University of Regensburg Summer Semester 2007

Quantum Theory of Condensed Matter

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Sheet 4

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1. Spin commutations

Write the spin operators s^+, s^-, and s^z operators in second quantization in terms of the fermionic operators $a^\dagger_{\uparrow,\downarrow}$ and $a_{\uparrow,\downarrow}$ (the indices $\uparrow$, $\downarrow$ characterize the electron possible spin states). Show they satisfy the commutation relations for spin components, that is

$$\begin{aligned} \left[s^+, s^-\right] &= 2\hbar s^z\,, \\ \left[s^\pm, s^z\right] &= \mp\hbar s^\pm\,. \end{aligned}$$

Hint: Use the fact that

$$\begin{aligned} [A, BC] &= [A, B]\, C + B\,[A, C]\;, \\ [AB, C] &= A\,[B, C]_+ - [A, C]_+\, B\,. \end{aligned}$$

2. Bose statistics

In the real world we never encounter zero temperature. Hence we will often need to use statistical physics and thermal averages. The quantum mechanical version of the thermal average reads:

$$\langle\hat{O}\rangle = \sum_{N=0}^{\infty}\sum_{\{n_\lambda\}_N}\left\langle \{n_\lambda\}_N \,\middle|\, \hat{\rho}\,\hat{O} \,\middle|\, \{n_\lambda\}_N\right\rangle\;,$$

where the density operator $\hat{\rho}$ is defined as:

$$\hat{\rho} = (1/Z)\exp[-\beta(\hat{H} - \mu\hat{N})]\,,$$

and for each N the sum $\sum_{\{n_\lambda\}_N}$ is taken only with respect to states with configuration $\{n_\lambda\}_N$ with a number of particles N. μ is the chemical potential and $\beta = 1/k_B T$ is the inverse temperature. Z is the grancanonical partition function:

$$Z = \sum_{N=0}^{\infty}\sum_{\{n_\lambda\}_N}\left\langle \{n_\lambda\}_N \,\middle|\, \exp[-\beta(\hat{H} - \mu\hat{N})] \,\middle|\, \{n_\lambda\}_N\right\rangle\;,$$

which normalizes the operator $\hat{\rho}$ and is a key quantity for the calculation of thermal averages. $\hat{N}$ is the number operator $\hat{N} = \sum_\lambda c^\dagger_\lambda c_\lambda = \sum_\lambda \hat{n}_\lambda$.

Let us consider the Hamiltonian for non-interacting bosons:

$$\hat{H}_{\mathrm{B}} = \sum_\lambda \hbar\omega_\lambda\left(a^\dagger_\lambda a_\lambda + \frac{1}{2}\right)$$

where the quantum number λ completely defines the single particle state. The chemical potential μ is taken to be lower than the lowest boson energy and independent of the temperature.

1. Prove that the grancanonical partition function Z for this system reads:

$$Z = \prod_\lambda \mathrm{e}^{-\beta\frac{\hbar\omega_\lambda}{2}}\frac{1}{1 - \mathrm{e}^{-\beta(\hbar\omega_\lambda - \mu)}}\,.$$

Hint: It is useful to remember the following identity:

$$\sum_{N=0}^{\infty} \sum_{\{n_\lambda\}_N} \prod_{\lambda} q_\lambda^{n_\lambda} = \prod_{\lambda} \sum_{n_\lambda=0}^{\infty} q_\lambda^{n_\lambda} \, ,$$

where q_λ is a set of complex numbers, one for each single particle state λ.

2. What is the average number of bosons in the state defined by the quantum number λ? Using the definition of average in terms of the density operator $\hat{\rho}$ prove the relation:

$$\langle \hat{n}_\lambda \rangle = -\frac{1}{\hbar\beta} \frac{\partial}{\partial \omega_\lambda} (\ln Z) - \frac{1}{2} \, .$$

3. Using points 1. and 2. calculate $\langle \hat{n}_\lambda \rangle$. This is called Bose-Einstein distribution n_{BE} and is a function of the single particle energy $\hbar\omega_\lambda$, the temperature T and the chemical potential μ .

4. Plot $n_{\mathrm{BE}}(\omega_\lambda, T, \mu)$ vs. ω_λ for different temperatures. Assume the chemical potential to be zero and the single particle energies ω_λ to be positive and very dense.

3. Fermi statistics

Let us now consider the Hamiltonian for non-interacting fermions:

$$\hat{H}_{\mathrm{F}} = \sum_{\lambda} \epsilon_\lambda c_\lambda^\dagger c_\lambda \, ,$$

where λ is a good quantum number for single particle states.

1. Prove that the grancanonical partition function Z for this system reads:

$$Z = \prod_{\lambda} \left[1 + \mathrm{e}^{-\beta(\hbar\omega_\lambda - \mu)} \right] \, .$$

Hint: Remember that for Fermions the Pauli exclusion principle holds. Formally $\{c^\dagger, c^\dagger\} = 0$ which implies that a single particle state can never be occupied by more than one fermion.

2. Calculate the average number of fermions in the state defined by the quantum number λ. You just rediscovered the Fermi-Dirac distribution n_{FD}. As a first step you must first extend to the fermionic case the relation of point 2.2.

3. Plot $n_{\mathrm{FD}}(\epsilon_\lambda, T, \mu)$ vs. ϵ_λ for different temperatures. This time take a positive chemical potential. Can you say what is the meaning of the chemical potential for very low temperatures?

Frohes Schaffen!