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

To be discussed on Friday, January 31, 2013.

Exercise 1: Bogoliubov transformation for fermions

Consider a bilinear Hamiltonian of the general form:

$$H = E_0(c^\dagger c + f^\dagger f) + E_1(c^\dagger f^\dagger + fc)$$

where c, f denote fermionic annihilation operators. We introduce a new set of operators denoted by α and β and seek a linear transformation of the form

$$c = u\alpha - v\beta^\dagger, \ f = u\beta + v\alpha^\dagger$$

that diagonalizes the Hamiltonian (assume that both u and v are real).

a. Show that one has to require $u^2 + v^2 = 1$ when inserting these operators into the anticommutation relations for the original fermions, in order for the transformation to be a canonical one (i.e., a transformation that preserves the anti-commutation relations).

b. Insert the transformation into the Hamiltonian and diagonalize it. Show that the eigenenergy Ω is given by $\Omega = \sqrt{E_0^2 + E_1^2}$.

c. Write down the ground state $|\psi_0\rangle$ and the groundstate energy ϵ_0.

Exercise 2: Specific heat of a spin system in a magnetic field

We consider a system of N uncoupled spin-$\frac{1}{2}$ moments in an external magnetic field B. The Hamiltonian is given by

$$H = \boldsymbol{B} \cdot \sum_j \boldsymbol{S}_j$$

a. Compute the specific heat c_V.

b. Discuss the high-temperature limit.

Exercise 3: Bose-Einstein distribution for phonons

The eigenenergies of phonons are given by

$$E = \sum_{\boldsymbol{k}s} (n_{\boldsymbol{k}s} + \frac{1}{2})\hbar\omega_s(\boldsymbol{k})$$

In this exercise we want to find out what kind of distribution the phonons obey. The free energy of a system is defined as

$$f = \frac{1}{V} \ln \left(\sum_i \mathrm{e}^{-\beta E_i} \right).$$

a. Show that the energy density

$$u = \frac{1}{V} \frac{\sum_i E_i \mathrm{e}^{-\beta E_i}}{\sum_i \mathrm{e}^{-\beta E_i}}, \quad \beta = \frac{1}{k_B T}$$

is given by $u = -\frac{\partial f}{\partial \beta}$.

b. Derive the free energy for phonons:

$$f = \frac{1}{V} \ln \left(\prod_{\boldsymbol{k}s} \frac{\mathrm{e}^{-\beta\omega_s(\boldsymbol{k})/2}}{1 - \mathrm{e}^{-\beta\omega_s(\boldsymbol{k})}} \right).$$

c. From this calculate $\langle n_{\boldsymbol{k}s} \rangle$.

Exercise 4: Heitler-London singlet-triplet splitting

Derive the Heitler-London estimate

$$\frac{1}{2}(E_s - E_t) = \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 [\phi_1(\boldsymbol{r}_1)\phi_2(\boldsymbol{r}_2)] \left(\frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} + \frac{e^2}{|\boldsymbol{R}_1 - \boldsymbol{R}_2|} - \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{R}_1|} - \frac{e^2}{|\boldsymbol{r}_2 - \boldsymbol{R}_2|} \right) [\phi_2(\boldsymbol{r}_1)\phi_1(\boldsymbol{r}_2)] \tag{1}$$

for the difference in singlet and triplet ground-state energies for the hydrogen molecule.

In showing that

$$E_s - E_t = \frac{(\bar{\psi}_s, H\bar{\psi}_s)}{(\bar{\psi}_s, \bar{\psi}_s)} - \frac{(\psi_t, H\psi_t)}{(\psi_t, \psi_t)} \tag{2}$$

reduces to Eq. (1) for well-separated protons, it is enssential to take into account the following points:

(a) The one-electron wave functions $\phi_1(\boldsymbol{r})$ and $\phi_2(\boldsymbol{r})$ out of which $\psi_t(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and $\bar{\psi}_s(\boldsymbol{r}_1, \boldsymbol{r}_2)$ are constructed are exact ground-state wave functions for a single electron in a hydrogen atom at $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, respectively.

(b) The criterion for well-separated protons is that they be far apart compared with the range of a one-electron hydrogenic wave function.

(c) The electrostatic field outside of a spherically symmetric distribution of charge is precisely the field one would have if all the charge were concentrated in a single point charge at the center of the sphere.

It is also convenient to include in the Hamiltonian the (constant) interaction energy $\frac{e^2}{|\boldsymbol{R}_1-\boldsymbol{R}_2|}$ of the two protons.