and the electron density $n(\mathbf{r})$ survives:

$$\frac{\partial E_\nu[n,\{\mathbf{R}_I\}]}{\partial \mathbf{R}_J} = \int \frac{\partial v(\mathbf{r},\{\mathbf{R}_I\})}{\partial \mathbf{R}_J} n(\mathbf{r},\{\mathbf{R}_I\}) d^3\mathbf{r}$$

Starting from density-functional theory proof that this equation is indeed valid when the electron density $n(\mathbf{r})$ is the fully self consistent result.

Exercise 13 (4 points): *Close-packed structures*

a) What is the packing density achieved by the bcc- and fcc-structure, respectively?

b) Show that a close-packed structure with ABC stacking is identical to the fcc-structure.

Exercise 14 (4 points): *Pointgroup O_h and that of diamond*
The full octrahedral group O_h contains the following symmetry elements: $3C_4$, $4C_3$, $6C_2$, $3\sigma_h$, $6\sigma_d$, i, $3S_4$ and $4S_6$. Determine the matrix representation for each of the following point transformations contained in the O_h group:
- Rotations C_3 (rotation angle $\frac{2\pi}{3}$ about the cube diagonals, e.g. $(1,1,1)$-axis,
- Rotations C_2 (rotation angle π) about the X, Y, Z axes,
- Reflections σ in the plane perpendicular to $\mathbf{n} = (-1,1,0)$ through the origin,
- Inversion,

a) with respect to the standard basis of $\mathbb{R}^3$;

b) with respect to the basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ of the fcc-lattice.

c) Show that while the inversion i is not a symmetry transformation of the diamond structure, C_3, C_2 and σ are (The pointgroup of diamond is the tetrahedral group T_d).

Note: Diamond has an fcc-lattice. The two-atom basis of the crystal is given by a C-atom at position $\mathbf{s}_1 = (0,0,0)$ and a C-atom at position $\mathbf{s}_2 = \frac{a}{4}(1,1,1)$, with a being the lattice constant.

Please turn over!⟶

- **Webpage of the lecture:** http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/
- **Lecture:** Tue. & Fri., 10:00 a.m.-12:00 p.m. in room EW 203, TU Berlin
- **Exercise:** Mon., 14:00 a.m. in room H 1029
- **Literature:**
  - Ashcroft, Mermin, David: Solid state physics, Saunders College, Philadelphia, 1981
  - Kittel: Quantum theory of solids,Wiley, New York, 1963
  - Ziman: Principles of the theory of solids, Cambridge University Press, Cambridge, 1964
  - Ibach, Lueth: Solid-state physics: an introduction to principles of materials science, Springer, Berlin, 1995
  - Madelung: Festk?rpertheorie, Springer, Berlin, 1972
  - Scherz: Quantenmechanik, Teubner, Stuttgart, 1999
  - Dreizler, Gross: Density functional theory: an approach to the quantum many-body problem, Springer, Berlin, 1990
  - Parr, Yang: Density-functional theory of atoms and molecules, Oxford University Press, Oxford, 1994
  - Anderson: Basic notations of condensed matter physics, Benjamin/Cummings, London, 1984
  - Marder: Condensed matter physics, Wiley, New York, 2000
  - Martin: Electronic Structure, Cambridge University Press, Cambridge, 2004
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler: on appointment
  - Dr. Volker Blum: on appointment
  - Philipp Zedler: Wed, 11:00 - 12:00 a.m. in room EW 711