Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Patrick Rinke, Dr. Alex Tkatchenko
Exercises: Dr. Volker Blum

April 11, 2012

http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/

Theoretical Material Science: Exercise Sheet 1

Please hand in solutions by: Wednesday, April 18, start of the exercise class

Exercise 1 (6 points): *Born-Oppenheimer approximation*
One version of the Born-Oppenheimer approximation is the static approximation, within which the electronic system is solved for a fixed reference coordinate $\{\mathbf{R}_l^0\}$ of the nuclei:

$$\begin{aligned}&[T^e(\{\mathbf{r}_k\sigma_k\}) + V^{e-e}(\{\mathbf{r}_k\sigma_k\})\\ &+V^{e-Ion}(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I^0\})]\phi_\nu(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I^0\}) \quad = \quad E^e_\nu(\{\mathbf{R}_I^0\})\phi_\nu(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I^0\}).\end{aligned}$$

The lattice equation within this approximation is then given by:

$$\begin{aligned}&[T^{Ion}(\{\Delta\mathbf{R}_I\}) + V^{ph}(\{\Delta\mathbf{R}_I\})\\ &+\langle\phi_\mu(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I^0\})|V^{e-ph}|\phi_\mu(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I^0\})\rangle]\Lambda_\mu(\{\mathbf{R}_I\}) \quad = \quad E^I_\mu\Lambda_\mu(\{\mathbf{R}_I\}).\end{aligned}$$

with

$$\begin{aligned}\Delta\mathbf{R}_I &:= \mathbf{R}_I - \mathbf{R}_I^0,\\ V^{ph}(\{\Delta\mathbf{R}_I\}) &:= V^{Ion-Ion}(\{\mathbf{R}_I\}) - V^{Ion-Ion}(\{\mathbf{R}_I^0\}),\\ V^{e-ph}(\{\mathbf{r}_k\sigma_k\},\{\Delta\mathbf{R}_I\}) &:= V^{e-Ion}(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I\}) - V^{e-Ion}(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I^0\}).\end{aligned}$$

Derive the lattice equation and indicate approximations used.
Hint: For the overall wavefunction, use the expansion:

$$\Psi(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I\}) = \sum_\nu \Lambda_\nu(\{\mathbf{R}_I\})\phi_\nu(\{\mathbf{r}_k\sigma_k\},\{\mathbf{R}_I^0\}).$$

Exercise 2 (4 points): *Ewald method*
In a crystal, the position of the nuclei and the density of the electrons define the electrostatic potential $\phi(\mathbf{r})$. With help of the Ewald method, the electrostatic potential can be written as:

$$\begin{aligned}\phi(\mathbf{r}) \quad = \quad &\frac{Z_\nu e}{4\pi\epsilon_0}\sum_{I=1}^{M}\frac{1-\mathrm{erf}(\sqrt{\alpha}|\mathbf{r}-\mathbf{R}_I|)}{|\mathbf{r}-\mathbf{R}_I|}\\ &+\frac{Z_\nu}{\Omega}\frac{e}{\epsilon_0}\sum_{\mathbf{G}_n}\frac{e^{-\mathbf{G}_n^2/(4\alpha)}e^{i\mathbf{G}_n\mathbf{r}}}{|\mathbf{G}_n^2|} - \frac{Z_\nu e}{4\pi\epsilon_0}\frac{1}{|\mathbf{r}-\mathbf{R}_1|} + C.\end{aligned}$$

Calculate the constant C, assuming that ϕ does not depend on α.
Hint: In a practical (numerical) calculation of the potential itself, there is no way to compute the $\mathbf{G}_n$=0 term in the sum above. The sum in the expression above is therefore defined to run only over the $\mathbf{G}_n \neq 0$ terms.

Exercise 3 (2 points): *Atomic units*
Schrödinger's equation contains several fundamental constants. For practical derivations, it would be convenient to use a system of units where all these constants take on simple values.

It is possible to find a set of units so that the relevant constants can be written as

$$\frac{e^2}{4\pi\epsilon_0} = 1, \quad \hbar = 1, \quad m_e = 1.$$

With this choice of units (Hartree atomic units), what is the (natural) unit of energy, of length, and what is the form of the Hamiltonian of the hydrogen atom. What would be the corresponding answers for Rydberg atomic units:

$$\frac{e^2}{4\pi\epsilon_0} = 2, \quad \hbar = 1, \quad m_e = 0.5$$

Please turn over!⟶

- **Webpage of the lecture:**
  http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/
  wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/
- **Lecture:** Tue. & Wed., 10:00 h -12:00 h (sharp!) in room EW 203, TU Berlin
- **Exercise:** Wed., 14:00 h in room EW 229
- **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: Festkörpertheorie, 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
  - Kohanoff: Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods, Cambridge University Press, Cambridge, 2006
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
  - Active participation in computational exercises
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler, Dr. Alex Tkatchenko, Dr. Patrick Rinke: by appointment
  - Dr. Volker Blum: Available Wed. 16:00 (after the exercise class) or by appointment