Answers

Physics 555	Fall 2007	HW 7

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 $\psi_{kn}=|kn>$. Show that the corresponding SCF dielectric function is

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

We need to find $\delta\rho_q = \int dr\, e^{-iq\cdot r}\delta\rho(r)$

where $\delta\rho(r) = -e\sum_k f_k\left[|\psi^1_{kn}|^2 - |\psi^0_{kn}|^2\right]$

$$\delta\rho_q = -e\sum_k f_k\Big[\langle\psi_{kn}|e^{-iq\cdot r}|\delta\psi_{kn}\rangle + \langle\delta\psi_{kn}|e^{-iq\cdot r}|\psi_{kn}\rangle\Big]$$

The perturbation is $\delta U(rt) = \sum_Q \delta U_Q\, e^{i(Q\cdot r-\omega t)}e^{\alpha t}$

where we take $\delta U_{-Q} = \delta U_Q$ since $\delta U(rt)$ is real.

Time-dependent perturbation theory gives

$$\delta\psi_{kn} = \sum_Q b_{kn,k+Qn'}\,\psi_{k+Qn'}$$

$$b_{kn,k+Qn'} = \frac{\langle k+Qn'|e^{iQ\cdot r}|kn\rangle U_Q e^{-i(\omega+i\alpha)t}}{\epsilon(kn)-\epsilon(k+Qn')+\hbar(\omega+i\alpha)}$$

Therefore we get

$$\delta\rho_q = -e\sum_{\substack{kn\\n'}} f_{kn}\Bigg\{\frac{\langle kn|e^{-iq\cdot r}|k+qn'\rangle\langle k+qn'|e^{iq\cdot r}|kn\rangle}{\epsilon(kn)-\epsilon(k+qn')+\hbar(\omega+i\alpha)}$$

$$+\frac{\langle k-qn'|e^{-iq\cdot r}|kn\rangle\langle kn|e^{iq\cdot r}|k-qn'\rangle}{\epsilon(kn)-\epsilon(k-qn')-\hbar(\omega+i\alpha)}\Bigg\}$$

redefining variables of summation in the 2nd term,

$$\delta\rho_q = +e\sum_{knn'}(f_{kn}-f_{k+qn'})\frac{|\langle k+qn'|e^{iq\cdot r}|kn\rangle|^2 U_q}{\epsilon(k+qn')-\epsilon(kn)-\hbar(\omega+i\alpha)}$$

Then using $\epsilon_{RPA}(q\omega) = 1 + \frac{4\pi e^2}{q^2} \frac{\delta \rho_q}{\delta U_{ext\,q}}$

we get the RPA or SCF dielectric function

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

$$\epsilon(q,0) = 1 + \frac{4\pi e^2}{q^2 V} \sum_{knn'} \left| \langle k+q\, n' | e^{iq\cdot r} | kn \rangle \right|^2 \left[\frac{f(kn) - f(k+q\, n')}{\epsilon(k+q\, n') - \epsilon(kn)} \right]$$

The matrix element simplifies when $q \to 0$

$$\lim_{q \to 0} \langle k+q\, n' | e^{iq\cdot r} | kn \rangle = \langle kn' | kn \rangle = \delta_{nn'} \, .$$

$$\epsilon(q,0) \longrightarrow 1 + \frac{4\pi e^2}{q^2 V} \sum_{kn} \left[\frac{f(kn) - f(k+q\, n)}{\epsilon(k+q\, n) - \epsilon(kn)} \right]$$

$[\;]$ has numerator and denominator smooth functions of q which $\to 0$ as $q \to 0$.

$$[\;] \longrightarrow -\frac{\partial f}{\partial \epsilon_{kn}} \longrightarrow \delta(\epsilon_{kn} - \mu) \quad \text{if } k_B T \ll \mu$$

$$\epsilon(q,0) = 1 + \frac{4\pi e^2}{V q^2} \sum_{kn} \delta(\epsilon_{kn} - \mu) = 1 + \frac{4\pi e^2}{q^2} D(\mu)$$

$$= 1 + \frac{k_{FT}^2}{q^2} \quad \text{where } k_{FT}^2 = 4\pi e^2 D(\mu)$$

3. For a system of massless Bosons (photons, phonons) the relevant space of states is spanned by the occupation number states, $|n_1,\ldots,n_i,\ldots\rangle$, 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

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

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

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

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 $|n_1,\ldots,n_i,\ldots\rangle$ is an eigenstates 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 $\beta\hbar\omega_i = 1$.

$$\langle n\rangle = \sum_n n P_n = \sum_n n e^{-nx}/(1-e^{-x})^{-1} \quad \text{where } x = \beta\hbar\omega$$
$$= -(1-e^{-x})\frac{d}{dx}\sum_n e^{-nx} = -(1-e^{-x})\frac{d}{dx}(1-e^{-x})^{-1}$$
$$= \frac{e^{-x}}{1-e^{-x}} = \boxed{\frac{1}{e^{x}-1} = \langle n\rangle}$$

$$\langle n^2\rangle = \sum_n n P_n = (1-e^{-x})\frac{d^2}{dx^2}\sum_n e^{-nx}$$
$$= (1-e^{-x})\frac{d}{dx}\left(\frac{-e^{-x}}{(1-e^{-x})^2}\right) = (1-e^{-x})\left[\frac{e^{-x}}{(1-e^{-x})^2} + \frac{2e^{-x}e^{-x}}{(1-e^{-x})^3}\right]$$
$$= \frac{e^{-x}}{1-e^{-x}}\left[1+\frac{2}{e^{x}-1}\right] = \langle n\rangle(2\langle n\rangle+1)$$

$$\boxed{\langle n^2\rangle - \langle n\rangle^2 = \langle n\rangle^2 + \langle n\rangle}$$

when $x=1$, $\langle n\rangle = \frac{1}{e^1-1} = \underline{0.58}$

$$\langle n^2\rangle - \langle n\rangle^2 = (0.58)^2 + (0.58) = \underline{0.92}$$

$$\frac{\sqrt{\langle n^2\rangle - \langle n\rangle^2}}{\langle n\rangle} = \sqrt{1+\frac{1}{\langle n\rangle}} \longrightarrow 1 \quad \text{at high } T$$

Massless Bosons have <u>large</u> number fluctuations if they are in thermal equilibrium (i.e. able to be emitted + absorbed by a black body.)

4. For massive Fermions, the same definitions work with a modification. The space of states is again spanned by the basis states $|n_1,\ldots,n_i,\ldots\rangle$, 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 $|n_1,\ldots,n_i,\ldots\rangle$, unrestricted as to total occupancy, is called "Fock space." The definition of creation and destruction operators is

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

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

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

where the partition function Z_i of the i$^{\text{th}}$ mode is the usual grand canonical ensemble result, $Z_i = 1+\exp[-\beta(\varepsilon_i-\mu)]$. Again, the operator $\hat{n}_i \equiv c_i^+c_i$ is the "number operator", because the state $|n_1,\ldots,n_i,\ldots\rangle$ is an eigenstates of $\hat{n}_i$ with eigenvalue n_i. Use the definitions above to prove that the thermal average occupancy is $\langle\hat{n}_i\rangle = [\exp(\beta(\varepsilon_i-\mu))+1]^{-1}$, 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 $\beta(\varepsilon_i-\mu)=1$. 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 $\sqrt{\langle\hat{N}^2\rangle-\langle\hat{N}\rangle^2}$ is small compared to N.

Let $x = \beta(\epsilon-\mu)$

$\langle n\rangle = \sum_n n P_n = 1\cdot P_1 + 2\cdot P_2 + \ldots = P_1$ since $P_n = 0$ for $n>1$

$= e^{-x}/Z = e^{-x}/(1+e^{-x}) = 1/(e^x+1) = f =$ Fermi-Dirac fn

$\langle n^2\rangle = \sum_n n^2 P_n = P_1 = \langle n\rangle = f.$ When $x=1$, $f = \frac{1}{e+1} = 0.27$

$\langle n^2\rangle - \langle n\rangle^2 = f(1-f)$ $\qquad f(1-f) = 0.20$

$\frac{\sqrt{\langle n^2\rangle-\langle n\rangle^2}}{\langle n\rangle} = \frac{\sqrt{0.20}}{0.27} = 1.65.$

Fluctuations of occupancy are large for states with $\epsilon_i-\mu$ of order k_BT.

$\langle N\rangle = \sum_i f_i \qquad \langle N^2\rangle = \sum_{ij}\langle n_i n_j\rangle = \sum_{i\neq j} f_i f_j + \sum_i f_i$

$\boxed{\langle N^2\rangle - \langle N\rangle^2 = \sum_i f_i(1-f_i)} < \sum_i f_i = \langle N\rangle$

$\sqrt{\langle N^2\rangle-\langle N\rangle^2} < \sqrt{\langle N\rangle} \ll \langle N\rangle$ QED.