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

April 18, 2012

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

Theoretical Material Science: Exercise Sheet 2

Please hand in solutions by: Wednesday, April 25, start of the exercise class

Exercise 4 (4 points): *Specific heat of metals and electron entropy*
We look at the electron contribution to the specific heat c_V, where we have defined the Energy and Entropy per volume $u = U/V$ and $s = S/V$. Both parts should be done for Jellium.

$$c_V = T\left(\frac{\partial s}{\partial T}\right)_V = \left(\frac{\partial u}{\partial T}\right)_V \tag{1}$$

a) Determine the electronic contribution to the specific heat (low-temperature expansion):

$$c_V = \left(\frac{\partial u}{\partial T}\right)_V = \frac{\pi^2}{3} k_B^2 T g(\epsilon_F).$$

g denotes the density of electronic levels per unit volume.
For comparison, in a crystal, the low-temperature contribution to c_v by phonons according to Debye's model (to be derived later in this lecture course) is:

$$c_V^{phonon} = \frac{12\pi^4}{5} n k_B \left(\frac{T}{\Theta_D}\right)^3.$$

Θ_D is known as the "Debye temperature" of a solid, and n denotes the number of ions in the solid per volume. Compare the electronic and phononic contributions to the specific heat.

b) Use equation 1 to determine the electron entropy, i.e. derive the equation

$$s = -k_B \sum_i \left\{ f(\epsilon_i) \ln f(\epsilon_i) + [1 - f(\epsilon_i)] \ln[1 - f(\epsilon_i)] \right\},$$

where $f(\epsilon)$ is the Fermi function and the index i runs over electronic states.

Exercise 5 (4 points): *Density of states*
Show that the density of energy states for an ideal noninteracting Fermi gas is

a) in one dimension

$$N^{1D}(\epsilon) = \frac{V_g}{\pi\hbar}\sqrt{\frac{m}{2}}\frac{1}{\sqrt{\epsilon}},$$

b) in two dimensions

$$N^{2D}(\epsilon) = \frac{m V_g}{\pi\hbar^2}$$

c) and in three dimensions

$$N^{3D}(\epsilon) = \frac{V_g}{\pi^2}\frac{\sqrt{2m^3}}{\hbar^3}\sqrt{\epsilon}.$$

Exercise 6 (4 points): *Hartree-Fock approximation*
The energy-functional in the Hartree-Fock approximation is given by the expression

$$\begin{aligned} E^{HF}[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}] &= T_s[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}] + E^{e-ion}[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}] \\ &\quad + E^{Hartree}[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}] + E^X[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}], \end{aligned}$$

with T_s and $E^{Hartree}$ defined as in the Hartree theory and

$$\begin{aligned} &E^X[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}] \\ &= -\frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\sum_{i,j}^{N,N} \delta_{s_i s_j} \int d^3\mathbf{r} \int d^3\mathbf{r}' \frac{\varphi^*_{o_i s_i}(\mathbf{r})\varphi^*_{o_j s_j}(\mathbf{r}')\varphi_{o_i s_i}(\mathbf{r}')\varphi_{o_j s_j}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|}. \end{aligned}$$

Please turn over!⟶

(Exercise 6 continued) Derive the effective single-particle Hartree-Fock equation by varying $E^{HF}[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}]$ under the constraint that $\varphi_{o_i s_i}$ is normalized and the requirement that the total energy assumes its minimum at the ground state, i.e:

$$\frac{\delta}{\delta \varphi^*_{o_i s_i}(\mathbf{r})} \left(E^{HF}[\{\varphi^*_{o_i s_i}, \varphi_{o_i s_i}\}] + \sum_{i,j}^{N,N} (\delta_{s_i s_j} - \lambda_{o_i o s_i, o_j s_j} \langle \varphi_{o_i s_i} | \varphi_{o_j s_j} \rangle) \right) = 0.$$

Keep in mind that the coefficients $\lambda_{o_i s_i, o_j s_j}$ are hermitian in i, j.

- **Webpage of the lecture:**
  http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/
  wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/
  http://th.fhi-berlin.mpg.de/sitesub/lectures/spring_2012/
- **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