

Theoretical Material Science: exercise sheet 2

Return: Monday, May 5 in the exercise

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.

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

a) Determine the electronic contribution to the specific heat:

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

Compare the result to the phonon contribution $c_V^{phonon} = \frac{12}{5} n k_B \left(\frac{T}{\Theta_D} \right)^3$.

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

$$s = -k_B T \int \frac{dk}{4\pi^3} [f \ln f + (1-f) \ln(1-f)],$$

where $f(\epsilon(k))$ is the Fermi function.

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

$$E^{HF}[\{\varphi_{o_i s_i}^*, \varphi_{o_i s_i}\}] = T_s[\{\varphi_{o_i s_i}^*, \varphi_{o_i s_i}\}] + E^{e-ion}[\{\varphi_{o_i s_i}^*, \varphi_{o_i s_i}\}] + E^{Hartree}[\{\varphi_{o_i s_i}^*, \varphi_{o_i s_i}\}] + E^X[\{\varphi_{o_i s_i}^*, \varphi_{o_i s_i}\}],$$

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

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

Derive the 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 variation on the ground state is 0, i.e:

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

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

Please turn over! →

- **Webpage of the lecture:** <http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfcp/>
- **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: 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
- **"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