

Due Friday December 7 **I. Screening and the Coulomb interaction**

1. Ziman derives the dielectric function explicitly only for the case of the free electron gas, where electron orbitals are plane waves. For the case of a real crystal, the orbitals are Bloch states $\psi_{kn} = |\mathbf{k}n\rangle$. Show that the corresponding SCF dielectric function is

$$\epsilon(\vec{q}, \omega) = 1 + \frac{4\pi e^2}{q^2} \sum_{\vec{k}, n, n'} \frac{\left| \langle \vec{k} + \vec{q}n' | e^{i\vec{q}\cdot\vec{r}} | \vec{k}n \rangle \right|^2 \left[f(\vec{k}n) - f(\vec{k} + \vec{q}n) \right]}{\epsilon(\vec{k} + \vec{q}n') - \epsilon(\vec{k}n) - \hbar(\omega + i\alpha)}$$

2. Show how to get the Fermi-Thomas limit ($\omega=0$ and \mathbf{q} small, $T=0$) with no further approximation, for real, not free electrons, and exhibit the formula.

II. Creation and Destruction operators (“2nd Quantization”)

3. For a system of massless Bosons (photons, phonons) the relevant space of states is spanned by the occupation number states, $|n_1, \dots, n_i, \dots\rangle$, where n_i is a (non-negative) integer interpreted as the number of Bose particles in the i^{th} mode (each boson in the i^{th} mode brings an energy $\hbar\omega_i$). Creation and destruction operators are defined by

$$a_i |n_1, \dots, n_i, \dots\rangle = \sqrt{n_i} |n_1, \dots, n_i - 1, \dots\rangle$$

$$a_i^+ |n_1, \dots, n_i, \dots\rangle = \sqrt{n_i + 1} |n_1, \dots, n_i + 1, \dots\rangle$$

In thermal equilibrium, the probability $P(n_1, \dots, n_i, \dots)$ of the system being in the state $|n_1, \dots, n_i, \dots\rangle$ is

$$P(n_1, \dots, n_i, \dots) = \prod_i e^{-n_i \beta \hbar \omega_i} / Z_i$$

where the partition function Z_i of the i^{th} mode is the usual grand canonical ensemble result, $Z_i = \prod_n \exp(-n \beta \hbar \omega_i) = [1 - \exp(-\beta \hbar \omega_i)]^{-1}$. The operator $\hat{n}_i \equiv a_i^+ a_i$ is the “number operator”, because the state $|n_1, \dots, n_i, \dots\rangle$ is an eigenstate of \hat{n}_i with eigenvalue n_i . Use the definitions above to prove that the thermal average occupancy is $\langle \hat{n}_i \rangle = [\exp(\beta \hbar \omega_i) - 1]^{-1}$, the usual Bose-Einstein function. Also evaluate the fluctuation $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$. Find the value of $\langle \hat{n}_i \rangle$ and $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$ at the temperature where $\beta \hbar \omega_i = 1$.

4. For massive Fermions, the same definitions work with a modification. The space of states is again spanned by the basis states $|n_1, \dots, n_i, \dots\rangle$, with the additional restriction that the integers n_i must be either 0 or 1. In a physical system of electrons, the total number is a fixed conserved quantity, but it is convenient to work in the grand canonical ensemble where the number is arbitrary, being determined by the chemical potential μ of a bath of particles in contact with the system. The space of all states $|n_1, \dots, n_i, \dots\rangle$, unrestricted as to total occupancy, is called “Fock space.” The definition of creation and destruction operators is

$$c_i |n_1, \dots, n_i, \dots\rangle = \sqrt{n_i} |n_1, \dots, n_i - 1, \dots\rangle$$

$$c_i^+ |n_1, \dots, n_i, \dots\rangle = \sqrt{1 - n_i} |n_1, \dots, n_i + 1, \dots\rangle$$

In thermal equilibrium, the probability $P(n_1, \dots, n_i, \dots)$ of the system being in the state $|n_1, \dots, n_i, \dots\rangle$ is

$$P(n_1, \dots, n_i, \dots) = \prod_i e^{-n_i \beta(\epsilon_i - \mu)} / Z_i$$

where the partition function Z_i of the i^{th} mode is the usual grand canonical ensemble result, $Z_i = 1 + \exp[-\beta(\epsilon_i - \mu)]$. Again, the operator $\hat{n}_i \equiv c_i^+ c_i$ is the “number operator”, because the state $|n_1, \dots, n_i, \dots\rangle$ is an eigenstate of \hat{n}_i with eigenvalue n_i . Use the definitions above to prove that the thermal average occupancy is $\langle \hat{n}_i \rangle = [\exp(\beta(\epsilon_i - \mu)) + 1]^{-1}$, the usual Fermi-Dirac function. Also evaluate the fluctuation $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$. Find the value of $\langle \hat{n}_i \rangle$ and $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$ at a temperature where $\beta(\epsilon_i - \mu) = 1$. Also find the general formula for the fluctuation $\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$ in the total number of Fermions (electrons, for example) in a system with $\langle \hat{N} \rangle = N$ total Fermions, in the grand canonical ensemble defined by β, μ . The total number operator is $\hat{N} = \sum_i \hat{n}_i$. Show that

$$\sqrt{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2} \text{ is small compared to } N.$$