Quantum theory of condensed matter I

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Tue	10:00 - 12:00	H33
Thu	10:00 - 12:00	H33
Tue	12:00 - 14:00	9.2.01

Sheet 7

1. Specific heat for Einstein model of optical phonons

Repeat all the steps as given in the lecture for the Debye model of acoustic phonons using now the Einstein model for optical phonons. As such, let all normal modes share the same frequency $\omega_j(\mathbf{q}) = \Omega$ independent of $\mathbf{q}$. As before, the total number of modes is the number of atoms in volume V times the dimensionality of the lattice d.
Calculate the internal energy E and the scecific heat $C_V = V^{-1}\partial E/\partial T$ of Einstein phonons being in thermal equilibrium at temperature T. Obtain an asymptotic expression for both quantities in the limits of large and low temperatures. Compare the results with the case of Debye acoustic phonons. **(2 Points)**

2. Bose statistics

In the real world we never encounter zero temperature. Hence we will often need to use statistical physics and thermal averages. For interacting system, general 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 $\hat{N} = \sum_\lambda a_\lambda^\dagger a_\lambda = \sum_\lambda \hat{n}_\lambda$.

Let us consider the Hamiltonian for non-interacting bosons:

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

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: Use commutation relations to show that operators $\hat{n}_\lambda$ and $\hat{n}_{\lambda'}$ commute, and factorize the exponential. Recall that $e^{X+Y} = e^X e^Y e^{-[X,Y]/2}$ provided the commutator commutes with both operators X and Y. You may also use the 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.

You have thus shown that different modes λ are statistically independent, $Z = \Pi_\lambda Z_\lambda$. **(3 Points)**

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:

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

(1 Point)

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 . **(2 Points)**

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.

   Note that $n_{\mathrm{BE}}(\omega_\lambda, T, \mu = 0)$ (Planck distribution) represents an equilibrium distribution for bosonic excitations like phonons or photons. Thermal equlibrium in such system is reached due to interaction with thermal bath via processes with creation and annihilation of individual quanta, hence the total numer of quanta N is not conserved. The equlibrium state corresponds to the minimum of free energy F with respect to N at fixed volume and temperature. Since $(\partial F/\partial N)_{T,V} = \mu$, it follows that the chemical potential μ ought to be zero. **(2 Points)**

3. Fermi statistics

(Oral) 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. The number operator $\hat{N} = \sum_\lambda c_\lambda^\dagger c_\lambda$.

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

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

   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, find the analogue of the relation in 2.2 in the fermionic case.

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

Frohes Schaffen!