LMU München
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Lehrstuhl für Theoretische Nanophysik
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9. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Tuesday, January 17, 2017.

Exercise 1:

Problem 1 from Chapter 17 in Ashcroft/Mermin (page 351).

Exercise 2: Hartree-Fock theory of the Jellium model

A simple model for a solid is found when the lattice-periodic potential is replaced by a constantly charged background with charge density $\rho_{\text{pos}} = \frac{Ne}{V}$. The lattice potential is then given by

$$V_G(\boldsymbol{r}) = -\frac{Ne^2}{V} \int \frac{d\boldsymbol{r}'}{|\boldsymbol{r} - \boldsymbol{r}'|}$$

and the Hartree-Fock equation for this model is:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_G(\boldsymbol{r}) + \sum_{\boldsymbol{k}'} \int d\boldsymbol{r}' \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r}'|} \left(2 \left| \psi_{\boldsymbol{k}'}(\boldsymbol{r}') \right|^2 - \frac{\psi^*_{\boldsymbol{k}'}(\boldsymbol{r}') \psi_{\boldsymbol{k}}(\boldsymbol{r}') \psi_{\boldsymbol{k}'}(\boldsymbol{r})}{\psi_{\boldsymbol{k}}(\boldsymbol{r})} \right) \right] \psi_{\boldsymbol{k}}(\boldsymbol{r}) = \epsilon^{\text{HF}}_{\boldsymbol{k}} \psi_{\boldsymbol{k}}(\boldsymbol{r}).$$

a. Explain the difference to the Hartree-Fock equations given in the lecture.

b. Show that, in the case of plane waves (i.e., $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \mathrm{e}^{i\boldsymbol{k}\boldsymbol{r}}$), the Hartree (direct) term in the Hartree-Fock equation compensates for the lattice potential V_G.

c. Show that plain waves solve the Hartree-Fock equation above.

d. Compute the eigenvalues $\epsilon^{\text{HF}}_{\boldsymbol{k}}$. You can use the following relation (from the Fourier transformation of the Coulomb potential):

$$\frac{1}{z} = \frac{1}{V} \sum_k \frac{4\pi}{k^2} \mathrm{e}^{i\boldsymbol{k}\boldsymbol{z}}.$$

The remaining sum over $\boldsymbol{k}$-space can be evaluated by transformation to an integral.