Condensed Matter - HW 8 :: Dielectric function.

PHSX 545

Problem 1

Collaborative effort: form a team that includes 'theorist' and 'experimentalist' (several people on the team is OK):

Tasks:

Theory: Find the imaginary part of dielectirc function $\varepsilon''(\mathbf{q},\omega)$ in RPA for classical electron gas obeying Maxwell-Boltzmann statistics.

Experiment: provided formula from theory, create a 3D (or better, 2D color plot) of $\omega\varepsilon''$ and $-\chi''$ in q,ω-plane and interpret them. Choose convenient dimensionless units in terms of temperature.

Problem 2

Calculate $\varepsilon(\mathbf{q},\omega)$ in RPA for the two-dimensional electron gas at zero temperature. Show that susceptibility can be given by analytic expression (hint: treat the two Dirac-Fermi distributions in χ_0 separately). Find the explicit expression for two non-vanishing terms of the plasmon dispersion $\omega(q)$ in the long wavelength limit.

(You may again form theory and experiment collaboration: the experimental people can plot the imaginary part of the susceptibility to determine where the plasmon mode is damped, and also graphically find the exact plasmon dispersion.)

Answer of exercise 1

The dielectric function in RPA approximation is

$$\varepsilon(\mathbf{q},\omega) = 1 - \frac{4\pi e^2}{q^2}\chi_0(\mathbf{q},\omega) \qquad\qquad \chi_0(\mathbf{q},\omega) = \sum_{\mathbf{p}} \frac{n_{\mathbf{p+q}} - n_{\mathbf{p}}}{\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}} - \hbar\omega - i0^+}$$

For this problem we will use Maxwell-Boltzmann distribution with chemical potential fixed by particle density

$$n_{\mathbf{p}} = e^{-\beta(\varepsilon_{\mathbf{p}}-\mu)} \qquad n_0 = \sum_{\mathbf{p}} n_{\mathbf{p}} = e^{\beta\mu}\int \frac{d^3p}{(h)^3} e^{-(\mathbf{p}^2/2mT)} = e^{\beta\mu}\left(\frac{2\pi mT}{h^2}\right)^{3/2}$$

The imaginary part of the dielectric function is

$$\varepsilon''(\mathbf{q},\omega) = -\frac{4\pi e^2}{q^2}\chi_0''(\mathbf{q},\omega) = -\frac{4\pi e^2}{q^2}\pi\sum_{\mathbf{p}}(n_{\mathbf{p+q}} - n_{\mathbf{p}})\delta(\varepsilon_{\mathbf{p+q}} - \varepsilon_{\mathbf{p}} - \hbar\omega)$$

The delta-function relates the energies of particle and hole excitations involved in the process of interacting with external field, and also gives constraints on the possible momenta $\mathbf{p}$. Since the system is isotropic we can choose $\mathbf{q}$ to be the z-axis direction, and one can write

$$\varepsilon''(\mathbf{q},\omega) = -\frac{4\pi e^2}{q^2}\pi\sum_{p_x,p_y,\,p_z}\left[n(\varepsilon_{\mathbf{p}} + \hbar\omega) - n(\varepsilon_{\mathbf{p}})\right]\delta\left(\frac{p_z\hbar q}{m} + \frac{\hbar^2q^2}{2m} - \hbar\omega\right)$$

$$= \frac{4\pi e^2}{q^2}\pi\left(1 - e^{-\beta\hbar\omega}\right)e^{\beta\mu}\int\frac{dp_xdp_ydp_z}{(h)^3}e^{-(\mathbf{p}^2/2mT)}\,\delta\left(\frac{p_z\hbar q}{m} + \frac{\hbar^2q^2}{2m} - \hbar\omega\right)$$

Do the x, y Gaussian integrals, and eliminate chemical potential,

$$\varepsilon''(\mathbf{q},\omega) = \frac{4\pi^2e^2}{q^2}\left(1 - e^{-\beta\hbar\omega}\right)n_0\int\frac{dp_z}{\sqrt{2\pi mT}}e^{-(p_z^2/2mT)}\,\delta\left(\frac{p_z\hbar q}{m} + \frac{\hbar^2q^2}{2m} - \hbar\omega\right)$$

$$= \frac{4\pi^2e^2}{q^2}\left(1 - e^{-\beta\hbar\omega}\right)n_0\frac{m}{\hbar q\sqrt{2\pi mT}}e^{-(p_z^2/2mT)}\Big|_{p_z=(m/\hbar q)(\hbar\omega - \frac{\hbar^2q^2}{2m})}$$

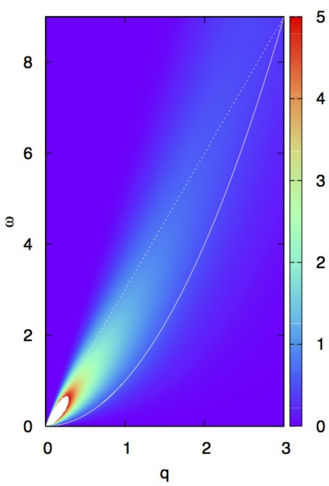
$$= \frac{4\pi^2e^2mn_0}{\hbar\sqrt{2\pi mT}\,q^3}\left(1 - e^{-\beta\hbar\omega}\right)\exp\left(-\frac{m}{2(\hbar q)^2T}\left[\hbar\omega - \frac{\hbar^2q^2}{2m}\right]^2\right)$$

Introduce dimensionless variables

$$y = \frac{\hbar\omega}{T} \qquad\qquad x = \frac{\hbar q}{\sqrt{2mT}}$$

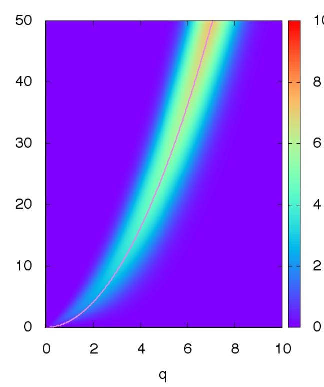
and write the imaginary part of dielectric function as

$$\omega\varepsilon''(q,\omega) = \frac{\pi^{3/2}n_0\hbar}{2mT}\frac{y}{x^3}\left(1 - e^{-y}\right)\exp\left(-\frac{(y - x^2)^2}{4x^2}\right)$$



Function $\omega\varepsilon''$ determines the rate of energy absorption by the medium in unit volume. The plot of this function is shown on the right. It indicates that the max absorption of EM waves will be just above $\hbar\omega = \hbar^2q^2/2m$ white line.

The better view is maybe from the second plot, that depicts $-\omega\chi''(q,\omega)$. This eliminates the extra $1/q^2$ factor in front and clearly shows the quadratic dispersion.



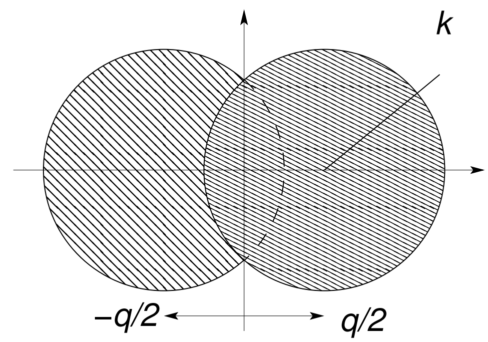
Answer of exercise 2

The dielectric function in RPA approximation is

$$\varepsilon(\mathbf{q},\omega) = 1 - \frac{4\pi e^2}{q^2}\chi_0(\mathbf{q},\omega)$$

and the susceptibility in 2D case is

$$\chi_0(\mathbf{q},\omega) = \int \frac{d^2p}{h^2}\frac{n_{\mathbf{p}+\mathbf{q}/2} - n_{\mathbf{p}-\mathbf{q}/2}}{\varepsilon_{\mathbf{p}+\mathbf{q}/2} - \varepsilon_{\mathbf{p}-\mathbf{q}/2} - \hbar\omega - i0^+}$$



The density of states in 2D gas is energy independent, and it is related to the particle density via:

$$N_f = \frac{2\pi m}{h^2} \qquad n_0 = \frac{\pi p_f^2}{h^2} = N_f \varepsilon_f$$

We split the integral in two, and integrate in polar coordinates centered at the origins of two Dirac-Fermi circles:

$$\chi_0(\mathbf{q},\omega) = \int \frac{d^2p}{h^2}\left[\frac{n_{\mathbf{p}+\mathbf{q}/2}}{\varepsilon_{\mathbf{p}+\mathbf{q}/2} - \varepsilon_{\mathbf{p}-\mathbf{q}/2} - \hbar\omega} - \frac{n_{\mathbf{p}-\mathbf{q}/2}}{\varepsilon_{\mathbf{p}+\mathbf{q}/2} - \varepsilon_{\mathbf{p}-\mathbf{q}/2} - \hbar\omega}\right]$$

$$= \int \frac{d^2p}{h^2}\left[\frac{n_{\mathbf{p}}}{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}-\mathbf{q}} - \hbar\omega} - \frac{n_{\mathbf{p}}}{\varepsilon_{\mathbf{p}+\mathbf{q}} - \varepsilon_{\mathbf{p}} - \hbar\omega}\right] = \frac{2\pi}{h^2}\int_0^{p_f} pdp \int_0^{2\pi}\frac{d\phi}{2\pi}\left[\frac{1}{\mathbf{pq}/m - (\hbar\omega + q^2/2m)} - \frac{1}{\mathbf{pq}/m - (\hbar\omega - q^2/2m)}\right]$$

and we remember that ω has small positive imaginary part.

$$\chi_0(\mathbf{q},\omega) = N_f \int_0^{p_f} pdp \frac{1}{pq}\int_0^{2\pi}\frac{d\phi}{2\pi}\left[\frac{1}{\cos\phi - m(\hbar\omega + q^2/2m)/pq} - \frac{1}{\cos\phi - m(\hbar\omega - q^2/2m)/pq}\right]$$

We take the angle integral first with standard sub $z = e^{i\phi}$:

$$\int_0^{2\pi}\frac{d\phi}{2\pi}\frac{1}{\cos\phi - a} = \frac{2}{2\pi i}\oint_{|z|=1}\frac{dz}{z^2 - 2az + 1} = \frac{2}{2\pi i}\oint_{|z|=1}\frac{dz}{(z-a)^2 + 1 - a^2} = \frac{2}{z_{in} - z_{out}}$$

where the $z_{in/out}$ are poles inside/outside the circle $|z| = 1$.

For $|Re(a)| > 1$ the poles are $z_{in} = sgn(a)(|a| - \sqrt{a^2-1})$, $z_{out} = sgn(a)(|a| + \sqrt{a^2-1})$;

For $|Re(a)| < 1$ we need to use the small positive imaginary part of a to determine which of the poles $z_\pm = a \pm i\sqrt{1-a^2}$ is inside the unit circle. Taking $a = a + i\varepsilon$ and expanding in ε we have $|z_\pm|^2 = |a + i\varepsilon \pm i\sqrt{1 - a^2 - i2a\varepsilon}|^2 \approx |a + i\varepsilon \pm i(\sqrt{1-a^2} - ia\varepsilon/\sqrt{1-a^2})|^2 = |a \pm a\varepsilon/\sqrt{1-a^2} + i\varepsilon \pm i\sqrt{1-a^2}|^2 = a^2(1 \pm \varepsilon/\sqrt{1-a^2})^2 + (\sqrt{1-a^2} \pm \varepsilon)^2 = a^2 \pm 2a^2\varepsilon/\sqrt{1-a^2} + (1-a^2) \pm 2\varepsilon\sqrt{1-a^2} = 1 \pm 2\varepsilon/\sqrt{1-a^2}$ So we have for $Re(a^2) < 1$: $z_{in} = a - i\sqrt{1-a^2}$ and $z_{out} = a + i\sqrt{1-a^2}$. Combining all together we can write the two cases in a unified way:

$$\int_0^{2\pi}\frac{d\phi}{2\pi}\frac{1}{\cos\phi - a} = \left\{\begin{array}{lll} -\dfrac{sgn(a)}{\sqrt{a^2-1}} & , \quad if & |Re(a)| > 1 \\ -\dfrac{1}{i\sqrt{1-a^2}} & , \quad if & |Re(a)| < 1 \end{array}\right\} = \frac{i}{\sqrt{1-a^2}} = -\frac{sgn(a)}{\sqrt{a^2-1}},$$

assuming the square root's branch-cut is along the negative real value of the argument.

For the susceptibility we get

$$\chi_0(\mathbf{q},\omega) = \frac{N_f}{q}\int_0^{p_f} pdp\left[\frac{sgn(\hbar\omega - q^2/2m)}{\sqrt{(m\hbar\omega/q - q/2)^2 - p^2}} - \frac{sgn(\hbar\omega + q^2/2m)}{\sqrt{(m\hbar\omega/q + q/2)^2 - p^2}}\right]$$

$$\chi_0(\mathbf{q},\omega) = -\frac{N_f}{q}\left[sgn(\hbar\omega - q^2/2m)\sqrt{(m\hbar\omega/q - q/2)^2 - p^2} - sgn(\hbar\omega + q^2/2m)\sqrt{(m\hbar\omega/q + q/2)^2 - p^2}\right]\Big|_0^{p_f}$$

$$\chi_0(\mathbf{q},\omega) = \frac{N_f}{q}\left[sgn(\hbar\omega + q^2/2m)\sqrt{(m\hbar\omega/q + q/2)^2 - p_f^2} - sgn(\hbar\omega - q^2/2m)\sqrt{(m\hbar\omega/q - q/2)^2 - p_f^2} - q\right] \qquad (1)$$

This is the exact general expression for susceptibility. The imaginary part $-\chi''$ gives the region (q,ω) of damped plasma oscillations. (Note 2 below).

In the long wavelength limit we expand in powers of q, foreseeing that the frequency is high:

$$\sqrt{(m\hbar\omega/q + q/2)^2 - p_f^2} - \sqrt{(m\hbar\omega/q - q/2)^2 - p_f^2} = \frac{m\hbar\omega}{q}\sqrt{\left(1+\frac{q^2}{2m\hbar\omega}\right)^2 - \frac{q^2v_f^2}{(\hbar\omega)^2}} - \frac{m\hbar\omega}{q}\sqrt{\left(1-\frac{q^2}{2m\hbar\omega}\right)^2 - \frac{q^2v_f^2}{(\hbar\omega)^2}}$$

$$\approx \frac{m\hbar\omega}{q}\frac{q^2}{m\hbar\omega}\left[1 + \frac{1}{2}\left(\frac{v_fq}{\hbar\omega}\right)^2 + \frac{3}{8}\left(\frac{v_fq}{\hbar\omega}\right)^4\right] = q\left[1 + \frac{1}{2}\left(\frac{v_fq}{\hbar\omega}\right)^2 + \frac{3}{8}\left(\frac{v_fq}{\hbar\omega}\right)^4\right]$$

and the plasmon dispersion is given by:

$$1 - \frac{4\pi e^2}{q^2}\chi_0(q,\omega) = 0 \qquad \Rightarrow \qquad 1 - \frac{4\pi e^2}{q^2}N_f\left[\frac{1}{2}\left(\frac{v_fq}{\hbar\omega}\right)^2 + \frac{3}{8}\left(\frac{v_fq}{\hbar\omega}\right)^4\right] = 0$$

and finally

$$1 - \frac{4\pi e^2 n_0}{m\omega^2}\left[1 + \frac{3}{4}\left(\frac{v_fq}{\omega}\right)^2\right] = 0 \qquad \Rightarrow \qquad \boxed{\omega^2(q) = \omega_p^2\left[1 + \frac{3}{4}\frac{v_f^2q^2}{\omega_p^2}\right]} \qquad \omega_p^2 = \frac{4\pi e^2 n_0}{m}$$

Note 1: We could have obtained this by doing q-expansion from the beginning:

$$\chi_0(\mathbf{q},\omega) = \int \frac{d^2p}{h^2}\frac{n_{\mathbf{p}+\mathbf{q}/2} - n_{\mathbf{p}-\mathbf{q}/2}}{\varepsilon_{\mathbf{p}+\mathbf{q}/2} - \varepsilon_{\mathbf{p}-\mathbf{q}/2} - \hbar\omega - i0^+} = \int \frac{d^2p}{h^2}\left(\frac{\partial n_\mathbf{p}}{\partial \varepsilon_\mathbf{p}}\right)\frac{\mathbf{vq}}{\mathbf{vq} - \hbar\omega} = \frac{N_f}{\hbar\omega}\int_0^{2\pi}\frac{d\phi}{2\pi}(\mathbf{v}_f\mathbf{q})\left[1 - \frac{\mathbf{v}_f\mathbf{q}}{\hbar\omega}\right]^{-1}$$

$$= \frac{N_f}{\hbar\omega}\int_0^{2\pi}\frac{d\phi}{2\pi}\left[\frac{(\mathbf{v}_f\mathbf{q})^2}{\hbar\omega} + \frac{(\mathbf{v}_f\mathbf{q})^4}{(\hbar\omega)^3}\right] = \frac{N_f}{(\hbar\omega)^2}q^2v_f^2\left[\frac{1}{2} + \frac{3}{8}\frac{(v_fq)^2}{(\hbar\omega)^2}\right]$$

- same limiting expression for susceptibility as before.

Note 2: The region of damping is given by the non-vanishing imaginary part of the susceptibility Eq.(1) which we write in this form now:

$$\chi_0(\mathbf{q},\omega) = \frac{N_f}{q}\left[i\sqrt{p_f^2 - (m\hbar\omega/q + q/2)^2} - i\sqrt{p_f^2 - (m\hbar\omega/q - q/2)^2} - q\right].$$

The damped region is found when the imaginary part of the susceptibility is negative. Since the second square root in this expression is always greater than the first one in the first quadrant of the (q,ω)-plane, the second square root determines the damping region:

$$p_f^2 > (m\hbar\omega/q - q/2)^2 \qquad \Rightarrow \qquad -v_fq < \hbar\omega - \frac{q^2}{2m} < v_fq \qquad \Rightarrow \qquad \boxed{-v_fq + \frac{q^2}{2m} < \hbar\omega < v_fq + \frac{q^2}{2m}}$$

which is the particle-hole continuum that we have also seen in 3D case.