

Ph225b
Problem Set #1 (Chapters IV.1. & IV.2.)

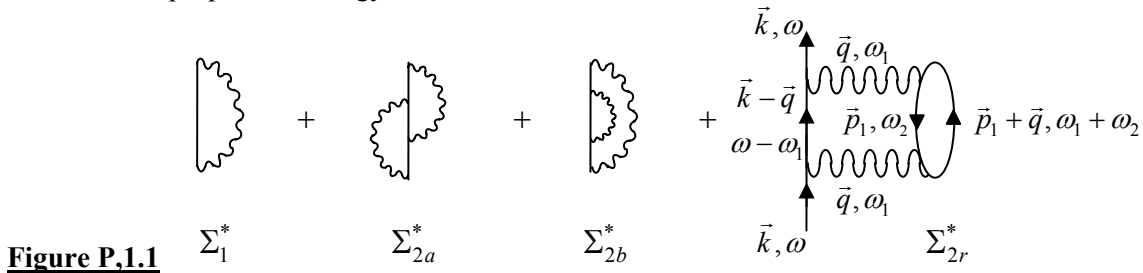
 January 5, 2005
 (due on January 24, 2005)

1. The Random Phase Approximation

In this problem we consider the diagrammatic representations of the random phase approximation that describes the dielectric response of electrons. An idealized approximation for the electronic response in a good metal, known as the “jellium model”, is to assume a high density (n) of electrons moving in the background of positive charge that ensures overall charge neutrality. The $1/r^2$ nature of the Coulomb interaction gives rise to an average potential energy per particle that is proportional to $n^{1/3}$; whereas the average kinetic energy per particle is proportional to $k_F^2/(2m) \propto n^{2/3}$ as the result of Pauli principle, with k_F being the momentum at the Fermi level. Thus, in contrast to ordinary gases, the kinetic energy dominates over the potential energy in the high-density electron system, and therefore the system behaves like a gas, known as the Fermi gas. On the other hand, in the low-density limit, the potential energy dominates, and the system becomes a solid, known as the Wigner crystal. For intermediate density, we have the Fermi liquid. We may quantify such descriptions by introducing a dimensionless quantity $r_s \equiv r_0/a_B$, where r_0 is defined as $4\pi r_0^3/3 = n = N/\Omega$, Ω is the volume of the system, and $a_B = \hbar^2/(me^2)$ is the Bohr radius. If we define the field operators $\psi = \sum_{\vec{k}} a_{\vec{k}} \psi_{\vec{k}}$ and $\psi^\dagger = \sum_{\vec{k}} a_{\vec{k}}^\dagger \psi_{\vec{k}}^*$ where $\psi_{\vec{k}}$ denotes the eigen-state, and introduce dimensionless quantities $\Omega' \equiv \Omega/r_0^3$, $k' \equiv kr_0$, $p' \equiv pr_0$, and $q' \equiv qr_0$, the Hamiltonian H of the electron system becomes

$$H = \frac{e^2}{a_B r_s^2} \left[\frac{1}{2} \sum_{\vec{k}'} k'^2 a_{\vec{k}'}^\dagger a_{\vec{k}'} + \frac{r_s}{2\Omega'} \sum_{\vec{k}', \vec{p}', \vec{q}' \neq 0} \frac{4\pi}{q'^2} a_{\vec{k}'+\vec{q}'}^\dagger a_{\vec{p}'-\vec{q}'}^\dagger a_{\vec{p}'} a_{\vec{k}'} \right], \quad (\text{P1.1})$$

We note that only Coulomb interactions with $\vec{q}' \neq 0$ are relevant. In the $r_s \rightarrow 0$ limit, the potential energy becomes negligible, and therefore we can limit contributions from the potential energy only up to second-order terms. Since diagrams with $\vec{q}' = 0$ are excluded, the remaining diagrams (see Fig. IV.1.1) that contribute to the proper self-energy are


Figure P.1.1

(a) Write down the explicit expressions for the diagrammatic contributions to Σ_{2a}^* and Σ_{2b}^* .

(b) The diagram Σ_{2r}^* is in fact troublesome and requires more careful analysis. It's contribution is given by

$$\Sigma_{2r}^*(\vec{k}, \omega) = i \int \frac{d^3 q}{(2\pi)^3} \frac{d\omega_1}{2\pi} g_0(\vec{k} - \vec{q}, \omega - \omega_1) V^2(\vec{q}) \Pi_0^*(\vec{q}, \omega_1), \quad (\text{P1.2})$$

where $-i\Pi_0^*$ is the contribution of the lowest order to the proper polarization:

$$\Pi_0^*(\vec{q}, \omega_1) = -i \int \frac{d^3 p_1}{(2\pi)^3} \frac{d\omega_2}{2\pi} g_0(\vec{p}_1, \omega_2) g_0(\vec{p}_1 + \vec{q}, \omega_1 + \omega_2). \quad (\text{P1.3})$$

If we define $\varepsilon_p = [p^2/(2m) - \varepsilon_F]$ with ε_F being the Fermi energy, prove that with the inclusion of spin degeneracy and at $T = 0$, we have

$$\Pi_0^*(\vec{q}, \omega_1) = 2 \int \frac{d^3 p_1}{(2\pi)^3} \theta(|\vec{q} + \vec{p}_1| - k_F) \theta(k_F - |\vec{p}_1|) \left[\frac{1}{\omega_1 - \omega_{\vec{q}}(\vec{p}_1) + i\eta} - \frac{1}{\omega_1 + \omega_{\vec{q}}(\vec{p}_1) - i\eta} \right], \quad (\eta > 0), \quad (\text{P1.4})$$

where $\omega_{\vec{q}}(\vec{p}) \equiv \varepsilon_{\vec{p}+\vec{q}} - \varepsilon_{\vec{p}}$. Also show that Eq. (P1.2) is logarithmically divergent in the small q limit.

(c) To prevent the divergence, we consider replacing the Coulomb potential by $[e^2 \exp(-\lambda r)/r]$ where λ is a small positive quantity, so that the Fourier transformation becomes:

$$V_\lambda(\vec{q}) = \frac{4\pi e^2}{q^2 + \lambda^2}. \quad (\text{P1.5})$$

Thus, we can use Eq. (P1.5) in the place of the interaction potential $V(q)$, sum the perturbation series in powers of V_λ , and take the limit $\lambda \rightarrow 0$ in the end. In other words, we are considering two independent small quantities, r_s and λ , and the expansion associated with λ has to sum over infinite series because the higher order terms cannot be dropped in the $\lambda \rightarrow 0$ limit. In general, for the l -th order term in V_λ , the corresponding diagram would give a contribution Σ_{lr}^* shown below and also illustrated in Figure P.1.2:

$$\Sigma_{lr}^* \sim r_s^{l-2} \int \frac{d^3 q}{(2\pi)^3} \frac{q}{(q^2 + \lambda^2)^l} \sim r_s^{l-2} \lambda^{2-l}, \quad (l = 3, 4, \dots), \quad (\text{P1.6})$$

while all other diagrams of the l -th order yields a contribution of the order $r_s^{l-2} \lambda^{3-l}$ or less. Thus, we can approximate the proper self-energy by the following:

$$\Sigma^* \simeq \Sigma_1^* + \Sigma_{2a}^* + \Sigma_{2b}^* + \sum_{l=2}^{\infty} (\Sigma_{lr}^*) = \Sigma_1^* + \Sigma_{2a}^* + \Sigma_{2b}^* + \Sigma_r^*. \quad (\text{P1.7})$$

Show that the random phase approximation (RPA) potential V_{RPA} can be obtained from the contributions of the interaction potential in Σ_1^* plus those in all the ring diagrams as follows:

$$V_{RPA} = \frac{V}{1 - V\Pi_0^*}, \quad (\text{P1.8})$$

and that the total contributions to the proper self-energy from the ring diagrams is given by:

$$\Sigma_r^*(\vec{k}, \omega) \equiv \Sigma_{2r}^*(\vec{k}, \omega) + \Sigma_{3r}^*(\vec{k}, \omega) + \dots = i \int \frac{d^3 q}{(2\pi)^3} \frac{d\omega_1}{2\pi} g_0(\vec{k} - \vec{q}, \omega - \omega_1) \frac{V^2(\vec{q}) \Pi_0^*(\vec{q}, \omega_1)}{1 - V(\vec{q}) \Pi_0^*(\vec{q}, \omega_1)}. \quad (\text{P1.9})$$

Comparing Eq. (P1.8) with Eq. (108) in Part IV.1, the random phase approximation is equivalent to replacing the proper polarization with its lowest order approximation in the interaction potential.

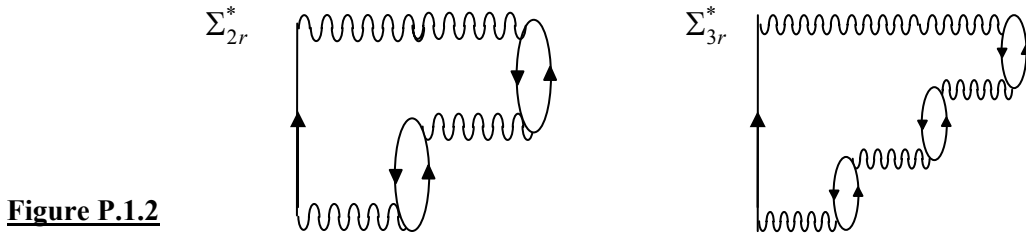


Figure P.1.2

(d) Show that the dielectric function in the random phase approximation is given by:

$$\varepsilon_{RPA}(\vec{q}, \omega) = 1 - V(\vec{q}) \Pi_0^*(\vec{q}, \omega), \quad (\text{P1.10})$$

and that in the static limit, i.e. for $\omega = 0$,

$$V_{RPA}(\vec{q}, \omega = 0) = \frac{4\pi e^2}{q^2 + q_{TF}^2 Y(q/k_F)}, \quad Y(x) \equiv \frac{1}{2} - \frac{1}{2x} \left(1 - \frac{1}{4} x^2 \right) \ln \left| \frac{2-x}{2+x} \right|, \quad (\text{P1.11})$$

where $(q_{TF})^{-1}$ is known as the Thomas-Fermi screening length.

2. Linear Response, Fluctuation-Dissipation Theorem & Kubo Formula

In a liquid or a gas under thermal equilibrium, the random impacts of molecules produce irregular driving forces. If the Brownian motion of particles is driven by an applied force, the same molecular impacts produce frictional resistive forces that can be described by certain macroscopic quantities. Since the random and systematic parts of the microscopic forces have the same physical origin, we expect a mathematical relation between them. In its general form, this relation is known as the fluctuation-dissipation theorem. [Ref.: R. Kubo, J. Phys. Soc. (Japan) **12**, 570 (1957)] In quantum mechanical terms, the fluctuations of a system in thermal equilibrium may be described by time correlation functions of the type $\langle A(t)B(0) \rangle$, where A and B are operators, or by the Fourier transforms of these correlation functions that characterize the fluctuation spectrum. The linear response to a driving force, such as the electrical conductivity to an applied electric field and the magnetic susceptibility to an applied magnetic field, is generally given by a function of the type of the retarded Green's function if we replace A and B by the field operators:

$$G^R(t) = -i\theta(t)\langle [A(t), B(0)] \rangle. \quad (\text{P1.12})$$

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

$$\langle A(t)B(0) \rangle = Z^{-1}\text{Tr}\{e^{-\beta H}e^{iHt}Ae^{-iHt}B\} = Z^{-1}\sum_n \langle n|e^{-\beta H}e^{iHt}Ae^{-iHt}B|n\rangle, \quad (\text{P1.13})$$

where Z is the partition function.

- (a) If the Fourier transform of $\langle A(t)B(0) \rangle$ is denoted by $J_1(\omega)$, which is also known as the spectral density function associated with the time correlation function $\langle A(t)B(0) \rangle$, show that the Fourier transform of the equivalent retarded Green's function has the following form:

$$G^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} (1 - e^{-\beta\omega'}) \frac{J_1(\omega')}{\omega - \omega' + i\eta}, \quad (\eta = 0^+). \quad (\text{P1.14})$$

We note that for $J_1(\omega)$ being real, which is true if A and B are the same operators or hermitian conjugates, Eq. (P1.14) gives

$$\text{Im} G^R(\omega) = -\frac{1}{2}(1 - e^{-\beta\omega})J_1(\omega), \quad \rightarrow \quad J_1(\omega \neq 0) = -\frac{2}{1 - e^{-\beta\omega}}\text{Im} G^R(\omega), \quad (\text{P1.15})$$

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

- (b) Now let's consider the dielectric response of a high-density electron gas (as described by the jellium model in the previous problem) to an external electrostatic potential $\phi_{\text{ext}}(r, t)$ that is turned on at $t = t_0$. In this case, both A and B operators can be replaced by the operator δn_I that denotes the density deviation of the electronic system from its equilibrium value n_0 in the interaction picture:

$$\delta n_I(\vec{r}, t) \equiv \psi_I^\dagger(\vec{r}, t)\psi_I(\vec{r}, t) - n_0, \quad (\text{P1.16})$$

and ψ_I is the field operator in the interaction picture. Using the fact that the external charge density is related to the external potential ϕ_{ext} through the Poisson's equation and that the dielectric function is defined as the ratio of the external charge density relative to the total charge density (*i.e.* the sum of the external and induced charge densities), show that the dielectric function is given by:

$$\varepsilon(\vec{k}, \omega) = \left[1 + \frac{4\pi e^2}{k^2} G^R(\vec{k}, \omega) \right]^{-1}. \quad (\text{P1.17})$$

- (c) The longitudinal conductivity σ is related to the dielectric function as follows:

$$\varepsilon(\vec{k}, \omega) = 1 + i(4\pi/\omega)\sigma(\vec{k}, \omega). \quad (\text{P1.18})$$

Therefore the longitudinal conductivity can be expressed in terms of G^R , or equivalently, the two-particle Green's function g_2 . Using Eqs. (P1.15), (P1.17) and the fact that δn is related to the current operator $\vec{J}(x)$ by the continuity equation,

$$\frac{\partial \rho(x)}{\partial t} + \vec{\nabla} \cdot \vec{J}(x) = 0, \quad \rho(x) \equiv \psi^\dagger(x)\psi(x), \quad (\text{P1.19})$$

find an explicit expression for the longitudinal conductivity $\sigma(\vec{k}, \omega)$ in terms of the current-current commutator. This result is a special case of the Kubo formula for longitudinal electrical conductivity in dielectric materials. [*Hint*: For simplicity, you may assume that the dielectric material under consideration is a poor conductor.]

3. Critical Dimension & Anisotropic Critical Phenomena

(a) Using the Ginzburg criterion, find the critical dimension D_c of the tri-critical point with following free energy density:

$$f = \frac{1}{2}r\phi^2 + u_6\phi^6. \quad (\text{P1.20})$$

(b) In the case of anisotropic systems, additional critical exponents must be introduced to describe the anisotropic critical phenomena. Consider an anisotropic system with the following correlation function:

$$G(x_{\parallel}, x_{\perp}, t) = b^{-(D-2+\eta)} G(b^{-(1+\mu_{\parallel})} x_{\parallel}, b^{-1} x_{\perp}, b^{1/\nu} t), \quad (\text{P1.21})$$

where $t = (T - T_c)/T_c$ is the reduced temperature, T_c denotes the critical point, and ν , η and μ_{\parallel} are critical exponents. Using Eq. (P1.21), determine the critical exponents governing the behavior of the following quantities in terms of ν , η and μ_{\parallel} : the correlation function $G(x_{\parallel}, x_{\perp} = 0, t = 0)$ and $G(x_{\parallel} = 0, x_{\perp}, t = 0)$, the correlation lengths ξ_{\parallel} and ξ_{\perp} , the magnetic susceptibility χ , and the order parameter ϕ for $t < 0$.