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

Theoretical Material Science: exercise sheet 1

Return: Monday, April 28 in the exercise

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:

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

The lattice equation within this approximation is then given by:

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

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: Use for the overall wavefunction 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*
With help of the Ewald method, the electric 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.

Exercise 3 (2 points): *Atomic units*
Starting from the assumptions

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

(Hartree atomic units), what is the (natural) unit of energy, of length, and what is the form of the Hamiltonian of the hydrogen atom. How does this look 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/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 PN 711