Ph223b **Problem Set #2 (Parts III.8 – III.9)** February 6, 2006
(Due: February 22, 2006)

1. Plasma oscillations in an electron gas

We have shown in Part III.9 that the linear response function of the density of an electron gas to an external perturbation is the retarded polarization propagator $\Pi^R(\mathbf{q},\omega)$, and that the poles of $\Pi^R(\mathbf{q},\omega)$ are associated with the excitation energies of collective modes in the interacting electron gas. In this problem we want to investigate a specific type of collective excitations of the degenerate electron gas known as the plasma oscillations. We shall restrict our consideration in the following to the ring diagrams.

(a) In the random phase approximation (RPA), the dielectric constant associated with the linear response of the density perturbation to an external impulsive potential $\varphi^{\text{ex}}(\mathbf{x},t) = e^{i\mathbf{q}\cdot\mathbf{x}}\varphi_0\,\delta(t)$ is given by $\varepsilon_r^R(\mathbf{q},\omega) = 1 - V(\mathbf{q})\Pi^{0R}(\mathbf{q},\omega)$, where $\Pi^{0R}(\mathbf{q},\omega)$ is the lowest order retarded polarization propagator. For $\omega = \Omega_p - i\gamma_p$ representing the poles so that $V(\mathbf{q})\Pi^{0R}(\mathbf{q},\Omega_p - i\gamma_p) = 1$, verify that in the limit of very small damping of the collective modes $\gamma_p \ll \Omega_p$ the following conditions are satisfied:

$$V(\mathbf{q})\,\text{Re}\left\{\Pi^{0R}(\mathbf{q},\Omega_p)\right\} = V(\mathbf{q})\,\text{Re}\left\{\Pi^{0}(\mathbf{q},\Omega_p)\right\} = 1,$$

$$\gamma_{\mathbf{q}} = \text{Im}\left\{\Pi^{0R}(\mathbf{q},\Omega_p)\right\}\left[\left.\frac{\partial\,\text{Re}\left\{\Pi^{0R}(\mathbf{q},\omega)\right\}}{\partial\omega}\right|_{\Omega_p}\right]^{-1}$$

$$= \text{sgn}(\Omega_p)\,\text{Im}\left\{\Pi^{0}(\mathbf{q},\Omega_p)\right\}\left[\left.\frac{\partial\,\text{Re}\left\{\Pi^{0}(\mathbf{q},\omega)\right\}}{\partial\omega}\right|_{\Omega_p}\right]^{-1}.$$

(b) Using the results derived for $\Pi^0(\mathbf{q},\omega)$ in the limit of a fixed frequency ω and for $|\mathbf{q}| \equiv q \to 0$, show that for a three-dimensional spherical Fermi surface, the dielectric constant associated with the RPA is real and is given by

$$\lim_{q\to 0}\varepsilon_r^R(\mathbf{q},\omega) = 1 - \frac{\left(4\pi ne^2/m\right)}{\omega^2} \equiv 1 - \left(\frac{\omega_p}{\omega}\right)^2.$$

Here n and m denotes the carrier density and mass, respectively, and ω_p is the plasma frequency.

(c) From the expression for $\text{Re}\{\Pi^0(\mathbf{q},\omega)\}$ in EQ. (III.599), show that in the small q limit

$$\text{Re}\left\{\Pi^{0R}(\mathbf{q},\omega)\right\} = \frac{k_F^3 q^2}{3\pi^2 m\omega^2}\left[1 + \frac{3}{5}\left(\frac{k_F q}{m\omega}\right)^2 + \cdots\right],$$

where k_F is the Fermi momentum, and the dispersion relation for the plasma oscillation is given by

$$\Omega_q = \pm\omega_p\left[1 + \frac{9}{10}\left(\frac{q^2\varepsilon_F}{6\pi ne^2}\right) + \cdots\right] \equiv \pm\omega_p\left[1 + \frac{9}{10}\left(\frac{q}{q_{TF}}\right)^2 + \cdots\right],$$

where q_{TF} is known as the Thomas-Fermi wave number. We remark that in the RPA, $\text{Im}\{\Pi^0(\mathbf{q},\Omega_q)\} = 0$ if $\left|\Omega_q\right| > (qk_F/m) + (q^2/2m)$, which implies that these plasma collective modes at long wavelengths are undamped in the lowest-order approximation. In reality, it can be shown that plasma oscillations are damped at all wavelengths if higher-order corrections are included.

2. Thomas-Fermi approximation and Friedel oscillations

In the previous problem we investigate the collective modes of a degenerate electron gas in response to an impulsive external perturbation. Here we consider another extreme case of the linear response of a degenerate electron gas to a static external perturbation. Specifically, we assume an impurity with positive point charge *Ze* locating at the origin, so that the external perturbation potential is given by

$$\varphi^{\text{ex}}(\mathbf{x},t)=\frac{Ze}{|\mathbf{x}|} \quad \Rightarrow \quad \varphi^{\text{ex}}(\mathbf{q},\omega)=\frac{8\pi^2 Ze}{|\mathbf{q}|^2}\delta(\omega).$$

(a) Under the assumption of random phase approximation, show that the dielectric constant associated with the retarded density-density correlation function is given by

$$\varepsilon_r^R(\mathbf{q},0)=\varepsilon_r(\mathbf{q},0)=1+\frac{4me^2k_F}{\pi q^2}\,g\left(\frac{q}{k_F}\right), \quad \text{where } g(x)\equiv\frac{1}{2}-\frac{1}{2x}\left(1-\frac{x^2}{4}\right)\ln\left|\frac{1-(x/2)}{1+(x/2)}\right|.$$

(b) From the result in part (a), show that the induced charge density due to the point charge impurity is

$$\delta\langle\rho(\mathbf{x})\rangle_r=-e\delta\langle n(\mathbf{x})\rangle_r=-Ze\int\frac{d^3q}{(2\pi)^3}e^{i\mathbf{q}\cdot\mathbf{x}}\left[\frac{4me^2(\pi k_F)^{-1}g(q/k_F)}{(q/k_F)^2+4me^2(\pi k_F)^{-1}g(q/k_F)}\right],$$

and that the total induced charge is

$$\delta Q_r\equiv\int d^3\mathbf{x}\,\delta\langle\rho(\mathbf{x})\rangle_r=-Ze.$$

In other words, the point charge impurity is completely screened by the electron gas at a long distance.

(c) In the long-wavelength limit, the induced charge density has a cutoff at the Thomas-Fermi wavelength

$$q_{TF}\equiv\left(4me^2k_F/\pi\right)^{1/2}.$$

If we neglect the singularity of $g(x)$ at $x = 2$, the induced charge density has the following asymptotic form in the $|\mathbf{x}|\to\infty$ limit, which is known as the *Thomas-Fermi approximation*:

$$\delta\langle\rho(\mathbf{x})\rangle_r\sim\delta\rho_{TF}(\mathbf{x})=-Zeq_{TF}^2\left(4\pi|\mathbf{x}|\right)^{-1}e^{-q_{TF}|\mathbf{x}|}.$$

Strictly speaking, however, the Thomas-Fermi approximation is not correct. A more complete consideration can be made by rewriting the induced charge density in part (b) as follows:

$$\delta\langle\rho(\mathbf{x})\rangle_r=\frac{Ze}{4\pi^2 i|\mathbf{x}|}\int_{-\infty}^{\infty}q\,dq\,e^{i\mathbf{q}\cdot\mathbf{x}}\left[\frac{q^2}{q^2+q_{TF}^2\,g(q/k_F)}-1\right].$$

Using the above expression for the induced charge density, show that its asymptotic form is given by

$$\lim_{|\mathbf{x}|\to\infty}\delta\langle\rho(\mathbf{x})\rangle_r\sim\frac{Ze}{\pi}\frac{2\left(q_{TF}^2/2k_F^2\right)}{\left[4+\left(q_{TF}^2/2k_F^2\right)\right]^2}\frac{\cos\left(2k_F|\mathbf{x}|\right)}{|\mathbf{x}|^3}$$

This long-wavelength oscillatory behavior in the induced charge density is well verified experimentally, which is known as the *Friedel oscillations*. In fact, this behavior is not limited to charge distributions. It is also found that in dilute magnetic alloys, the conduction electrons induce an indirect exchange interaction with the magnetic impurities via the same spatial dependence. This type of long-range oscillations in the screening charge density is the consequence of a sharp Fermi surface, so that it is not possible to construct a smooth function out of a restricted set of wave vectors with $q > k_F$.

3. Linear response, fluctuation-dissipation theorem & correlation functions

We have seen in Part III.9 that the general theory of linear response can be applied to the collective excitations of a system in response to external perturbation and also to the fluctuation-dissipation theorem. To investigate these issues further, we define a generalized retarded Green's function $\mathcal{G}^R$ and a generalized time-ordered Green's function $\mathcal{G}$ for operators A and B as follows:

$$\mathcal{G}^R(t) = -i\,\theta(t)\left\langle\left[A(t), B(0)\right]\right\rangle, \quad \mathcal{G}(t) = -i\left\langle T\left[A(t)B(0)\right]\right\rangle.$$

For a system with a Hamiltonian $\mathcal{H}$ and a complete set of eigen-states $\{|n\rangle\}$ such that $\mathcal{H}|n\rangle = \varepsilon_n|n\rangle$, the thermal average $\langle A(t)B(0)\rangle$ is given by

$$\left\langle A(t)B(0)\right\rangle = Z^{-1}\mathrm{Tr}\left\{e^{-\beta\mathcal{H}}e^{i\mathcal{H}t}Ae^{-i\mathcal{H}t}B\right\} = Z^{-1}\sum_n\left\langle n\right|e^{-\beta\mathcal{H}}e^{i\mathcal{H}t}Ae^{-i\mathcal{H}t}B\left|n\right\rangle,$$

where Z is the partition function.

(a) If we denote the Fourier transform of $\langle A(t)B(0)\rangle$ by $J_1(\omega)$, which is also known as the spectral density function associated with the time-ordered Green's function $\langle A(t)B(0)\rangle$, show that the Fourier transforms of the equivalent retarded Green's function $\mathcal{G}^R$ and the time-ordered Green's function $\mathcal{G}$ at $T = \beta^{-1}$ have the following forms (with $\eta = 0^+$):

$$\mathcal{G}^R(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left(1-e^{-\beta\omega'}\right)\frac{J_1(\omega')}{\omega-\omega'+i\eta}, \text{ and } \mathcal{G}(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}J_1(\omega')\left[\frac{1}{\omega-\omega'+i\eta} - \frac{e^{-\beta\omega'}}{\omega-\omega'-i\eta}\right].$$

If A and B are hermitian conjugates so that $J_1(\omega)$ is real, verify that

$$\mathrm{Im}\left\{\mathcal{G}^R(\omega)\right\} = -\frac{1}{2}\left(1-e^{-\beta\omega}\right)J_1(\omega) = \tanh\left(\frac{1}{2}\beta\omega\right)\mathrm{Im}\left\{\mathcal{G}(\omega)\right\},$$

$$\Rightarrow \quad J_1(\omega\neq 0) = -\frac{2}{1-e^{-\beta\omega}}\mathrm{Im}\left\{\mathcal{G}^R(\omega)\right\}.$$

The last line is a form of the fluctuation-dissipation theorem. In other words, the spectral response of the system (*i.e.* fluctuations) to an external perturbation at $t > 0$ gives rise to dissipation manifested by the imaginary part of the retarded Green's function.

(b) Now let's consider an explicit example with $A(t)$ and $B(0)$ replaced by the density operators of a free Fermi gas:

$$A(t) \Rightarrow c^\dagger(\mathbf{x},t)\,c(\mathbf{x},t), \quad B(0) \Rightarrow c^\dagger(0,0)\,c(0,0),$$

so that the corresponding retarded Green's function becomes the lowest-order retarded polarization Π^{0R}. Assuming $T = 0$ and in the small $\mathbf{q}$ and ω limit with $\omega/|\mathbf{q}|$ fixed, verify that the Fourier transforms of the retarded correlation functions for different spatial dimensions $d = 3, 2, 1$ satisfy the following relations:

$$\Pi^{0R}(\mathbf{q},\omega) = -\frac{mk_F}{2\pi^2}\left\{\left[1-\left(\frac{\omega}{2qv_F}\right)\ln\left|\frac{\omega+qv_F}{\omega-qv_F}\right|\right] + i\left[\frac{\pi\omega}{2qv_F}\theta\left(qv_F-|\omega|\right)\right]\right\} \qquad \text{for } d = 3,$$

$$= -\frac{m}{2\pi}\left\{\left[1-\frac{\omega\,\theta\left(|\omega|-qv_F\right)}{\sqrt{\omega^2-(qv_F)^2}}\right] + i\left[\frac{\omega\theta\left(qv_F-|\omega|\right)}{\sqrt{(qv_F)^2-\omega^2}}\right]\right\} \qquad \text{for } d = 2,$$

$$= \frac{1}{\pi}\frac{v_F q^2}{\left(\omega+i0^+\right)^2-\left(qv_F\right)^2} \qquad \text{for } d = 1.$$

4. Magnetic susceptibility in the generalized Hartree-Fock approximation

We have introduced the transverse magnetic susceptibility χ^{-+} in Part III.9 as the linear response function of a spin system to an external magnetic field. Here we want to evaluate χ^{-+} explicitly under the generalized Hartree-Fock approximation, which involves summing over the ladder diagrams containing repeated interactions of electron and hole lines, as shown in Fig. III.9.1. Thus, for

$$\chi^{-+}(\mathbf{x}-\mathbf{x}',t-t') = i\theta(t-t')\left\langle\left[\sigma^{-}(\mathbf{x},t),\sigma^{+}(\mathbf{x}',t')\right]\right\rangle = \sum_{\mathbf{p},\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}\chi^{-+}(\mathbf{p},\mathbf{q};t-t')$$
$$= \sum_{\mathbf{p},\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} i\theta(t-t')\left\langle\left[a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}(t-t')\,a_{\mathbf{p}\uparrow}(t-t'),\,\sigma^{+}(0,0)\right]\right\rangle,$$

where $\sigma^{+}(\mathbf{x}) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}\sum_{\mathbf{p}} a^{\dagger}_{\mathbf{p}+\mathbf{q}\uparrow}a_{\mathbf{p}\downarrow}$ and $\sigma^{-}(\mathbf{x}) = \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}\sum_{\mathbf{p}} a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}a_{\mathbf{p}\uparrow}$, the equation of motion for $\chi^{-+}(\mathbf{p},\mathbf{q};t)$ under a Hamiltonian $\mathcal{H}$ becomes:

$$i\frac{\partial}{\partial t}\chi^{-+}(\mathbf{p},\mathbf{q};t) = -\delta(t)\left\langle\left[a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}a_{\mathbf{p}\uparrow},\,\sigma^{+}(0,0)\right]\right\rangle + i\theta(t)\left\langle\left[\left[a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}(t)\,a_{\mathbf{p}\uparrow}(t),\mathcal{H}\right],\sigma^{+}(0,0)\right]\right\rangle.$$

(a) For a model Hamiltonian (known as the Hubbard model)

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I = \left(\sum_{\mathbf{p}\sigma}\omega_{\mathbf{p}}a^{\dagger}_{\mathbf{p}\sigma}a_{\mathbf{p}\sigma}\right) + \left(\frac{U}{N}\sum_{\mathbf{p}\mathbf{p}'\mathbf{q}} a^{\dagger}_{\mathbf{p}+\mathbf{q}\uparrow}a_{\mathbf{p}\uparrow}a^{\dagger}_{\mathbf{p}'-\mathbf{q}\downarrow}a_{\mathbf{p}'\downarrow}\right),$$

with U representing an on-site repulsion potential, show that under the generalized Hartree-Fock approximation, where one sums over all Wick contractions, using the expectation value

$$\left\langle a^{\dagger}_{\mathbf{p}\alpha}a_{\mathbf{p}'\beta}\right\rangle = \delta_{\mathbf{p}\mathbf{p}'}\delta_{\alpha\beta}\,f_{\mathbf{p}\alpha}\ ,$$

the following relation holds:

$$\left[a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}(t)\,a_{\mathbf{p}\uparrow}(t),\mathcal{H}\right] = -\left(\omega_{\mathbf{p}+\mathbf{q}}-\omega_{\mathbf{p}}\right)a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}a_{\mathbf{p}\uparrow}$$
$$+\frac{U}{N}\sum_{\mathbf{p}'}\left\{\left(f_{\mathbf{p}\uparrow}-f_{\mathbf{p}+\mathbf{q}\downarrow}\right)a^{\dagger}_{\mathbf{p}+\mathbf{p}'+\mathbf{q}\downarrow}a_{\mathbf{p}+\mathbf{p}'\uparrow} + \left(f_{\mathbf{p}'\downarrow}-f_{\mathbf{p}'\uparrow}\right)a^{\dagger}_{\mathbf{p}+\mathbf{q}\downarrow}a_{\mathbf{p}\uparrow}\right\}.$$

(b) From the result in part (a) and the definitions

$$\chi(\omega) = \int_{-\infty}^{\infty} dt\,\chi(t)\,e^{i\omega t}, \qquad \chi(\mathbf{q}) = \sum_{\mathbf{p}}\chi(\mathbf{p},\mathbf{q}), \qquad \tilde{\omega}_{\mathbf{p}\sigma} \equiv \omega_{\mathbf{p}} - \frac{U}{N}\sum_{\mathbf{p}'} f_{\mathbf{p}',-\sigma}$$

verify that the Fourier transform of the transverse magnetic susceptibility satisfies the following relation:

$$\chi^{-+}(\mathbf{q},\omega) = \frac{\Gamma^{-+}(\mathbf{q},\omega)}{1-U\Gamma^{-+}(\mathbf{q},\omega)}, \text{ where } \Gamma^{-+}(\mathbf{q},\omega) = \frac{1}{N}\sum_{\mathbf{p}}\frac{f_{\mathbf{p}\uparrow}-f_{\mathbf{p}+\mathbf{q}\downarrow}}{\omega-\left(\tilde{\omega}_{\mathbf{p}\downarrow}-\tilde{\omega}_{\mathbf{p}+\mathbf{q}\uparrow}\right)+i\eta}.$$

We note that $\chi^{-+}(\mathbf{q},\omega)$ given above is the general expression for the frequency- and momentum-dependent magnetic susceptibility of an interacting electron gas, whereas the function $\Gamma^{-+}(\mathbf{q},\omega)$ is the same unperturbed particle-hole polarization propagator as appeared in the Coulomb interaction. It is worth noting that for $\omega = 0$ and $\mathbf{q} = 0$, $\Gamma^{-+}(\mathbf{q},\omega)$ reduces to the well known Pauli susceptibility, which is proportional to the density of states at the Fermi level.