

## II.8. Hartree-Fock and Random Phase Approximations

The general expression for Green's functions in EQ. (II.452) in principle enables evaluations of Green's functions to all orders for given interaction potential. In practice, however, we need to devise proper approximations to solve realistic physical problems.

We have described in the previous section the diagrammatic representation of the Hartree-Fock approximation in Fig. II.7.10. In this section, we shall examine the Hartree-Fock approximation in more details, followed by discussion of the random phase approximation (RPA) for treating long-range Coulomb interaction in degenerate (i.e. high-density) Fermi gas.

### [Self-consistent solutions to the Hartree-Fock approximation]

Despite the apparent simplicity of the Hartree-Fock approximation, self-consistent solutions to the corresponding Dyson's equation are already highly non-trivial. As a heuristic example for diagrammatic analysis of many-body physics, we go over the necessary steps in the following to obtain the self-consistent solutions to a many-body system under the Hartree-Fock approximation. This approximation is also widely used in the calculations of electronic bandstructures of crystalline materials.

We begin with setting up a more generalized non-perturbed Hamiltonian  $\mathcal{H}_0$  that includes an external potential  $U_{\text{ext}}(\mathbf{r})$  and a perturbation  $\mathcal{H}_I$  that incorporates the inter-particle interaction  $U(x, x')_{\lambda\lambda', \mu\mu'}$ . For simplicity, we assume that both  $U_{\text{ext}}(\mathbf{r})$  and  $U(x, x')_{\lambda\lambda', \mu\mu'}$  are spin-independent, so that

$$U(x, x')_{\lambda\lambda', \mu\mu'} = V(\mathbf{x} - \mathbf{x}') \delta(t - t') \delta_{\lambda\lambda'} \delta_{\mu\mu'}.$$

Hence, we have

$$\mathcal{H}_0 = \int d^3\mathbf{x} \psi_\alpha^\dagger(\mathbf{x}) \left[ -\frac{\nabla^2}{2m} + U_{\text{ext}}(\mathbf{x}) \right] \psi_\alpha(\mathbf{x}), \quad (\text{II.476})$$

$$\mathcal{H}_I = \frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{x}' \psi_\alpha^\dagger(\mathbf{x}) \psi_\beta^\dagger(\mathbf{x}') V(\mathbf{x} - \mathbf{x}') \psi_\beta(\mathbf{x}') \psi_\alpha(\mathbf{x}). \quad (\text{II.477})$$

The Green's function can be obtained via the Dyson's equation represented in Fig. II.7.7 (b):

$$g(x, y) = G^0(x, y) + \int d^3\mathbf{x}_1 d^3\mathbf{x}'_1 G^0(x, x_1) \Sigma^*(x_1, x'_1) g(x'_1, y), \quad (\text{II.478})$$

where the Kronecker delta function for spin indices has been factored out. The proper self-energy under the Hartree-Fock approximation (see Fig. II.7.10) is therefore given by

$$\Sigma^*(x_1, x'_1) = -i \delta(t_1 - t'_1) \left[ \delta(\mathbf{x}_1 - \mathbf{x}'_1) (2s + 1) \int d^3\mathbf{x}_2 V(\mathbf{x}_1 - \mathbf{x}_2) g(\mathbf{x}_2, t_2; \mathbf{x}_2, t_2^+) \right. \\ \left. - V(\mathbf{x}_1 - \mathbf{x}'_1) g(\mathbf{x}_1, t_1; \mathbf{x}'_1, t_1^+) \right] \quad (\text{II.479})$$

for spin- $s$  fermions. The Fourier transformed Green's function for the above time-independent  $\mathcal{H}_0$  and  $\mathcal{H}_I$  thus becomes:

$$g(\mathbf{x}, \mathbf{y}; \omega) = G^0(\mathbf{x}, \mathbf{y}; \omega) + \int d^3\mathbf{x}_1 d^3\mathbf{x}'_1 G^0(\mathbf{x}, \mathbf{x}_1; \omega) \Sigma^*(\mathbf{x}_1, \mathbf{x}'_1) g(\mathbf{x}'_1, \mathbf{y}; \omega), \quad (\text{II.480})$$

where

$$\Sigma^*(\mathbf{x}_1, \mathbf{x}'_1) = -i \delta(\mathbf{x}_1 - \mathbf{x}'_1) (2s + 1) \int d^3\mathbf{x}_2 V(\mathbf{x}_1 - \mathbf{x}_2) (2\pi)^{-1} \int d\omega e^{i\omega\eta} g(\mathbf{x}_2, \mathbf{x}_2; \omega)$$

$$+iV(\mathbf{x}_1 - \mathbf{x}'_1)(2\pi)^{-1} \int d\omega e^{i\omega\eta} g(\mathbf{x}_1, \mathbf{x}'_1, \omega) \quad (\text{II.481})$$

For a complete set of orthonormal eigenfunctions of  $\mathcal{H}_0$  given by

$$\mathcal{H}_0 \varphi_j^0(\mathbf{x}) = \left[ -\frac{\nabla^2}{2m} + U(\mathbf{x}) \right] \varphi_j^0(\mathbf{x}) = \varepsilon_j^0 \varphi_j^0(\mathbf{x}), \quad (\text{II.482})$$

the unperturbed Green's function becomes:

$$\begin{aligned} iG^0(\mathbf{x}t, \mathbf{x}'t') &= \sum_j \varphi_j^0(\mathbf{x}) \varphi_j^0(\mathbf{x}')^* e^{-i\varepsilon_j^0(t-t')} \left[ \theta(t-t') \langle \Phi_0 | a_j a_j^\dagger | \Phi_0 \rangle - \theta(t'-t) \langle \Phi_0 | a_j^\dagger a_j | \Phi_0 \rangle \right] \\ &= \sum_j \varphi_j^0(\mathbf{x}) \varphi_j^0(\mathbf{x}')^* e^{-i\varepsilon_j^0(t-t')} \left[ \theta(t-t') \theta(\varepsilon_j^0 - \varepsilon_F^0) - \theta(t'-t) \theta(\varepsilon_F^0 - \varepsilon_j^0) \right], \end{aligned} \quad (\text{II.483})$$

where  $\varepsilon_F^0$  is the Fermi energy of the unperturbed system. Therefore, the Fourier transform EQ. (II.483) is

$$G^0(\mathbf{x}, \mathbf{y}; \omega) = \sum_j \varphi_j^0(\mathbf{x}) \varphi_j^0(\mathbf{y})^* \left[ \frac{\theta(\varepsilon_j^0 - \varepsilon_F^0)}{\omega - \varepsilon_j^0 + i\eta} + \frac{\theta(\varepsilon_F^0 - \varepsilon_j^0)}{\omega - \varepsilon_j^0 - i\eta} \right], \quad (\text{II.484})$$

and the particle density in the unperturbed ground state is [from EQ. (II.389) except now restoring the spin degrees of freedom]

$$n^0(\mathbf{x}) = -i(2s+1)(2\pi)^{-1} \int d\omega e^{i\omega\eta} G^0(\mathbf{x}, \mathbf{x}, \omega) = (2s+1) \sum_j |\varphi_j^0(\mathbf{x})|^2 \theta(\varepsilon_F^0 - \varepsilon_j^0), \quad (\text{II.485})$$

so that the total number of particles is

$$N^0 = \int d^3\mathbf{x} n^0(\mathbf{x}) = (2s+1) \sum_j \theta(\varepsilon_F^0 - \varepsilon_j^0). \quad (\text{II.486})$$

Equations (II.480), (II.482) and (II.484) form a set of coupled equations for the self-consistent Green's function  $g$ . Noting that  $\Sigma^*$  in EQ. (II.480) is not dependent on  $\omega$ , we expect that the frequency dependence of  $g$  is similar to that of  $G^0$ :

$$g(\mathbf{x}, \mathbf{y}; \omega) = \sum_j \varphi_j(\mathbf{x}) \varphi_j(\mathbf{y})^* \left[ \frac{\theta(\varepsilon_j - \varepsilon_F)}{\omega - \varepsilon_j + i\eta} + \frac{\theta(\varepsilon_F - \varepsilon_j)}{\omega - \varepsilon_j - i\eta} \right], \quad (\text{II.487})$$

where  $\{\varphi_j(\mathbf{x})\}$  denotes a complete set of single-particle wave functions with eigen-energies  $\varepsilon_j$  and  $\varepsilon_F$  is the Fermi energy of the interacting system. Similar to EQs. (II.485) and (II.486), the particle density of the interacting system is

$$n(\mathbf{x}) = (2s+1) \sum_j |\varphi_j(\mathbf{x})|^2 \theta(\varepsilon_F - \varepsilon_j), \quad (\text{II.488})$$

and the total number of particles is

$$N = N^0 = \int d^3\mathbf{x} n(\mathbf{x}) = (2s+1) \sum_j \theta(\varepsilon_F - \varepsilon_j), \quad (\text{II.489})$$

which is the same as that of the unperturbed system because the interaction Hamiltonian  $\mathcal{H}_I$  conserves the total number of particles.

Using EQ. (II.487), we can evaluate the proper self-energy in EQ. (II.481) and find:

$$\begin{aligned} \Sigma^*(\mathbf{x}_1, \mathbf{x}_1') &= \delta(\mathbf{x}_1 - \mathbf{x}_1') (2s+1) \int d^3\mathbf{x}_2 V(\mathbf{x}_1 - \mathbf{x}_2) \sum_j |\varphi_j(\mathbf{x}_2)|^2 \theta(\varepsilon_F - \varepsilon_j) \\ &\quad - V(\mathbf{x}_1 - \mathbf{x}_1') \sum_j \varphi_j(\mathbf{x}_1) \varphi_j(\mathbf{x}_1')^* \theta(\varepsilon_F - \varepsilon_j). \end{aligned} \quad (\text{II.490})$$

We note that the proper self-energy thus given depends on  $\{\varphi_j(\mathbf{x})\}$  rather than  $\{\varphi_j^0(\mathbf{x})\}$ . Therefore, combining EQs. (II.480) and (II.490) yields a non-linear integral equation for  $\{\varphi_j(\mathbf{x})\}$  if we assume that  $\{\varphi_j^0(\mathbf{x})\}$  is known. Our objective is to find the solutions to  $\{\varphi_j(\mathbf{x})\}$  and  $\{\varepsilon_j\}$ .

For simplicity, we define the following differential operator

$$L_1 = \omega - \left[ -\frac{\nabla_1^2}{2m} + U(\mathbf{x}_1) \right] = \omega - \mathcal{H}_0, \quad (\text{II.491})$$

so that

$$L_1 G^0(\mathbf{x}_1, \mathbf{x}_1'; \omega) = \delta(\mathbf{x}_1 - \mathbf{x}_1')$$

and

$$L_1 g(\mathbf{x}_1, \mathbf{x}_1'; \omega) = \delta(\mathbf{x}_1 - \mathbf{x}_1') + \int d^3\mathbf{x}_2 \Sigma^*(\mathbf{x}_1, \mathbf{x}_2) g(\mathbf{x}_2, \mathbf{x}_1'; \omega). \quad (\text{II.492})$$

Inserting EQs. (II.487) and (II.491) into EQ. (II.492), we find

$$\begin{aligned} &\left[ \omega + \frac{\nabla_1^2}{2m} - U(\mathbf{x}_1) \right] \sum_j \varphi_j(\mathbf{x}_1) \varphi_j(\mathbf{x}_1')^* \left[ \frac{\theta(\varepsilon_j - \varepsilon_F)}{\omega - \varepsilon_j + i\eta} + \frac{\theta(\varepsilon_F - \varepsilon_j)}{\omega - \varepsilon_j - i\eta} \right] \\ &- \int d^3\mathbf{x}_2 \Sigma^*(\mathbf{x}_1, \mathbf{x}_2) \sum_j \varphi_j(\mathbf{x}_2) \varphi_j(\mathbf{x}_1')^* \left[ \frac{\theta(\varepsilon_j - \varepsilon_F)}{\omega - \varepsilon_j + i\eta} + \frac{\theta(\varepsilon_F - \varepsilon_j)}{\omega - \varepsilon_j - i\eta} \right] = \delta(\mathbf{x}_1 - \mathbf{x}_1'), \end{aligned} \quad (\text{II.493})$$

Multiplying EQ. (II.493) by  $\varphi_i(\mathbf{x}_1')$ , integrating over  $\mathbf{x}_1'$ , using the orthogonality of  $\{\varphi_j(\mathbf{x}_1)\}$ , and taking the  $\eta \rightarrow 0$  limit, we obtain the following Schrödinger-like equation for  $\varphi_j(\mathbf{x}_1)$ :

$$\left[ -\frac{\nabla_1^2}{2m} + U(\mathbf{x}_1) \right] \varphi_j(\mathbf{x}_1) + \int d^3\mathbf{x}_2 \Sigma^*(\mathbf{x}_1, \mathbf{x}_2) \varphi_j(\mathbf{x}_2) = \varepsilon_j \varphi_j(\mathbf{x}_1). \quad (\text{II.494})$$

The physical significance of the proper self-energy  $\Sigma^*$  becomes evident from EQ. (II.494), which is effectively a static non-local potential. Given that  $\Sigma^*$  is hermitian and independent of the index  $j$ , the orthogonality of  $\{\varphi_j(\mathbf{x}_1)\}$  remains. Moreover, from EQ. (II.490) we note that  $\Sigma^*$  contains two terms, a direct term proportional to the local particle density, and an exchange term involving non-local interaction of particles.

Equations (II.490) and (II.494) are known as the Hartree-Fock equations used for finding self-consistent solutions to  $\{\varphi_j(\mathbf{x})\}$  and  $\{\varepsilon_j\}$  for a given potential  $U(\mathbf{x})$ . The general approach is to first insert a set of known wavefunctions  $\{\varphi_j^0(\mathbf{x})\}$  into EQ. (II.490) to obtain the proper self-energy  $\Sigma^*$ , which is then used in EQ. (II.494) to solve for  $\{\varphi_j(\mathbf{x})\}$ . The newly obtained  $\{\varphi_j(\mathbf{x})\}$  are then applied to EQ. (II.490) to compute  $\Sigma^*$ , the resulting proper self-energy inserted back to EQ. (II.494), and so on, until self-consistent solutions are found for both  $\{\varphi_j(\mathbf{x})\}$  and  $\{\varepsilon_j\}$ . Evidently it is a complicated computation procedure for arbitrary potential  $U(\mathbf{x})$ . Therefore, the Hartree-Fock solutions to the eigenfunctions, eigen-energies and bandstructures of realistic materials are generally carried out with large computers.

Finally, recall that the ground state energy can be evaluated from Green's functions, we obtain the corresponding ground state energy for a given potential  $U(\mathbf{x})$  using Eqs. (II.393) and (II.494):

$$\begin{aligned}
 E_0 &= -\frac{i}{2}(2s+1) \int d^3\mathbf{x}_1 \lim_{\mathbf{x}'_1 \rightarrow \mathbf{x}_1} \int \frac{d\omega}{(2\pi)} e^{i\omega\eta} \left[ \omega - \frac{\nabla_1^2}{2m} + U(\mathbf{x}_1) \right] g(\mathbf{x}_1, \mathbf{x}'_1; \omega) \\
 &= -i(2s+1) \int d^3\mathbf{x}_1 \sum_j \varphi_j(\mathbf{x}_1)^* \int \frac{d\omega}{(2\pi)} e^{i\omega\eta} \left\{ \frac{1}{2} \omega \varphi_j(\mathbf{x}_1) + \left[ \frac{1}{2} \varepsilon_j \varphi_j(\mathbf{x}_1) - \frac{1}{2} \int d^3\mathbf{x}_2 \Sigma^*(\mathbf{x}_1, \mathbf{x}_2) \varphi_j(\mathbf{x}_2) \right] \right. \\
 &\quad \left. \times \left[ \frac{\theta(\varepsilon_j - \varepsilon_F)}{\omega - \varepsilon_j + i\eta} + \frac{\theta(\varepsilon_F - \varepsilon_j)}{\omega - \varepsilon_j - i\eta} \right] \right\} \\
 &= (2s+1) \sum_j \varepsilon_j \theta(\varepsilon_F - \varepsilon_j) - \frac{1}{2}(2s+1) \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 \sum_j \varphi_j(\mathbf{x}_1)^* \Sigma^*(\mathbf{x}_1, \mathbf{x}_2) \varphi_j(\mathbf{x}_2) \theta(\varepsilon_F - \varepsilon_j). \\
 &= (2s+1) \sum_j \varepsilon_j \theta(\varepsilon_F - \varepsilon_j) - \frac{1}{2}(2s+1) \sum_{jj'} \theta(\varepsilon_F - \varepsilon_j) \theta(\varepsilon_F - \varepsilon_{j'}) \int d^3\mathbf{x}_1 d^3\mathbf{x}_2 V(\mathbf{x}_1 - \mathbf{x}_2) \\
 &\quad \times \left[ (2s+1) |\varphi_j(\mathbf{x}_1)|^2 |\varphi_{j'}(\mathbf{x}_2)|^2 - \varphi_j(\mathbf{x}_1)^* \varphi_{j'}(\mathbf{x}_1) \varphi_{j'}(\mathbf{x}_2)^* \varphi_j(\mathbf{x}_2) \right] \quad (\text{II.495})
 \end{aligned}$$

Equation (II.495) is the usual Hartree-Fock result, where the first term is the simple sum of the energies of all occupied states. The second term involving the proper self-energy includes both the direct and exchange interactions. In general for short-range potentials, the direct and exchange interactions are comparable in magnitude, whereas for long-range potentials, the exchange interaction is much smaller than the direct interaction. In the special case of a uniform system so that the potential  $U(\mathbf{x})$  vanishes, plane-wave solutions satisfy the self-consistent equations, and the corresponding self-consistent single particle energy becomes:

$$\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{k}}^0 + \Sigma^*(\mathbf{k}), \quad (\text{II.496})$$

where the proper self-energy is

$$\begin{aligned}
 \Sigma^*(\mathbf{k}) &= \int d^3(\mathbf{x} - \mathbf{x}') e^{-i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')} \Sigma^*(\mathbf{x} - \mathbf{x}') \\
 &= nV(0) - (2\pi)^{-3} \int d^3\mathbf{k}' V(\mathbf{k} - \mathbf{k}') \theta(k_F - |\mathbf{k}'|), \quad (\text{II.497})
 \end{aligned}$$

and the ground-state energy reduces to

$$\begin{aligned}
 E_0 &= (2s+1)V(2\pi)^{-3} \int d^3\mathbf{k} \left[ \varepsilon_{\mathbf{k}} - \frac{1}{2}\Sigma^*(\mathbf{k}) \right] \theta(k_F - |\mathbf{k}|) \\
 &= (2s+1)V(2\pi)^{-3} \int d^3\mathbf{k} \left[ \varepsilon_{\mathbf{k}}^0 + \frac{1}{2}\Sigma^*(\mathbf{k}) \right] \theta(k_F - |\mathbf{k}|).
 \end{aligned} \tag{II.498}$$

Therefore, in a uniform system the proper self-energy provides a simple correction to the ground-state energy of an interacting system. However, it should be kept in mind that the simple correction given in EQ. (II.498) is no longer valid for non-uniform systems.

### [The Random Phase Approximation (RPA) for degenerate Fermi gas]

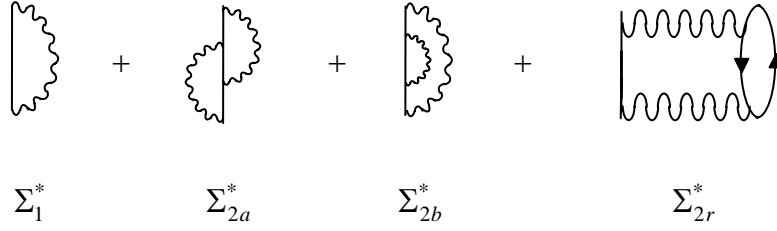
Here we want to consider the diagrammatic representation of the random phase approximation that describes the dielectric response of high-density (or, degenerate) electrons. The primary reason for considering degenerate electrons (which is a valid approximation for good conductors) is that the potential energy of such a system can be assumed to be nearly uniform, which greatly simplifies the diagrammatic analysis despite the apparent difficulties in dealing with the long-range Coulomb interaction among electrons. Specifically, we consider an idealized approximation for the electronic response in a good metal, known as the ‘‘jellium model’’, which assumes a high density ( $n$ ) of electrons moving in a uniform 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 the above descriptions by introducing a dimensionless quantity  $r_s \equiv r_0/a_B$ , where  $r_0$  is defined as  $(4\pi r_0^3/3)^{-1} = n = N/\Omega$ ,  $\Omega$  is the volume of the system, and  $a_B = \hbar^2/(me^2)$  is the Bohr radius. If we define the field operators  $\psi = \sum_{\mathbf{k}} a_{\mathbf{k}}\psi_{\mathbf{k}}$  and  $\psi^\dagger = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger\psi_{\mathbf{k}}^*$  where  $\psi_{\mathbf{k}}$  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  $\mathcal{H}$  of the electron system becomes

$$\mathcal{H} = \frac{e^2}{a_B r_s^2} \left[ \frac{1}{2} \sum_{\mathbf{k}'} k'^2 a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} + \frac{r_s}{2\Omega'} \sum_{\mathbf{k}', \mathbf{p}', \mathbf{q}' \neq 0} \frac{4\pi}{q'^2} a_{\mathbf{k}'+\mathbf{q}'}^\dagger a_{\mathbf{p}'-\mathbf{q}'}^\dagger a_{\mathbf{p}'} a_{\mathbf{k}'} \right], \tag{II.499}$$

We note that only Coulomb interactions with  $\mathbf{q}' \neq 0$  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  $\mathbf{q}' = 0$  do not contribute to the inter-particle interaction (because of charge neutrality for the entire system), the remaining diagrams (see Fig. II.7.5) up to second order in Coulomb interaction that contribute to the proper self-energy are given in Fig. II.8.1.

The diagrammatic contributions to  $\Sigma_1^*$ ,  $\Sigma_{2a}^*$  and  $\Sigma_{2b}^*$  are finite, whereas the diagram  $\Sigma_{2r}^*$  is in fact troublesome and requires more careful analysis. Specifically, the diagram  $\Sigma_{2r}^*$  involves a polarization loop. The polarization loop is the dominant response of a degenerate electron gas to Coulomb interaction and can be associated with the density correlation function, as we shall demonstrate below.



**Figure II.8.1** Diagrams relevant to the proper self-energy of degenerate Fermi gas up to second-order.

For simplicity we restrict our consideration to a spatially homogeneous system of particles with a spin-independent interaction potential:

$$U_0(x, x')_{\lambda\lambda', \mu\mu'} = V(\mathbf{x} - \mathbf{x}') \delta(t - t') \delta_{\lambda\lambda'} \delta_{\mu\mu'}. \quad (\text{II.500})$$

The interaction energy evaluated relative to the exact ground state becomes

$$\begin{aligned} \langle V \rangle &= \frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{x}' V(\mathbf{x} - \mathbf{x}') \langle \psi_\alpha^\dagger(\mathbf{x}) \psi_\beta^\dagger(\mathbf{x}') \psi_\beta(\mathbf{x}') \psi_\alpha(\mathbf{x}) \rangle \\ &= \frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{x}' V(\mathbf{x} - \mathbf{x}') [\langle n(\mathbf{x}) n(\mathbf{x}') \rangle - \delta(\mathbf{x} - \mathbf{x}') \langle n(\mathbf{x}) \rangle], \end{aligned} \quad (\text{II.501})$$

where  $n(\mathbf{x}) \equiv \psi_\alpha^\dagger(\mathbf{x}) \psi_\alpha(\mathbf{x})$  is the particle density operator. If we introduce the density fluctuation operator:

$$\tilde{n}(\mathbf{x}) \equiv n(\mathbf{x}) - \langle n(\mathbf{x}) \rangle, \quad (\text{II.502})$$

EQ. (II.501) can be rewritten into the following:

$$\langle V \rangle = \frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{x}' V(\mathbf{x} - \mathbf{x}') [\langle \tilde{n}(\mathbf{x}) \tilde{n}(\mathbf{x}') \rangle + \langle n(\mathbf{x}) \rangle \langle n(\mathbf{x}') \rangle - \delta(\mathbf{x} - \mathbf{x}') \langle n(\mathbf{x}) \rangle], \quad (\text{II.503})$$

where we have used the identity  $\langle \tilde{n}(\mathbf{x}) \rangle = 0$ . Although EQ. (II.503) is generally complicated for an arbitrary interacting system, it can be greatly simplified for a uniform system because the second and third terms in EQ. (II.503) become trivial. In this special case,  $\langle n(\mathbf{x}) \rangle = n_0 = (N/\Omega)$  is a constant, so we can concentrate on the correlation function for the density fluctuation operator  $\langle \tilde{n}(\mathbf{x}) \tilde{n}(\mathbf{x}') \rangle$ :

$$i\Pi(x, x') \equiv \frac{\langle \Psi_0 | T[\tilde{n}(x) \tilde{n}(x')] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = i\Pi(x', x). \quad (\text{II.504})$$

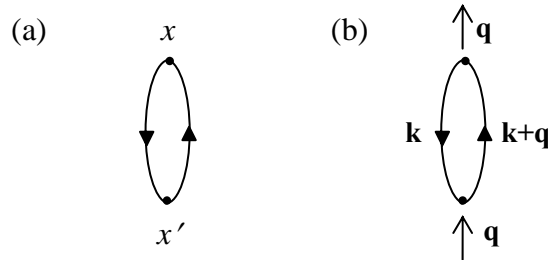
Similarly, we may define the density fluctuation operator for the non-interacting system as follows:

$$\begin{aligned} i\Pi^0(x, x') &\equiv \langle \Phi_0 | T[\psi_\alpha^\dagger(x) \psi_\beta^\dagger(x') \psi_\beta(x') \psi_\alpha(x)] | \Phi_0 \rangle \\ &\quad - \langle \Phi_0 | \psi_\alpha^\dagger(x) \psi_\alpha(x) | \Phi_0 \rangle \langle \Phi_0 | \psi_\beta^\dagger(x') \psi_\beta(x') | \Phi_0 \rangle = i\Pi^0(x', x), \\ &= iG_{\alpha\alpha}^0(x, x^+) iG_{\beta\beta}^0(x', x'^+) - iG_{\alpha\beta}^0(x, x') iG_{\beta\alpha}^0(x', x) - \langle n(\mathbf{x}) \rangle \langle n(\mathbf{x}') \rangle, \end{aligned} \quad (\text{II.505})$$

where we have employed Wick's theorem in the last line of EQ. (II.505). For a uniform fermion system of spin  $s$ , the first and the third terms in the last line of EQ. (II.505) exactly cancel, so we obtain

$$i\Pi^0(x, x') = (2s + 1)G^0(x, x')G^0(x', x). \quad (\text{II.506})$$

The physical meaning of  $\Pi^0$  is the lowest-order contribution to the density correlation function of the interacting system,  $\Pi$ , which is also known as the polarization propagator. The diagrammatic representations for  $\Pi^0$  in the coordinate space and in momentum space are respectively shown in Figs. II.8.2 (a) and II.8.2 (b). For a degenerate electron gas, the lowest-order polarization insertion  $\Pi^0$  is analogous to the creation and subsequent annihilation of an electron-hole pair, which is consistent with the notion of density fluctuations in an otherwise uniform system.

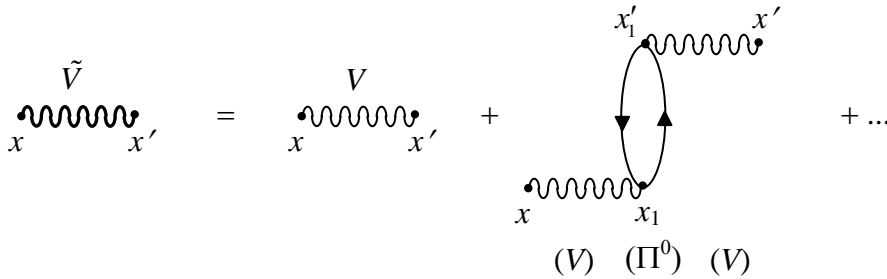


**Figure II.8.2** Lowest-order contribution  $\Pi^0$  to the density correlation function (a) in coordinate space, and (b) in momentum space.

Therefore, following the convention in EQs. (II.469) and (II.470), we have the effective interaction:

$$\tilde{V}(x, x') = V(x, x') + \int d^4x_1 d^4x'_1 V(x, x_1)\Pi^0(x_1, x'_1)V(x'_1, x') + \dots, \quad (\text{II.507})$$

and the corresponding Feynman diagrams in coordinate space are shown in Fig. II.8.3.



**Figure II.8.3** Diagrammatic expansion of the effective interaction in coordinate space.

Having introduced the polarization propagator, we may rewrite the expectation value for the interaction potential in a uniform system into:

$$\begin{aligned} \langle V \rangle = & \frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{x}' V(\mathbf{x} - \mathbf{x}') [i\Pi^0(\mathbf{x}, t; \mathbf{x}', t') + n^2 - \delta(\mathbf{x} - \mathbf{x}')n] \\ & + \frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{x}' V(\mathbf{x} - \mathbf{x}') [i\Pi(\mathbf{x}, t; \mathbf{x}', t') - i\Pi^0(\mathbf{x}, t; \mathbf{x}', t')] \end{aligned}$$

$$= \langle \Phi_0 | V | \Phi_0 \rangle + \frac{1}{2} \int d^3 \mathbf{x} d^3 \mathbf{x}' V(\mathbf{x} - \mathbf{x}') \left[ i \Pi(\mathbf{x}, t; \mathbf{x}', t') - i \Pi^0(\mathbf{x}, t; \mathbf{x}', t') \right]. \quad (\text{II.508})$$

Hence, the ground-state energy of the interacting system can be evaluated as follows:

$$\begin{aligned} E &= \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle + \frac{1}{2} \int_0^1 \frac{d\lambda}{\lambda} \int d^3 \mathbf{x} d^3 \mathbf{x}' \lambda V(\mathbf{x} - \mathbf{x}') \left[ i \Pi^\lambda(\mathbf{x}, t; \mathbf{x}', t') - i \Pi^0(\mathbf{x}, t; \mathbf{x}', t') \right] \\ &= \langle \Phi_0 | \mathcal{H} | \Phi_0 \rangle + E_{\text{corr}}, \end{aligned} \quad (\text{II.509})$$

where  $\Pi^\lambda$  denotes the renormalized polarization associated with an interaction strength  $\lambda$ , and the correlation energy is given by

$$\begin{aligned} E_{\text{corr}} &= \frac{1}{2} \int_0^1 \frac{d\lambda}{\lambda} \int d^3 \mathbf{x} d^3 \mathbf{x}' \lambda V(\mathbf{x} - \mathbf{x}') \left[ i \Pi^\lambda(\mathbf{x}, t; \mathbf{x}', t') - i \Pi^0(\mathbf{x}, t; \mathbf{x}', t') \right] \\ &= \frac{1}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4 q \lambda V(\mathbf{q}) \left[ i \Pi^\lambda(\mathbf{q}, \omega) - i \Pi^0(\mathbf{q}, \omega) \right], \end{aligned} \quad (\text{II.510})$$

and we have used the identity

$$\Pi^\lambda(x, x') = \Pi^\lambda(\mathbf{x} - \mathbf{x}', t - t') = (2\pi)^{-4} \int d^4 q e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}') - i\omega(t - t')} \Pi^\lambda(\mathbf{q}, \omega). \quad (\text{II.511})$$

We also note that the expression in EQ. (II.509) has been obtained through a “trick” by Pauli, which asserts that the exact ground state energy ( $E$ ) of an interacting system is related to the ground state energy ( $E_0$ ) of the unperturbed non-interacting system by the following relation

$$E - E_0 = \int_0^1 \frac{d\lambda}{\lambda} \langle \Psi_0(\lambda) | \lambda \mathcal{H}_I | \Psi_0(\lambda) \rangle,$$

where we have defined  $\mathcal{H}(\lambda) \equiv \mathcal{H}_0 + \lambda \mathcal{H}_I$ , so that  $\mathcal{H}(1) \equiv \mathcal{H}_0 + \mathcal{H}_I = \mathcal{H}$  and  $\mathcal{H}(0) = \mathcal{H}_0$ . In addition,  $\mathcal{H}(\lambda) | \Psi_0(\lambda) \rangle = E(\lambda) | \Psi_0(\lambda) \rangle$ ,  $E(0) = E_0$ ,  $E(1) = E$ , and  $\langle \Psi_0(\lambda) | \Psi_0(\lambda) \rangle = 1$ . Therefore, we have  $E(\lambda) = \langle \Psi_0(\lambda) | \mathcal{H}(\lambda) | \Psi_0(\lambda) \rangle$  and

$$\begin{aligned} \frac{d}{d\lambda} E(\lambda) &= \left\langle \frac{d\Psi_0(\lambda)}{d\lambda} | \mathcal{H}(\lambda) | \Psi_0(\lambda) \right\rangle + \left\langle \Psi_0(\lambda) | \mathcal{H}(\lambda) | \frac{d\Psi_0(\lambda)}{d\lambda} \right\rangle + \left\langle \Psi_0(\lambda) | \frac{d\mathcal{H}(\lambda)}{d\lambda} | \Psi_0(\lambda) \right\rangle \\ &= E(\lambda) \frac{d}{d\lambda} \langle \Psi_0(\lambda) | \Psi_0(\lambda) \rangle + \langle \Psi_0(\lambda) | \mathcal{H}_I | \Psi_0(\lambda) \rangle = \langle \Psi_0(\lambda) | \mathcal{H}_I | \Psi_0(\lambda) \rangle \end{aligned}$$

for  $0 \leq \lambda \leq 1$ , which leads to the solution for  $(E - E_0)$  through integration over the coupling constant  $\lambda$ .

Next, if we further incorporate Dyson’s equation that allows the following conversion through the introduction of a proper polarization propagator  $\Pi^*$ ,

$$\int d^4 x_1 V(x, x_1) \Pi(x_1, x') = \int d^4 x_1 \tilde{V}(x, x_1) \Pi^*(x_1, x'), \quad (\text{II.512})$$

the correlation energy in EQ. (II.510) becomes:

$$E_{\text{corr}} = \frac{i}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4q \left[ \tilde{V}^\lambda(\mathbf{q}) \Pi^{*\lambda}(\mathbf{q}) - \lambda V(\mathbf{q}) \Pi^0(\mathbf{q}) \right], \quad (\text{II.513})$$

where  $\tilde{V}^\lambda$  denotes the effective interaction under an interaction strength  $\lambda$ . Finally, using EQs. (II.474) and (II.475), we find

$$\tilde{V}(\mathbf{q}) \Pi^*(\mathbf{q}) = \frac{V(\mathbf{q}) \Pi^*(\mathbf{q})}{1 - V(\mathbf{q}) \Pi^*(\mathbf{q})} = \frac{1 - \varepsilon^c(\mathbf{q})}{\varepsilon^c(\mathbf{q})} = \frac{1}{\varepsilon^c(\mathbf{q})} - 1. \quad (\text{II.514})$$

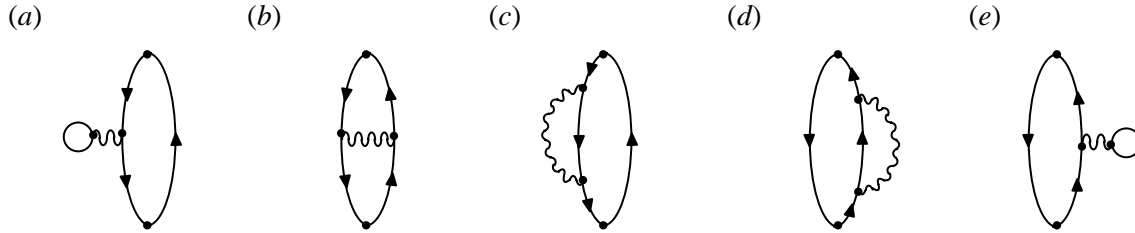
where  $\varepsilon^c(\mathbf{q})$  is the dielectric constant, which can be determined empirically. Hence, EQ. (II.513)

$$E_{\text{corr}} = \frac{i}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4q \left\{ \left[ \varepsilon^c(\mathbf{q}) \right]^{-1} - 1 - \lambda V(\mathbf{q}) \Pi^0(\mathbf{q}) \right\}. \quad (\text{II.515})$$

To proceed further, we expand the proper polarization propagator  $\Pi^*$  in a perturbation series so that  $\Pi^* = \Pi_{(0)}^* + \Pi_{(1)}^* + \dots$  where  $\Pi_{(0)}^* = \Pi^0$ . Thus, EQ. (II.473) can be rewritten into the following:

$$\begin{aligned} \tilde{V}(\mathbf{q}) \Pi^*(\mathbf{q}) &= \frac{V(\mathbf{q}) \Pi^*(\mathbf{q})}{1 - V(\mathbf{q}) \Pi^*(\mathbf{q})} = V \Pi^* + V \Pi^* V \Pi^* + \dots \\ &= V \left[ \Pi_{(0)}^* + \Pi_{(1)}^* \right] + V \Pi_{(0)}^* V \Pi_{(0)}^* + \dots \\ &= V \Pi^0 + V \Pi_{(1)}^* + V \Pi^0 V \Pi^0 + \dots \end{aligned} \quad (\text{II.516})$$

The first-order proper polarization  $\Pi_{(1)}^*$  contains first-order interaction potential  $V$ , and the contributions are shown in Fig. II.8.4 (a) – (e).



**Figure II.8.4** All first-order diagrammatic contributions to the proper polarization propagator.

In reality, the diagrams in (a) and (e) do not contribute to the correlation energy because for a neutral system we have  $V(0) = 0$ . Consequently, if we keep the leading terms to  $V^2$ , the correlation energy becomes

$$E_{\text{corr}} = E_2^r + E_2^b + E_2^c + E_2^d + \dots \quad (\text{II.517})$$

where the superscript “r” refers to ring diagrams, and

$$E_2^r = \frac{i}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4q \left[ \lambda V(\mathbf{q}) \Pi^0(\mathbf{q}) \right]^2, \quad (\text{II.518})$$

$$E_2^{b,c,d} = \frac{i}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4 q \left[ \lambda V(\mathbf{q}) \Pi_{(1)b,c,d}^*(\mathbf{q}) \right]. \quad (\text{II.519})$$

Here the subscript “2” refers to second-order in  $V$ . It turns out that the contributions in EQ. (II.519) are finite, which you may try to verify. On the other hand, the contribution in EQ. (II.518) diverges logarithmically because  $E_2^r \sim [V(\mathbf{q})]^2 \propto q^{-4}$ . In fact, all terms of the form  $E_n^r$  in the perturbation expansion with  $n \geq 2$  diverge. Nonetheless, if we keep in EQ. (II.516) all the terms of the form  $E_n^r$  with  $n \geq 2$  such that

$$\tilde{V}\Pi^* = (V\Pi^0 + V\Pi^0 V\Pi^0 + \dots) + V\Pi_{(1)}^* + \dots = \frac{V\Pi^0}{1 - V\Pi^0} + V\Pi_{(1)}^* + \dots$$

we have

$$E_{\text{corr}} = E_r + E_2^b + E_2^c + E_2^d + \dots = \left( \sum_{n=2}^{\infty} E_n^r \right) + E_2^b + E_2^c + E_2^d + \dots, \quad (\text{II.520})$$

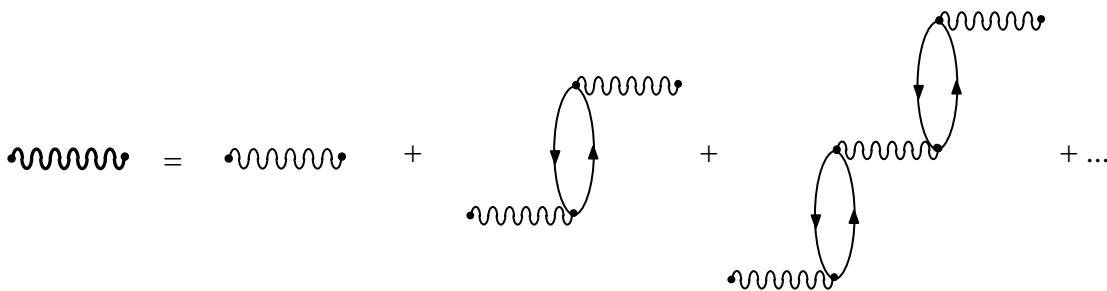
where

$$\begin{aligned} E_r &= \sum_{n=2}^{\infty} E_n^r = \frac{i}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4 q \sum_{n=2}^{\infty} \left[ \lambda V(\mathbf{q}) \Pi^0(\mathbf{q}) \right]^n \\ &= \frac{i}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4 q \frac{\left[ \lambda V(\mathbf{q}) \Pi^0(\mathbf{q}) \right]^2}{1 - \lambda V(\mathbf{q}) \Pi^0(\mathbf{q})} \\ &\equiv \frac{i}{2} \Omega (2\pi)^{-4} \int_0^1 \frac{d\lambda}{\lambda} \int d^4 q \lambda V(\mathbf{q}) \Pi^0(\mathbf{q}) \tilde{V}_r^\lambda(\mathbf{q}) \Pi^0(\mathbf{q}), \end{aligned} \quad (\text{II.521})$$

and

$$\tilde{V}_r(\mathbf{q}) \equiv \frac{V(\mathbf{q})}{1 - V(\mathbf{q}) \Pi^0(\mathbf{q})} \equiv \frac{V(\mathbf{q})}{\varepsilon_r(\mathbf{q})}. \quad (\text{II.522})$$

The “ring approximation” for the interaction potential given in EQ. (II.522) consists of an infinite series of ring (*i.e.* polarization propagator) diagrams, with each ring approximated by its lowest-order term  $\Pi^0$ , as shown in Fig. II.8.5. The diagrammatic expressions for the correlation energy in EQ. (II.520) are illustrated in Fig. II.8.6. These results based on summing over the ring diagrams are known as the random phase approximation.



**Figure II.8.5** Ring approximation for effective interaction  $\tilde{V}_r = V + V\Pi^0 V + V\Pi^0 V\Pi^0 V + \dots$

Next, we must evaluate the lowest-order polarization  $\Pi^0$  explicitly because many important physical quantities in the random phase approximation are given in terms of  $\Pi^0$ . Since it is generally more convenient to evaluate  $\Pi^0$  in momentum space, we Fourier transform EQ. (II.506), which yields

$$\begin{aligned}
\Pi^0(\mathbf{q}) &= \Pi^0(\mathbf{q}, q_0) = -i(2s+1)(2\pi)^{-4} \int d^4k G^0(k)G^0(k+\mathbf{q}) \\
&= -i \frac{(2s+1)}{(2\pi)^4} \int d^3k \int d\omega \left[ \frac{\theta(|\mathbf{k}|-k_F)}{\omega-\omega_{\mathbf{k}}+i\eta} + \frac{\theta(k_F-|\mathbf{k}|)}{\omega-\omega_{\mathbf{k}}-i\eta} \right] \left[ \frac{\theta(|\mathbf{k}+\mathbf{q}|-k_F)}{(\omega+q_0)-\omega_{\mathbf{k}+\mathbf{q}}+i\eta} + \frac{\theta(k_F-|\mathbf{k}+\mathbf{q}|)}{(\omega+q_0)-\omega_{\mathbf{k}+\mathbf{q}}-i\eta} \right] \\
&= \frac{2}{(2\pi)^3} \int d^3k \left[ \frac{\theta(|\mathbf{k}+\mathbf{q}|-k_F)\theta(k_F-|\mathbf{k}|)}{q_0+\omega_{\mathbf{k}}-\omega_{\mathbf{k}+\mathbf{q}}+i\eta} - \frac{\theta(k_F-|\mathbf{k}+\mathbf{q}|\theta(|\mathbf{k}|-k_F))}{q_0+\omega_{\mathbf{k}}-\omega_{\mathbf{k}+\mathbf{q}}-i\eta} \right]. \tag{II.523}
\end{aligned}$$

In the last line of EQ. (II.523), we have assumed spin-1/2 particles and note that the frequency integral reduces four terms in EQ. (II.523) down to two, because those with poles on the same side of the complex frequency plane do not contribute to the integration. For non-interacting systems, the eigen-energies are given by  $\omega_{\mathbf{k}} = \varepsilon_{\mathbf{k}}^0 = k^2/(2m)$ , so that  $\omega_{\mathbf{qk}} \equiv \omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}} = (\mathbf{k} \cdot \mathbf{q} + q^2/2)/m$ . We may further simplify EQ. (II.523) with the change of variables  $\mathbf{k}' \rightarrow -(\mathbf{k} + \mathbf{q})$  in the second term, so that

$$\Pi^0(\mathbf{q}, q_0) = \frac{2}{(2\pi)^3} \int d^3k \theta(|\mathbf{k}+\mathbf{q}|-k_F)\theta(k_F-|\mathbf{k}|) \left[ \frac{1}{q_0+\omega_{\mathbf{k}}-\omega_{\mathbf{k}+\mathbf{q}}+i\eta} - \frac{1}{q_0+\omega_{\mathbf{k}+\mathbf{q}}-\omega_{\mathbf{k}}-i\eta} \right]. \tag{II.524}$$

In the limit of  $|q_0| \rightarrow \infty$ , EQ. (II.524) yields  $\Pi^0(\mathbf{q}, q_0) \sim O(q_0^{-2})$  so that the polarization propagator is an even function of large  $q_0$ . By employing the following relation for the step function

$$\theta(x) = 1 - \theta(-x), \tag{II.525}$$

we find

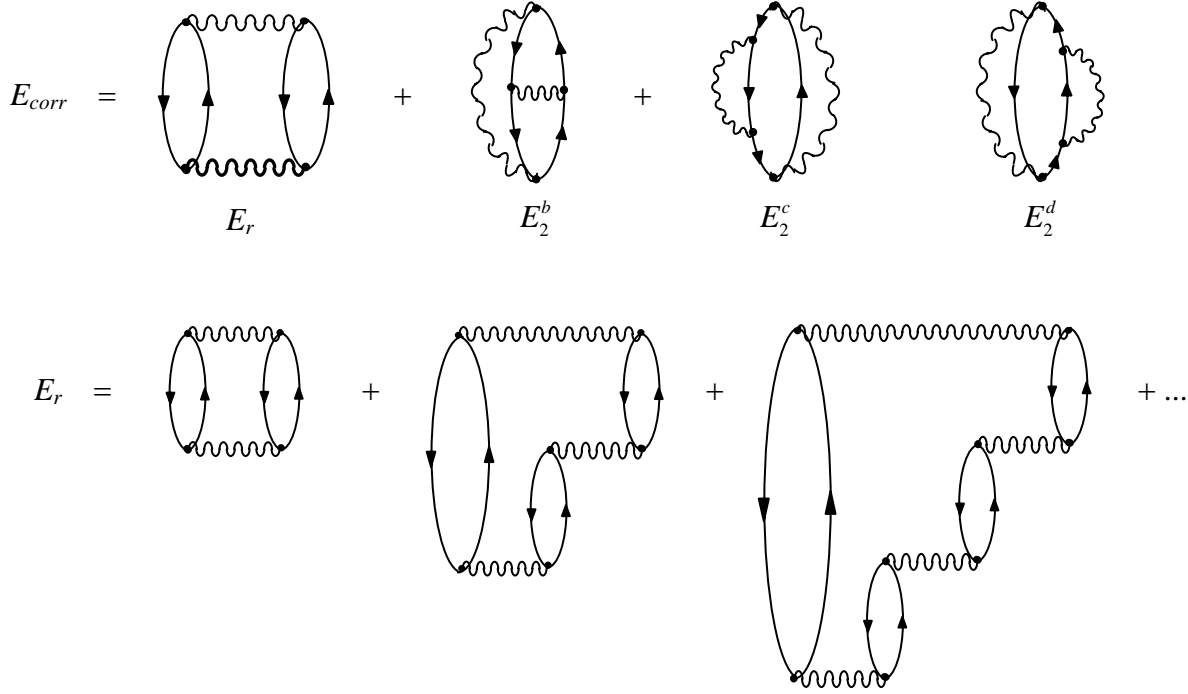
$$\begin{aligned}
\text{Re}\{\Pi^0(\mathbf{q}, q_0)\} &= \frac{2}{(2\pi)^3} \mathcal{P} \int d^3k [1 - \theta(k_F - |\mathbf{k} + \mathbf{q}|)] \theta(k_F - |\mathbf{k}|) \left[ \frac{1}{q_0 - \omega_{\mathbf{qk}}} - \frac{1}{q_0 + \omega_{\mathbf{qk}}} \right] \\
&= \frac{2}{(2\pi)^3} \mathcal{P} \int d^3k \theta(k_F - |\mathbf{k}|) \left[ \frac{1}{q_0 - \omega_{\mathbf{qk}}} - \frac{1}{q_0 + \omega_{\mathbf{qk}}} \right] \\
\left( v \equiv \frac{mq_0}{k_F^2} \Rightarrow \right) &= \frac{2mk_F}{(2\pi)^3} \mathcal{P} \int d^3k \theta(1-k) \left[ \frac{1}{v - qk \cos \vartheta - (q^2/2)} - \frac{1}{v + qk \cos \vartheta + (q^2/2)} \right], \tag{II.526}
\end{aligned}$$

where in the last line of EQ. (II.526) we measure all wave vectors in units of  $k_F$ . We also note that the following term in the first line of EQ. (II.526) vanishes by exchanging  $\mathbf{k}+\mathbf{q}$  and  $\mathbf{k}$  so that:

$$\begin{aligned}
&\mathcal{P} \int d^3k \theta(k_F - |\mathbf{k} + \mathbf{q}|) \theta(k_F - |\mathbf{k}|) \left[ \frac{1}{q_0 - \omega_{\mathbf{qk}}} - \frac{1}{q_0 + \omega_{\mathbf{qk}}} \right] \\
&= \mathcal{P} \int d^3k \theta(k_F - |\mathbf{k}|) \theta(k_F - |\mathbf{k} + \mathbf{q}|) \left[ \frac{1}{q_0 + \omega_{\mathbf{qk}}} - \frac{1}{q_0 - \omega_{\mathbf{qk}}} \right] \\
&\Leftrightarrow \mathcal{P} \int d^3k \theta(k_F - |\mathbf{k} + \mathbf{q}|) \theta(k_F - |\mathbf{k}|) \left[ \frac{1}{q_0 - \omega_{\mathbf{qk}}} - \frac{1}{q_0 + \omega_{\mathbf{qk}}} \right] = 0
\end{aligned}$$

Integrating over the momentum space yields

$$\text{Re}\{\Pi^0(\mathbf{q}, \nu)\} = \frac{2mk_F}{4\pi^2} \left\{ -1 + \frac{1}{2q} \left[ 1 - \left( \frac{\nu - q}{q} \right)^2 \right] \ln \left| \frac{1 + \left( \frac{\nu - q}{q} \right)}{1 - \left( \frac{\nu - q}{q} \right)} \right| - \frac{1}{2q} \left[ 1 - \left( \frac{\nu + q}{q} \right)^2 \right] \ln \left| \frac{1 + \left( \frac{\nu + q}{q} \right)}{1 - \left( \frac{\nu + q}{q} \right)} \right| \right\} \quad (\text{II.527})$$



**Figure II.8.6** Leading diagrammatic contributions to the correlation energy  $E_{corr}$ .

In addition, from EQ. (II.524) we obtain the imaginary part of  $\Pi^0(\mathbf{q}, q_0)$ :

$$\text{Im}\{\Pi^0(\mathbf{q}, q_0)\} = -\frac{1}{4\pi^2} \int d^3k \theta(|\mathbf{k} + \mathbf{q}| - k_F) \theta(k_F - |\mathbf{k}|) [\delta(q_0 - \omega_{\mathbf{qk}}) + \delta(q_0 + \omega_{\mathbf{qk}})]. \quad (\text{II.528})$$

The physical significance of EQ. (II.528) is associated with the energy absorption required to move a particle from under the Fermi sea ( $|\mathbf{k}| < k_F$ ) to outside the Fermi sea ( $|\mathbf{k} + \mathbf{q}| > k_F$ ) via conservation of energy.

To evaluate EQ. (II.528), we only have to consider the positive value of  $q_0$  because the polarization is an even function of  $q_0$ . If we measure all wave vectors in units of  $k_F$ , EQ. (II.528) reduces to

$$\text{Im}\{\Pi^0(\mathbf{q}, \nu > 0)\} = -\frac{mk_F}{4\pi^2} \int d^3k [\theta(|\mathbf{k} + \mathbf{q}| - 1) \theta(1 - k)] \delta\left(\nu - \mathbf{k} \cdot \mathbf{q} - \frac{1}{2} q^2\right). \quad (\text{II.526})$$

The integration in EQ. (II.529) may be evaluated by considering two unit Fermi spheres with their centers separated by  $|\mathbf{q}|$ . We define the upper Fermi sphere as one determined by  $k < 1$  and lower Fermi sphere as one associated with momentum transfer  $|\mathbf{q}|$ . The non-trivial integration over  $k$  must ensure that  $|\mathbf{k} + \mathbf{q}| > 1$

and that the integration area involves the intersection between the Fermi sphere  $k < 1$  and a plane defined by the energy conservation condition  $\nu = \mathbf{k} \cdot \mathbf{q} + (q^2/2)$ . There are three distinct possibilities of  $\mathbf{q}$  and  $\nu$  for evaluating the integration in EQ. (II.529).

$$1) \quad q > 2, \quad \frac{1}{2}q^2 + q \geq \nu \geq \frac{1}{2}q^2 - q:$$

In this case, the two Fermi spheres do not intersect, and the integration becomes (taking  $z = \cos \vartheta$ )

$$\begin{aligned} \text{Im}\{\Pi^0(\mathbf{q}, \nu)\} &= -\frac{mk_F}{4\pi^2} 2\pi \int_{\frac{\nu-q}{q}}^1 k^2 dk \int_{-1}^1 dz \frac{1}{qk} \delta\left(\frac{\nu}{qk} - \frac{q}{2k} - z\right) \\ &= -\frac{mk_F}{4\pi q} \left[ 1 - \left(\frac{\nu}{q} - \frac{q}{2}\right)^2 \right]. \end{aligned} \quad (\text{II.530})$$

$$2) \quad q < 2, \quad \frac{1}{2}q^2 + q \geq \nu \geq \frac{1}{2}q^2 - q:$$

Here the two Fermi spheres intersect so that the intersection regime of the two Fermi spheres is forbidden. However, the intersection area between the upper Fermi sphere with  $k < 1$  and the plane is not affected as long as  $\nu \geq (q^2/2) - q$ . Consequently, the integration yields the same result as in case 1):

$$\text{Im}\{\Pi^0(\mathbf{q}, \nu)\} = -\frac{mk_F}{4\pi q} \left[ 1 - \left(\frac{\nu}{q} - \frac{q}{2}\right)^2 \right]. \quad (\text{II.531})$$

$$3) \quad q < 2, \quad 0 \leq \nu \leq q - \frac{1}{2}q^2:$$

In this case, the two Fermi spheres intersect, and the intersecting plane passes through the forbidden Fermi sphere at the bottom, so the allowed region of intersection becomes an annulus. The area of the annulus has a minimum value of  $k$  allowed by the conservation of energy:

$$k_{\min}^2 = \left(\frac{q}{2} - \frac{\nu}{q}\right)^2 + \left[ 1 - \left(\frac{q}{2} + \frac{\nu}{q}\right)^2 \right] = 1 - 2\nu$$

while the maximum value of  $k$  is 1. Thus, the integration becomes

$$\begin{aligned} \text{Im}\{\Pi^0(\mathbf{q}, \nu)\} &= -\frac{mk_F}{4\pi^2} 2\pi \int_{(1-2\nu)^{1/2}}^1 \frac{k dk}{q} \int_{-1}^1 dz \delta\left(\frac{\nu}{qk} - \frac{q}{2k} - z\right) \\ &= -\frac{mk_F}{4\pi q} [1 - (1 - 2\nu)] = -\frac{mk_F \nu}{2\pi q}. \end{aligned} \quad (\text{II.532})$$

Given EQs. (II.527) and (II.530) – (II.532) for  $\Pi^0(\mathbf{q}, q_0)$ , we can obtain estimates for the correlation energy, dielectric constant, and other useful physical properties under the random phase approximation (RPA). For instance, it can be shown from EQs. (II.522) and (II.524) that the dielectric constant under the RPA is given by

$$\begin{aligned} \frac{1}{\varepsilon_r(\mathbf{q}, q_0)} &= \frac{1}{1 - V(\mathbf{q})\Pi^0(\mathbf{q}, q_0)} \\ &= 1 - \frac{4\pi e^2}{q^2} \sum_n \left| \langle \Phi_n | \sum_{\mathbf{k}} c_{\mathbf{k}-\mathbf{q}}^\dagger c_{\mathbf{k}} | \Phi_0 \rangle \right|^2 \left\{ \frac{1}{q_0 + \omega_{n0} + i\eta} + \frac{1}{-q_0 + \omega_{n0} - i\eta} \right\}, \end{aligned} \quad (\text{II.533})$$

where  $|\Phi_0\rangle$  and  $|\Phi_n\rangle$  refer to the unperturbed ground and excited states, and  $\omega_{n0}$  denotes the energy difference between the states  $|\Phi_0\rangle$  and  $|\Phi_n\rangle$ . The sum over the expectation values of density fluctuations associated with all excitations as given in EQ. (II.533) lends the notation of “random phase” and hence the random phase approximation. Later in one of the problem sets you’ll be asked to consider various interesting limits of the random phase approximation.

Finally, we summarize in the following a few limiting forms of the zero-order polarization propagator, which are often useful for various applications:

1) Fixing the momentum  $|\mathbf{q}| \equiv q$  and taking  $\nu \rightarrow 0$ :

$$\begin{aligned} \text{Im}\{\Pi^0(\mathbf{q}, 0)\} &= 0, \\ \text{Re}\{\Pi^0(\mathbf{q}, 0)\} &= \frac{mk_F}{2\pi^2} \left[ -1 + \frac{1}{q} \left( 1 - \frac{1}{4}q^2 \right) \ln \left| \frac{1 - \frac{1}{2}q}{1 + \frac{1}{2}q} \right| \right]. \end{aligned} \quad (\text{II.534})$$

2) Fixing the energy transfer  $\nu$  and taking the momentum transfer  $q \rightarrow 0$ :

$$\begin{aligned} \text{Im}\{\Pi^0(0, \nu)\} &= 0, \\ \text{Re}\{\Pi^0(\mathbf{q}, \nu)\} &\approx \frac{mk_F}{3\nu^2\pi^2} q^2 \quad \text{for } q \rightarrow 0. \end{aligned} \quad (\text{II.535})$$

3) Fixing the ratio of energy transfer to momentum transfer  $\nu/q \equiv x$ , and taking  $q \rightarrow 0$ :

$$\begin{aligned} \text{Im}\{\Pi^0(q, qx)\} &= -\frac{mk_F x}{2\pi} && \text{for } q \rightarrow 0, 0 \leq x \leq 1, \\ &= 0 && \text{for } q \rightarrow 0, x > 1 \\ \text{Re}\{\Pi^0(\mathbf{q}, \nu)\} &\approx -\frac{mk_F}{2\pi^2} \left( 2 - x \ln \left| \frac{1+x}{1-x} \right| \right) && \text{for } q \rightarrow 0. \end{aligned} \quad (\text{II.536})$$

## II.9. Linear Response and Correlation Functions

Thus far we have focused on descriptions for a many-body system with internal interactions. In this section we want to investigate how a many-body system responds to external perturbation, which is very important for associating the physical properties of a many-body system with empirically measurable quantities. We shall restrict to the limit of small perturbation, so that it is valid to assume linear response to external fields. In this section we first develop a general theory for linear response, and then apply the linear response formalism, known as the Kubo formula related to correlation functions, to empirically detectable physical quantities of electrical conductivity, dielectric constant, and magnetic susceptibility. In addition, we consider the general formalism for fluctuation-dissipation theorem in the context of linear response and correlation functions.

### [Theory of linear response to an external perturbation]

Consider an interacting many-body system with a time-independent Hamiltonian  $\mathcal{H}_0$  at  $t \leq t_0$ . As discussed in Part I, the exact state vector in the Schrödinger picture satisfies the Schrödinger equation

$$i \frac{\partial |\Psi_s(t)\rangle}{\partial t} = \mathcal{H}_0 |\Psi_s(t)\rangle, \quad (\text{II.537})$$

so that

$$|\Psi_s(t)\rangle = e^{-i\mathcal{H}_0 t} |\Psi_s(0)\rangle \quad \text{for } t \leq t_0. \quad (\text{II.538})$$

Next, if we turn on a time-dependent external Hamiltonian  $\mathcal{H}^{\text{ex}}(t)$  at  $t = t_0$ , the new state vector  $|\bar{\Psi}_s(t)\rangle$  for the modified Schrödinger equation

$$i \frac{\partial |\bar{\Psi}_s(t)\rangle}{\partial t} = [\mathcal{H}_0 + \mathcal{H}^{\text{ex}}(t)] |\bar{\Psi}_s(t)\rangle \quad (\text{II.539})$$

becomes

$$|\bar{\Psi}_s(t)\rangle = e^{-i\mathcal{H}_0 t} A(t) |\Psi_s(0)\rangle, \quad (\text{II.540})$$

where the operator  $A(t)$  satisfies

$$i \frac{\partial A(t)}{\partial t} = e^{i\mathcal{H}_0 t} \mathcal{H}^{\text{ex}}(t) e^{-i\mathcal{H}_0 t} A(t) \equiv \mathcal{H}^{\text{ex}}(t) A(t) \quad \text{for } t > t_0, \quad (\text{II.541})$$

$$A(t) = 1 \quad \text{for } t \leq t_0, \quad (\text{II.542})$$

and  $\mathcal{H}^{\text{ex}}(t)$  denotes the external Hamiltonian operator in the interaction picture. We further note that our following consideration does not require  $\mathcal{H}^{\text{ex}}(t)$  commute with  $\mathcal{H}_0$ .

Noting that  $\mathcal{H}^{\text{ex}}(t \leq t_0) = 0$  and assuming small perturbation at  $t > t_0$ , we obtain the solution to  $A(t)$  in EQs. (II.541) and (II.542) iteratively to the first order of  $\mathcal{H}^{\text{ex}}(t)$ :

$$A(t) = 1 - i \int_{t_0}^t dt' \mathcal{H}^{\text{ex}}(t') + \dots \quad (\text{II.543})$$

From EQs. (II.540) and (II.543), the perturbed state vector is given by

$$|\bar{\Psi}_s(t)\rangle = e^{-i\mathcal{H}_0 t} |\Psi_s(0)\rangle - i e^{-i\mathcal{H}_0 t} \int_{t_0}^t dt' \mathcal{H}^{\text{ex}}(t') |\Psi_s(0)\rangle + \dots \quad (\text{II.544})$$

Consequently, in the presence of  $\mathcal{H}^{\text{ex}}(t)$  the matrix elements of operators in Schrödinger picture become

$$\begin{aligned} \langle O(t) \rangle_{\text{ex}} &= \langle \bar{\Psi}'_s(t) | O_s(t) | \bar{\Psi}_s(t) \rangle \\ &= \langle \Psi'_s(0) | \left[ 1 + i \int_{t_0}^t dt' \mathcal{H}^{\text{ex}}(t') \right] e^{i\mathcal{H}_0 t} O_s(t) e^{-i\mathcal{H}_0 t} \left[ 1 - i \int_{t_0}^t dt' \mathcal{H}^{\text{ex}}(t') \right] | \Psi_s(0) \rangle + \dots \\ &= \langle \Psi'_H(0) | O_H(t) | \Psi_H(0) \rangle + i \langle \Psi'_H(0) | \int_{t_0}^t dt' [\mathcal{H}^{\text{ex}}(t'), O_H(t)] | \Psi_H(0) \rangle + \dots, \end{aligned} \quad (\text{II.545})$$

where we have only retained terms up to first-order in  $\mathcal{H}^{\text{ex}}(t)$ . If we evaluate the matrix elements of the operators in the exact ground state in the presence of  $\mathcal{H}^{\text{ex}}(t)$ , so that  $|\Psi_H(0)\rangle = |\Psi'_H(0)\rangle = |\Psi_0\rangle$ , we arrive at the linear response of the ground-state expectation value of an operator to an external perturbation:

$$\begin{aligned} \delta \langle O(t) \rangle &\equiv \langle O(t) \rangle_{\text{ex}} - \langle O(t) \rangle \\ &= i \langle \Psi_0 | \int_{t_0}^t dt' [\mathcal{H}^{\text{ex}}(t'), O_H(t)] | \Psi_0 \rangle. \end{aligned} \quad (\text{II.546})$$

As an explicit example, let us consider the linear response of a system with charge  $e$  per particle to an external scalar potential  $\varphi^{\text{ex}}(\mathbf{x}, t)$ , which is turned on at  $t = t_0$ . If the exact particle density operator in the unperturbed system is denoted by  $n(\mathbf{x}, t)$ , the external perturbation Hamiltonian becomes:

$$\mathcal{H}^{\text{ex}}(t) = \int d^3 \mathbf{x} n(\mathbf{x}, t) e \varphi^{\text{ex}}(\mathbf{x}, t), \quad (\text{II.547})$$

and the corresponding linear response of the system, following EQs. (II.546) and (II.547), is given by

$$\begin{aligned} \delta \langle n(\mathbf{x}, t) \rangle &= i \int_{t_0}^t dt' \int d^3 \mathbf{x}' e \varphi^{\text{ex}}(\mathbf{x}', t') \langle \Psi_0 | [n(\mathbf{x}', t'), n(\mathbf{x}, t)] | \Psi_0 \rangle \\ &= i \int_{t_0}^t dt' \int d^3 \mathbf{x}' e \varphi^{\text{ex}}(\mathbf{x}', t') \langle \Psi_0 | [\tilde{n}(\mathbf{x}', t'), \tilde{n}(\mathbf{x}, t)] | \Psi_0 \rangle, \end{aligned} \quad (\text{II.548})$$

where in the second line we have used the definition in EQ. (II.502) for the density fluctuation function. Next, we define the retarded density correlation function in analogy with that for the retarded Green's function so that

$$i\mathcal{G}_n^R(x, x') = \theta(t - t') \frac{\langle \Psi_0 | [\tilde{n}(x), \tilde{n}(x')] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \quad (\text{II.549})$$

and EQ. (II.548) is rewritten into

$$\delta \langle n(\mathbf{x}, t) \rangle = \int_{-\infty}^{\infty} dt' \int d^3 \mathbf{x}' \mathcal{G}_n^R(\mathbf{x}, t; \mathbf{x}', t') e \varphi^{\text{ex}}(\mathbf{x}', t'), \quad (\text{II.550})$$

which enforces the causal behavior of the linear response through the retarded density correlation function.

The expression given in EQ. (II.550) can be generalized to the linear response of a many-body system to an external perturbation through a retarded correlation function  $\mathcal{G}^R$ . In particular, if the system under consideration is spatially homogeneous, we have  $\mathcal{G}^R(x, x') = \mathcal{G}^R(x - x')$  and the following Fourier transformed functions

$$\delta\langle n(\mathbf{k}, \omega) \rangle = \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}} \delta\langle n(\mathbf{x}, t) \rangle, \quad (\text{II.551})$$

$$\varphi^{\text{ex}}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}} \varphi^{\text{ex}}(\mathbf{x}, t), \quad (\text{II.552})$$

$$\mathcal{G}^R(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}} \mathcal{G}^R(\mathbf{x}, t). \quad (\text{II.553})$$

Hence, the Fourier transformed equivalence to the linear response function of EQ. (II.550)

$$\delta\langle n(\mathbf{k}, \omega) \rangle = \mathcal{G}_n^R(\mathbf{k}, \omega) e\varphi^{\text{ex}}(\mathbf{k}, \omega). \quad (\text{II.554})$$

From the relation given in EQ. (II.554) we may identify the retarded correlation function  $\mathcal{G}^R$  as a generalized susceptibility representing the linear response of a many-body system to an external perturbation.

### [Kubo formula for dielectric response, conductivity and magnetic susceptibility]

Having defined the general theory of linear response to external perturbation, we are ready to consider several explicit examples.

#### 1. The dielectric response of a degenerate electron gas

Following the discussion that leads to EQ. (II.554), if we assume that the external perturbation potential is due to the presence of an external charge density  $n_{\text{ex}}(\mathbf{x}, t)$ , we have

$$\mathcal{H}^{\text{ex}}(\mathbf{x}, t) = \int d^3\mathbf{x}' n(\mathbf{x}, t) V(\mathbf{x} - \mathbf{x}') n_{\text{ex}}(\mathbf{x}', t), \quad (\text{II.555})$$

where  $V(\mathbf{x} - \mathbf{x}')$  denotes the Coulomb potential. From EQs. (II.554) and (II.555), we obtain the induced charge density in response to the external charge density:

$$\delta\langle n(\mathbf{q}, \omega) \rangle = \mathcal{G}_n^R(\mathbf{q}, \omega) V(\mathbf{q}) n_{\text{ex}}(\mathbf{q}, \omega) \equiv \frac{n_{\text{ex}}(\mathbf{q}, \omega)}{\varepsilon(\mathbf{q}, \omega)} - n_{\text{ex}}(\mathbf{q}, \omega), \quad (\text{II.556})$$

which leads to a dielectric constant

$$\frac{1}{\varepsilon(\mathbf{q}, \omega)} = 1 + \mathcal{G}_n^R(\mathbf{q}, \omega) V(\mathbf{q}) = 1 + \frac{4\pi e^2}{|\mathbf{q}|^2} \mathcal{G}_n^R(\mathbf{q}, \omega), \quad (\text{II.557})$$

where  $\mathcal{G}_n^R$  is defined according to EQ. (II.549) and is therefore related to the polarization propagator. Thus, if the external charge density is specified, we may use the corresponding  $\Pi^0(\mathbf{q}, \omega)$  in Part II.8 to derive related physical quantities such as the dielectric constant, the induced charge density, the total induced charge, etc. Equation (II.557) represents the linear response of a degenerate electron gas to external charge density, which is given in terms of the density correlation function and is also known as a generalized Kubo formula for dielectric response.

Next, we consider the linear response of a degenerate electron gas to an impulsive external perturbation of the following form:

$$\varphi^{\text{ex}}(\mathbf{x}, t) = e^{i\mathbf{q}\cdot\mathbf{x}} \varphi_0 \delta(t) \quad \Rightarrow \quad \varphi^{\text{ex}}(\mathbf{k}, \omega) = (2\pi)^3 \varphi_0 \delta(\mathbf{k} - \mathbf{q}). \quad (\text{II.558})$$

The corresponding induced density perturbation becomes

$$\begin{aligned}\delta\langle n(\mathbf{x}, t) \rangle &= -e \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{(2\pi)} e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\omega t} \Pi^R(\mathbf{k}, \omega) \varphi^{\text{ex}}(\mathbf{k}, \omega) \\ &= -e\varphi_0 e^{i\mathbf{q}\cdot\mathbf{x}} \int \frac{d\omega}{(2\pi)} e^{-i\omega t} \Pi^R(\mathbf{q}, \omega) = -e\varphi_0 e^{i\mathbf{q}\cdot\mathbf{x}} \int \frac{d\omega}{(2\pi)} e^{-i\omega t} [V(\mathbf{q})]^{-1} \left\{ [\varepsilon^R(\mathbf{q}, \omega)]^{-1} - 1 \right\}\end{aligned}\quad (\text{II.559})$$

and the poles of the integrand in EQ. (II.559) represent the frequency and lifetime of the collective modes of the degenerate electron gas.

If we restrict to the ring diagrams, we find the dielectric constant is given by

$$\varepsilon_r^R(\mathbf{q}, \omega) = 1 - V(\mathbf{q}) \Pi^{0R}(\mathbf{q}, \omega), \quad (\text{II.560})$$

and the linear response function associated with the retarded density correlation function is

$$\begin{aligned}\Pi^{0R}(\mathbf{q}, \omega) &= \text{Re} \left\{ \Pi^0(\mathbf{q}, \omega) \right\} + i \text{sgn}(\omega) \text{Im} \left\{ \Pi^0(\mathbf{q}, \omega) \right\} \\ &= 2 \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{[1 - \theta(k_F - |\mathbf{k} + \mathbf{q}|)] \theta(k_F - |\mathbf{k}|)}{\omega + \omega_{\mathbf{k}} - \omega_{\mathbf{k} + \mathbf{q}} + i\eta} - \frac{\theta(k_F - |\mathbf{k} + \mathbf{q}|) [1 - \theta(k_F - |\mathbf{k}|)]}{\omega + \omega_{\mathbf{k}} - \omega_{\mathbf{k} + \mathbf{q}} + i\eta} \right\} \\ &= -2 \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{\theta(k_F - |\mathbf{k} + \mathbf{q}|) - \theta(k_F - |\mathbf{k}|)}{\omega + \omega_{\mathbf{k}} - \omega_{\mathbf{k} + \mathbf{q}} + i\eta} \right\}\end{aligned}\quad (\text{II.561})$$

Suppose that the poles of the integrand in EQ. (II.559) are denoted by  $\omega = \Omega_p - i\gamma_p$ , we have

$$V(\mathbf{q}) \Pi^{0R}(\mathbf{q}, \Omega_p - i\gamma_p) = 1. \quad (\text{II.562})$$

In general, EQ. (II.562) can only be solved numerically. However, in the special case of small damping so that  $\gamma_p \ll \Omega_p$ , the real and imaginary parts of EQ. (II.562) can be separated so that we obtain the following conditions (see Problem Set 3) the following conditions are satisfied:

$$V(\mathbf{q}) \text{Re} \left\{ \Pi^{0R}(\mathbf{q}, \Omega_p) \right\} = V(\mathbf{q}) \text{Re} \left\{ \Pi^0(\mathbf{q}, \Omega_p) \right\} = 1, \quad (\text{II.563})$$

$$\begin{aligned}\gamma_p &= \text{Im} \left\{ \Pi^{0R}(\mathbf{q}, \Omega_p) \right\} \left[ \frac{\partial \text{Re} \left\{ \Pi^{0R}(\mathbf{q}, \omega) \right\}}{\partial \omega} \Big|_{\Omega_p} \right]^{-1} \\ &= \text{sgn}(\Omega_p) \text{Im} \left\{ \Pi^0(\mathbf{q}, \Omega_p) \right\} \left[ \frac{\partial \text{Re} \left\{ \Pi^0(\mathbf{q}, \omega) \right\}}{\partial \omega} \Big|_{\Omega_p} \right]^{-1}.\end{aligned}\quad (\text{II.564})$$

In the small  $q$  limit, it can be shown that a specific collective mode known as the plasma oscillations exists by finding the solution  $\Omega_p$  to EQ. (II.563), and  $\Omega_p$  satisfies

$$\Omega_q = \pm \left( \frac{4\pi n e^2}{m} \right)^{1/2} \left[ 1 + \frac{9}{10} \left( \frac{q^2 \varepsilon_F}{6\pi n e^2} \right) + \dots \right] \equiv \pm \omega_p \left[ 1 + \frac{9}{10} \left( \frac{q^2 \varepsilon_F}{6\pi n e^2} \right) + \dots \right], \quad (\text{II.565})$$

which you'll examine in Problem Set 3.

In EQ. (II.556), we note that the total charge density is given by  $n_{\text{tot}} = (n_{\text{ex}}/\epsilon)$ . Furthermore, we may relate the dielectric screening response to the longitudinal conductivity  $\sigma_\ell \equiv \delta\langle J \rangle / E = (J_{\text{tot}} - J_{\text{ex}}) / E$ , where  $E$  denotes the electric field,  $\delta\langle J \rangle$  is the induced current in response to an external current  $J_{\text{ex}}$ , and the total current is related to the total charge density via the continuity equation

$$\frac{\partial n_{\text{tot}}(x)}{\partial t} e + \nabla \cdot \mathbf{J}_{\text{tot}}(x) = 0 \Rightarrow \delta\langle n(\mathbf{q}, \omega) \rangle = \frac{\mathbf{q} \cdot \delta\langle \mathbf{J}(\mathbf{q}, \omega) \rangle}{\omega e} = \frac{q\sigma_\ell E(\mathbf{q}, \omega)}{\omega e}. \quad (\text{II.566})$$

Recall the Maxwell's equation:

$$\nabla \cdot \mathbf{E} = 4\pi e n_{\text{tot}}(x) = 4\pi e \frac{\delta\langle n(x) \rangle}{1 - \epsilon} \Rightarrow \delta\langle n(\mathbf{q}, \omega) \rangle = iq \frac{1 - \epsilon(\mathbf{q}, \omega)}{4\pi e} E(\mathbf{q}, \omega), \quad (\text{II.567})$$

so that EQs. (II.566) and (II.567) lead to a simple relation between the dielectric constant and the longitudinal conductivity:

$$\epsilon(\mathbf{q}, \omega) = 1 + i \frac{4\pi\sigma_\ell}{\omega}. \quad (\text{II.568})$$

## 2. The Kubo formula for transverse electrical conductivity

Historically the theory for electrical conduction prior to the development of many-body physics was based on the semi-classical one-particle approach that assumes random scattering of single-electron wavefunctions governed by the Boltzmann equation. With the introduction of Green's function techniques and the aforementioned linear response theory, we can derive the electrical conductivity of a system directly from the current-current correlation function with only one simple assumption that the induced current is linear in the applied voltage, as first discussed by Kubo.

To derive the Kubo formula for electrical conductivity, we consider a perturbation field  $\mathcal{H}_{\text{ex}}$  associated with an applied vector potential  $\mathbf{A}(\mathbf{x}, t)$  so that  $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{ex}}$  and

$$\mathcal{H}_{\text{ex}} = - \int d^3\mathbf{x} [\mathbf{A}(\mathbf{x}) \cdot \mathbf{J}(\mathbf{x})], \quad (\text{II.569})$$

where  $\mathbf{J}(\mathbf{x})$  is the total current density operator (including the external and induced current densities):

$$\begin{aligned} \mathbf{J}(\mathbf{x}) &= \frac{1}{2m} \sum_i \{ [\mathbf{p}_i - ne\mathbf{A}(\mathbf{x})] \delta(\mathbf{x} - \mathbf{x}_i) + \delta(\mathbf{x} - \mathbf{x}_i) [\mathbf{p}_i - ne\mathbf{A}(\mathbf{x})] \} \\ &= -\frac{e}{2im} \left[ \psi^\dagger(\mathbf{x}) \nabla \psi(\mathbf{x}) - (\nabla \psi^\dagger(\mathbf{x})) \psi(\mathbf{x}) \right] - \frac{e^2}{m} \mathbf{A}(\mathbf{x}) \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}). \end{aligned} \quad (\text{II.570})$$

We also have  $\mathcal{H}_{\text{ex}}(t) = e^{i\mathcal{H}_0 t} \mathcal{H}_{\text{ex}} e^{-i\mathcal{H}_0 t}$  and  $\mathbf{J}(\mathbf{x}, t) = e^{i\mathcal{H}_0 t} \mathbf{J}(\mathbf{x}) e^{-i\mathcal{H}_0 t}$  in the interaction picture. To compute the average of the current density operator in the presence of a specific external field, we use the density matrix  $\rho(\mathbf{x}, t)$  such that

$$\langle \mathbf{J}(\mathbf{x}, t) \rangle = \text{Tr} \{ \rho(\mathbf{x}) \mathbf{J}(\mathbf{x}) \} = \text{Tr} \{ \rho(\mathbf{x}, t) \mathbf{J}(\mathbf{x}, t) \}, \quad (\text{II.571})$$

where

$$\rho(\mathbf{x}, t) \equiv e^{i\mathcal{H}_0 t} \rho(\mathbf{x}) e^{-i\mathcal{H}_0 t} \quad \text{and} \quad i \frac{\partial \rho}{\partial t} = [\mathcal{H}_0 + \mathcal{H}_{\text{ex}}, \rho]. \quad (\text{II.572})$$

From EQ. (II.572), we find

$$i \frac{\partial \rho(\mathbf{x}, t)}{\partial t} = [\mathcal{H}_{\text{ex}}(t), \rho(\mathbf{x}, t)], \quad (\text{II.573})$$

so that

$$\begin{aligned} \rho(\mathbf{x}, t) &= \rho_0 - i \int_{-\infty}^t dt' [\mathcal{H}_{\text{ex}}(t'), \rho(\mathbf{x}, t')] \\ &\approx \rho_0 - i \int_{-\infty}^t dt' [\mathcal{H}_{\text{ex}}(t'), \rho_0], \end{aligned} \quad (\text{II.574})$$

where  $\rho_0$  is the equilibrium density matrix, which is only a function of  $\mathcal{H}_0$ , and we have assumed linear response in arriving at the second line of EQ. (II.574).

Inserting EQ. (II.574) into EQ. (II.571), we obtain

$$\begin{aligned} \langle \mathbf{J}(\mathbf{x}, t) \rangle &\approx \text{Tr} \{ \rho_0 \mathbf{J}(\mathbf{x}, t) \} - i \int_{-\infty}^t dt' \text{Tr} \{ [\mathcal{H}_{\text{ex}}(t'), \rho_0] \mathbf{J}(\mathbf{x}, t') \} \\ &= -\frac{ne^2}{m} \mathbf{A}(\mathbf{x}, t) - i \int_{-\infty}^t dt' \text{Tr} \{ [\mathbf{J}(\mathbf{x}, t'), \mathcal{H}_{\text{ex}}(t')] \rho_0 \} \\ &\equiv -\frac{ne^2}{m} \mathbf{A}(\mathbf{x}, t) - i \int_{-\infty}^t dt' \langle [\mathbf{J}(\mathbf{x}, t'), \mathcal{H}_{\text{ex}}(t')] \rangle_0, \end{aligned} \quad (\text{II.575})$$

where we have used the following relations to arrive at the second line of EQ. (II.575):

$$\text{Tr} \{ \rho_0 \psi^\dagger \psi \} \equiv n, \quad (\text{II.576})$$

$$\text{Tr} \{ ABC \} = \text{Tr} \{ BCA \} = \text{Tr} \{ CAB \}, \quad (\text{II.577})$$

and  $n$  is the number of electrons per unit volume. Finally, inserting the interaction picture of EQ. (II.569) into EQ. (II.575), we obtain:

$$\begin{aligned} \langle J_\alpha(\mathbf{x}, t) \rangle &= -\frac{ne^2}{m} A_\alpha(\mathbf{x}, t) - i \int_{-\infty}^{\infty} dt' \int d^3 \mathbf{x}' \theta(t-t') \langle [J_\alpha(\mathbf{x}, t), J_\beta(\mathbf{x}', t')] \rangle_0 A_\beta(\mathbf{x}', t'), \\ &= -\int_{-\infty}^{\infty} dt' \int d^3 \mathbf{x}' \left\{ \frac{ne^2}{m} \delta_{\alpha\beta} \delta(\mathbf{x}-\mathbf{x}') \delta(t-t') + i\theta(t-t') \langle [J_\alpha(\mathbf{x}, t), J_\beta(\mathbf{x}', t')] \rangle_0 \right\} A_\beta(\mathbf{x}', t') \\ &\equiv \int_{-\infty}^{\infty} dt' \int d^3 \mathbf{x}' R_{\alpha\beta}(\mathbf{x}-\mathbf{x}', t-t') A_\beta(\mathbf{x}', t'), \end{aligned} \quad (\text{II.578})$$

which is the Kubo formula for transverse electrical conductivity in coordinate space, where  $\alpha$  and  $\beta$  refer to different Cartesian suffixes, the response function  $R_{\alpha\beta}$  is proportional to the conductivity, and we have assumed transverse perturbation so that  $\mathbf{q} \cdot \mathbf{A}(\mathbf{q}) = 0$  and there is no need to worry about the internal fields arising from induced charge density as in the previous case for dielectric response.

We may further Fourier transform EQ. (II.578) and recall the relation between the electric field and the vector potential and the definition of electrical conductivity  $\sigma_{\alpha\beta}(\mathbf{q}, \omega)$ :

$$\begin{aligned}\mathbf{E}(\mathbf{x}, t) &= -\frac{\partial \mathbf{A}(\mathbf{x}, t)}{\partial t} \Rightarrow \mathbf{E}(\mathbf{q}, \omega) = i\omega \mathbf{A}(\mathbf{q}, \omega), \\ J_\alpha(\mathbf{q}, \omega) &= \sigma_{\alpha\beta}(\mathbf{q}, \omega) E_\beta(\mathbf{q}, \omega),\end{aligned}$$

so that EQ. (II.578) becomes

$$\langle J_\alpha(\mathbf{q}, \omega) \rangle = -\frac{ne^2}{i\omega m} E_\alpha(\mathbf{q}, \omega) + \frac{1}{\omega} \int_{-\infty}^0 dt' e^{-i\omega t'} \langle [J_\alpha(\mathbf{q}, 0), J_\beta(-\mathbf{q}, t')] \rangle_0 E_\beta(\mathbf{q}, \omega), \quad (\text{II.579})$$

and the final Kubo formula for electrical conductivity is therefore given by

$$\sigma_{\alpha\beta}(\mathbf{q}, \omega) = -\frac{ne^2}{i\omega m} \delta_{\alpha\beta} + \frac{1}{\omega} \int_{-\infty}^0 dt' e^{-i\omega t'} \langle [J_\alpha(\mathbf{q}, 0), J_\beta(-\mathbf{q}, t')] \rangle_0. \quad (\text{II.580})$$

### 3. The Kubo formula for magnetic susceptibility tensor

The magnetic susceptibility of a many-body system can be obtained by considering the linear response of spins to an applied magnetic field  $\mathbf{H}(\mathbf{x}, t)$ . The external perturbation Hamiltonian may be written as:

$$\mathcal{H}_{\text{ex}} = -\int d^3x \mathbf{H}(\mathbf{x}, t) \cdot \mathbf{m}(\mathbf{x}), \quad (\text{II.581})$$

where  $\mathbf{m}(\mathbf{x})$  is the magnetic moment density operator defined as

$$\mathbf{m}(\mathbf{x}) = \sum_i \delta(\mathbf{x} - \mathbf{x}_i) \boldsymbol{\sigma}(\mathbf{x}_i), \quad (\text{II.582})$$

and  $\boldsymbol{\sigma}(\mathbf{x}_i)$  denotes the spin operator at the position  $\mathbf{x}_i$ , with the components of the vector  $\boldsymbol{\sigma}(\mathbf{x}_i)$  represented by the Pauli matrices.

The expectation value of the induced magnetic moment  $\langle \mathbf{m}(\mathbf{x}, t) \rangle_H$  under a finite magnetic field  $\mathbf{H}$  can be obtained via the linear response theory outlined previously, which yields:

$$\langle m_\alpha(\mathbf{x}, t) \rangle_H = \langle m_\alpha(\mathbf{x}, t) \rangle_0 + \sum_\beta \int dt' \int d^3x' \chi_{\alpha\beta}(\mathbf{x} - \mathbf{x}', t - t') H_\beta(\mathbf{x}', t'), \quad (\text{II.583})$$

where the susceptibility tensor is given by the retarded correlation function of the magnetic moment operator:

$$\chi_{\alpha\beta}(\mathbf{x} - \mathbf{x}', t - t') = i\theta(t - t') \langle [\sigma_\alpha(\mathbf{x}, t), \sigma_\beta(\mathbf{x}', t')] \rangle. \quad (\text{II.584})$$

If we further define

$$\sigma^\pm \equiv \frac{1}{2} (\sigma_x \pm i\sigma_y), \quad (\text{II.585})$$

then we have the transverse and longitudinal susceptibility  $\chi^+$  and  $\chi^z$  given by:

$$\chi^+(\mathbf{x} - \mathbf{x}', t - t') = i\theta(t - t') \langle [\sigma^-(\mathbf{x}, t), \sigma^+(\mathbf{x}', t')] \rangle = \sum_{\mathbf{p}, \mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}')} \chi^+(\mathbf{p}, \mathbf{q}; t - t'), \quad (\text{II.586})$$

$$\chi^z(\mathbf{x} - \mathbf{x}', t - t') = i\theta(t - t') \langle [\sigma_z(\mathbf{x}, t), \sigma_z(\mathbf{x}', t')] \rangle = \sum_{\mathbf{p}, \mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}')} \chi^z(\mathbf{p}, \mathbf{q}; t - t'). \quad (\text{II.587})$$

For isotropic or cubic media in the paramagnetic state (*i.e.*,  $T > T_{\text{Curie}}$ ),  $\chi_{\alpha\beta}$  is diagonal and isotropic from symmetry consideration, and therefore

$$\chi_{\alpha\beta} = 2\chi^+ \delta_{\alpha\beta}, \quad (\text{II.588})$$

implying that  $\chi^+$  determines the magnetic susceptibility completely. On the other hand, for  $T < T_{\text{Curie}}$ ,  $\chi^z$  differs from  $\chi^+$  and must be calculated separately. In Problem Set 3 you are asked to consider the transverse magnetic susceptibility in the generalized Hartree-Fock approximation.

### [Fluctuation-dissipation theorem]

In addition to the derivation of linear response functions, the aforementioned linear response theory can be applied to the fluctuation-dissipation theorem. Consider a liquid or a gas under thermal equilibrium in which 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. As we have discussed previously, 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:

$$\mathcal{G}^R(t) = -i\theta(t)\langle [A(t), B(0)] \rangle. \quad (\text{II.589})$$

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

$$\langle A(t)B(0) \rangle = Z^{-1}\text{Tr}\left\{e^{-\beta\mathcal{H}}e^{i\mathcal{H}t}Ae^{-i\mathcal{H}t}B\right\} = Z^{-1}\sum_n \langle n|e^{-\beta\mathcal{H}}e^{i\mathcal{H}t}Ae^{-i\mathcal{H}t}B|n\rangle, \quad (\text{II.590})$$

where  $Z$  is the partition function.

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  $\langle A(t)B(0) \rangle$ , it can be shown that the Fourier transform of the equivalent retarded Green's function at  $T = \beta^{-1}$  (see Problem Set 3) has the following form:

$$\mathcal{G}^R(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} (1 - e^{-\beta\omega'}) \frac{J_1(\omega')}{\omega - \omega' + i\eta}, \quad (\eta = 0^+). \quad (\text{II.591})$$

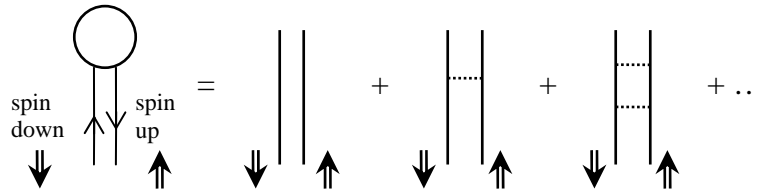
We note that for  $A$  and  $B$  being hermitian conjugates at different times,  $J_1(\omega)$  is real so that EQ. (II.591) gives

$$\text{Im}[\mathcal{G}^R(\omega)] = -\frac{1}{2}(1 - e^{-\beta\omega})J_1(\omega), \quad \Rightarrow \quad J_1(\omega \neq 0) = -\frac{2}{1 - e^{-\beta\omega}}\text{Im}[\mathcal{G}^R(\omega)], \quad (\text{II.592})$$

which 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 that is manifested by the imaginary part of the retarded Green's function.

**[Remarks on interacting electrons]**

Before closing our discussion on the Green’s function techniques, it is worth noting that in Part II.8 and Part II.9 we have primarily focused on many-body interaction in high-density electron gas where the ring diagrams associated with the long-range Coulomb interaction are important. In the limit of a dilute Fermi gas, on the other hand, a different type of diagrams known as the ladder diagrams that are associated with short-range repulsive potentials are prominent. (An example of the ladder diagram contribution to the proper self-energy can be found in two of the diagrams on the right of Fig. II.7.9.) While the potentials may be strong, the scattering amplitude can be small for the short-range “hard-core” interactions. This type of interaction forms the basis for studying nuclear matter and  $^3\text{He}$ . Moreover, the ladder diagrams are reasonable approximations to studying impurity scattering in an electron gas if we assume that electron-hole pairs associated with the polarization propagators are simultaneously scattered by impurities without interacting directly with each other. For comprehensive discussions on the ladder diagrams and impurity scattering, see, for example, the books by Fetter & Walecka and Doniach & Sondheimer. In Fig. II.9.1 we illustrate an example of ladder diagrams that contain repeated interactions of electron and hole lines contribute to the transverse magnetic susceptibility  $\chi^{-+}(\mathbf{p}, \mathbf{q})$ .



**Fig. II.9.1** Ladder diagrams contributing to the transverse magnetic susceptibility  $\chi^{-+}(\mathbf{p}, \mathbf{q})$ .

Having studied interacting electrons, we want to understand how electrons in a solid interact with the background ions characterized by their quantized modes, the phonons. Diagrammatically, we can consider the electron-phonon interaction as a vertex contribution to electrons. This interaction can lead to scattering of electrons, which gives rise to electrical resistivity. On the other hand, under special circumstances, the electron-phonon interaction can also lead to an effective attractive potential for electrons, thus giving rise to Cooper pairing and conventional superconductivity.