Chapter 3

Correlation and Response Functions

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When studying a many-body system, we rarely try to compute the N-particle wavefunction $\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_N)$. This calculation is usually hardly feasible, and we do not need all the information which is contained in the wavefunction. A reduced description in terms of a few variables is often sufficient if it allows one to explain the response of the system to an experimental probe. Correlation functions offer such a description. In Sec. 3.1, we show that the linear response of the system to an external field is given by a correlation function. In Sec. 3.2, we study the basic properties of correlation (or response) functions and show that they contain information about the excitations of the system. Furthermore, they are simply related to the imaginary-time Green functions introduced in Sec. 1.2.3 and can therefore be calculated perturbatively using the methods discussed in Chap. 1. In Secs. 3.3 and 3.4, we study the density-density and electromagnetic response functions. From the properties of the latter, we deduce a number of general features of electron systems (metals and superconductors). The one-particle Green function is just one type of correlation function and is studied in Sec. 3.5. Finally, in Sec. 3.6, we consider systems with a spontaneous broken symmetry and derive two important theorems due to Goldstone, and Mermin and Wagner.

3.1 Linear response theory

We consider a physical system in the presence of an external field $h_i(\mathbf{r}, t)$ which couples to observables of the system described by the operators $\hat{A}_i(\mathbf{r})$. The total Hamiltonian can be written as

$$\hat{H} + \hat{H}'(t) = \hat{H} - \int d^d r \sum_i h_i(\mathbf{r}, t) \hat{A}_i(\mathbf{r}), \tag{3.1}$$

where $\hat{H}$ is the Hamiltonian in the absence of the external field. In the grand canonical ensemble, $\hat{H}$ includes the term $-\mu \hat{N}$. The perturbation term $\hat{H}'(t)$ comes from the coupling to the external field which is assumed to be local in space. If we are dealing with a physical external field, e.g. an electromagnetic field, the operators $\hat{A}_i(\mathbf{r})$ correspond to observables of the system and are Hermitian, while $h_i(\mathbf{r}, t)$ is real. It is useful to consider a more general perturbation Hamiltonian $\hat{H}'(t)$ where the operator $\hat{A}_i(\mathbf{r})$ is bosonic but not necessary Hermitian. In order to ensure that $\hat{H}'(t)$ is Hermitian, one has to include the Hermitian conjugate part $h_i^*(\mathbf{r}, t)\hat{A}_i^\dagger(\mathbf{r})$ in $\hat{H}'(t)$. The functional integral formalism allows a further generalization where $\hat{A}_i$ is fermionic and the field h_i a Grassmann variable (Sec. 3.2.7).

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3.1.1 Kubo's formula

We are interested in the response of the system in the limit of a vanishing external field, $h_i(\mathbf{r},t) \to 0$. At finite temperature T, the mean value of the operator $\hat{A}_i(\mathbf{r})$ is given by[1]

$$\langle \hat{A}_i(\mathbf{r}) \rangle(t) = \mathrm{Tr}[\hat{\rho}(t)\hat{A}_i(\mathbf{r})], \tag{3.2}$$

where $\hat{\rho}(t)$ is the density matrix of the whole system (including the external field) at time t. We assume that the external field is turned on adiabatically and vanishes for $t \to -\infty$. These boundary conditions ensure that the external perturbation remains small – provided the system is stable – and that nonlinear effects do not play an important role.

The time evolution of the density matrix is obtained under the assumption of adiabaticity: $\hat{\rho}(t) = \sum_n |\Psi_n(t)\rangle p_n \langle \Psi_n(t)|$ where $\{|\Psi_n(t=-\infty)\rangle, \epsilon_n\}$ is a complete set of eigenvectors of $\hat{H}$ and the probability occupations $p_n \propto e^{-\beta\epsilon_n}$ are time independent. This assumption of unitary evolution is justified for time evolutions that are fast on the scale of the thermal equilibrium time. When the time evolution is sufficiently slow, it is possible for the system to exchange energy (heat) with the reservoir, thus modifying the population of the energy levels.[2] Since $i\partial_t|\Psi_n(t)\rangle = (\hat{H} + \hat{H}'(t))|\Psi_n(t)\rangle$, the adiabaticity assumption leads to

$$i\frac{\partial \hat{\rho}(t)}{\partial t} = [\hat{H} + \hat{H}'(t), \hat{\rho}(t)], \tag{3.3}$$

with $\hat{\rho}(-\infty) = \hat{\rho}_{\mathrm{eq}} = e^{-\beta\hat{H}}/\mathrm{Tr}(e^{-\beta\hat{H}})$ the density matrix of the system in thermal equilibrium. To linear order in the external fields, $\delta\hat{\rho}(t) = \hat{\rho}(t) - \hat{\rho}_{\mathrm{eq}}$ satisfies the equation

$$i\frac{\partial \delta\hat{\rho}(t)}{\partial t} = [\hat{H}, \delta\hat{\rho}(t)] + [\hat{H}'(t), \hat{\rho}_{\mathrm{eq}}], \tag{3.4}$$

the solution of which is given by

$$\delta\hat{\rho}(t) = -i\int_{-\infty}^{t} dt' e^{-i\hat{H}(t-t')}[\hat{H}'(t'), \hat{\rho}_{\mathrm{eq}}]e^{i\hat{H}(t-t')}, \tag{3.5}$$

as can be verified by direct substitution into (3.4).

> This result can also be derived by writing the evolution operator (Sec. 2.2.4) in the interaction representation (Sec. 1.G.1.1):
>
> $$|\Psi_n(t)\rangle = \hat{T}(t,t_0)|\Psi_n(t_0)\rangle, \qquad \hat{T}(t,t_0) = e^{-i\hat{H}t}\hat{T}_I(t,t_0)e^{i\hat{H}t_0}, \tag{3.6}$$
>
> where $\hat{T}$ and $\hat{T}_I$ satisfy
>
> $$\begin{aligned} \hat{T}^\dagger(t,t_0)\hat{T}(t,t_0) &= \hat{T}_I^\dagger(t,t_0)\hat{T}_I(t,t_0) = 1, \\ i\partial_t\hat{T}(t,t_0) &= [\hat{H} + \hat{H}'(t)]\hat{T}(t,t_0), \\ i\partial_t\hat{T}_I(t,t_0) &= \hat{H}'_I(t)\hat{T}_I(t,t_0) \end{aligned} \tag{3.7}$$
>
> with
>
> $$\hat{H}'_I(t) = e^{i\hat{H}t}\hat{H}'(t)e^{-i\hat{H}t}. \tag{3.8}$$

[1] We shall use the notation $\langle \hat{A}_i(\mathbf{r}) \rangle(t)$ or $\langle A_i(\mathbf{r},t) \rangle$ to denote the expectation value of the (time-independent) operator $\hat{A}_i(\mathbf{r})$ in the presence of a (time-dependent) external perturbation. The notation $\langle A_i(\mathbf{r},t) \rangle$ is indeed natural when one computes $\langle A_i(\mathbf{r},\tau) \rangle$ in the Euclidean formalism before performing the analytic continuation to real time (see Sec. 3.2.7).

[2] See the discussion in Sec. 3.2.7.

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To linear order in the external perturbation,

$$\hat{T}_I(t,t_0) = 1 - i\int_{t_0}^{t} dt'\, \hat{H}'_I(t'). \tag{3.9}$$

Equation (3.5) then follows from $\hat{\rho}(t) = \hat{T}(t,-\infty)\hat{\rho}_{\rm eq}\hat{T}^\dagger(t,-\infty)$.

From the cyclic invariance of the trace, we then deduce

$$\begin{aligned}
\delta\langle\hat{A}_i(\mathbf{r})\rangle(t) &= {\rm Tr}[\delta\hat{\rho}(t)\hat{A}_i(\mathbf{r})] \\
&= -i\int_{-\infty}^{t} dt'\, {\rm Tr}\Big\{e^{-i\hat{H}(t-t')}[\hat{H}'(t'),\hat{\rho}_{\rm eq}]e^{i\hat{H}(t-t')}\hat{A}_i(\mathbf{r})\Big\} \\
&= -i\int_{-\infty}^{t} dt'\, {\rm Tr}\Big\{\hat{\rho}_{\rm eq}\Big[\hat{A}_i(\mathbf{r},t), e^{i\hat{H}t'}H'(t')e^{-i\hat{H}t'}\Big]\Big\} \\
&= i\int_{-\infty}^{t} dt' \int d^dr' \sum_j {\rm Tr}\{\hat{\rho}_{\rm eq}[\hat{A}_i(\mathbf{r},t),\hat{A}_j(\mathbf{r},t')]\}h_j(\mathbf{r}',t').
\end{aligned} \tag{3.10}$$

Here $\hat{A}_i(\mathbf{r},t) = e^{i\hat{H}t}\hat{A}_i(\mathbf{r})e^{-i\hat{H}t}$ denotes the operator $\hat{A}_i(\mathbf{r})$ in the Heisenberg representation (with respect to the Hamiltonian $\hat{H}$). Equation (3.10) can be written in terms of a "retarded" (causal) response function (or susceptibility) $\chi^R_{A_iA_j}$ as

$$\begin{aligned}
\delta\langle\hat{A}_i(\mathbf{r})\rangle(t) &= \int_{-\infty}^{\infty} dt' \int d^dr' \sum_j \chi^R_{A_iA_j}(\mathbf{r},t;\mathbf{r}',t')h_j(\mathbf{r}',t'), \\
\chi^R_{A_iA_j}(\mathbf{r},t;\mathbf{r}',t') &= i\Theta(t-t')\langle[\hat{A}_i(\mathbf{r},t),\hat{A}_j(\mathbf{r}',t')]\rangle,
\end{aligned} \tag{3.11}$$

where the average $\langle[.,.]\rangle$ is taken with the equilibrium density matrix $\hat{\rho}_{\rm eq}$. Equation (3.11), which expresses the linear response function as an equilibrium correlation function, is known as Kubo's formula. It is convenient to introduce the correlation function $\chi''_{A_iA_j}$ defined by

$$\begin{aligned}
\chi''_{A_iA_j}(\mathbf{r},t;\mathbf{r}',t') &= \frac{1}{2}\langle[\hat{A}_i(\mathbf{r},t),\hat{A}_j(\mathbf{r}',t')]\rangle, \\
\chi^R_{A_iA_j}(\mathbf{r},t;\mathbf{r}',t') &= 2i\Theta(t-t')\chi''_{A_iA_j}(\mathbf{r},t;\mathbf{r}',t').
\end{aligned} \tag{3.12}$$

In the following, we include the $\mathbf{r}$ dependence of the operator $\hat{A}_i$ in the i index unless explicitly written. Accordingly, the response function is denoted by $\chi^R_{A_iA_j}(t,t') = 2i\Theta(t-t')\chi''_{A_iA_j}(t,t')$. We also write $\hat{\rho}$ instead of $\hat{\rho}_{\rm eq}$ for the equilibrium density matrix $e^{-\beta\hat{H}}/{\rm Tr}(e^{-\beta\hat{H}})$ as only equilibrium thermal averages will now be considered.

In addition to the retarded response function, we shall also discuss the "advanced" (anticausal) response function, defined by

$$\chi^A_{A_iA_j}(t,t') = -2i\Theta(-t+t')\chi''_{A_iA_j}(t,t'). \tag{3.13}$$

To make $\chi^A_{A_iA_j}$ well defined, one has to assume that the external field is switched off adiabatically and vanishes for $t \to \infty$.

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3.1.2 Periodic perturbations

Both experimentally and theoretically, one often considers the response to a periodic perturbation. A field $h_i(t) = h_i(\omega)e^{-i\omega t}$ would violate the assumption that the perturbation is turned on – or switched off when considering the advanced response – adiabatically. This difficulty is avoided by choosing

$$h_i(t) = h_i(\omega)e^{-i\omega t+\eta t} \qquad (\eta \to 0^+) \tag{3.14}$$

when calculating the retarded response function. η^{-1} determines the adiabatic switching time of the external perturbation. The limit $\eta \to 0^+$ must be taken at the end of the calculation. A straightforward calculation then gives

$$\delta\langle \hat{A}_i\rangle(t) = \sum_j \chi^R_{A_iA_j}(\omega)h_j(\omega)e^{-i\omega t+\eta t}, \tag{3.15}$$

where the Fourier transform of χ^R is defined by[3]

$$\chi^R_{A_iA_j}(\omega) = \int_{-\infty}^{\infty} dt\, \chi^R_{A_iA_j}(t)e^{i(\omega+i\eta)t}. \tag{3.16}$$

Similarly, we obtain

$$\chi^A_{A_iA_j}(\omega) = \int_{-\infty}^{\infty} dt\, \chi^A_{A_iA_j}(t)e^{i(\omega-i\eta)t} \tag{3.17}$$

for the advanced response function, with $h_i(t) = h_i(\omega)e^{-i\omega t-\eta t}$.

3.2 Properties of response functions

3.2.1 Symmetry properties

In this section, we discuss the symmetry properties of $\chi''(\omega)$. These imply analogous properties for χ^R and χ^A which are most easily derived from their spectral representation (Sec. 3.2.3). As the derivation does not raise any difficulty, we merely summarize the symmetry properties of χ^R and χ^A in Table 3.1.

3.2.1.1 Properties following from the definition

Some properties of χ'' directly follow from its definition (3.12). The cyclic invariance of the trace implies that $\chi''_{A_iA_j}(t,t') = \chi''_{A_iA_j}(t-t')$ depends only on the time difference $t-t'$, as expected for a system in thermal equilibrium. We denote its Fourier transform by $\chi''_{A_iA_j}(\omega)$. $\chi''_{A_iA_j}(t)$ being defined by a commutator, it satisfies $\chi''_{A_iA_j}(t) = -\chi''_{A_jA_i}(-t) = [\chi''_{A_j^\dagger A_i^\dagger}(-t)]^*$. In frequency space, this gives

$$\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega) = [\chi''_{A_j^\dagger A_i^\dagger}(\omega)]^*. \tag{3.18}$$

[3] Equation (3.16) is actually unchanged if we replace $\omega + i\eta$ by ω in the rhs, i.e. if we forget that the external field is switched on adiabatically. The reason is that $\chi^R(\omega) = \int_{-\infty}^{\infty} dt\, \chi^R(t)e^{i\omega t}$ is analytic in the upper-half complex plane so that $\chi^R(\omega) = \chi^R(\omega + i\eta)$.

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3.2.1.2 Properties following from symmetries of the system

To most symmetry transformations we can associate a unitary operator $\hat{U}$ (Chap. 2); time-reversal symmetry, where the Wigner operator $\hat{U}$ is antiunitary, will be discussed below. If the system is invariant under the symmetry transformation, then the transformed Hamiltonian $\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger + i(\partial_t\hat{U})\hat{U}^\dagger$ is identical to the original Hamiltonian $\hat{H}$. In this section, except for the time-reversal symmetry discussed below, we restrict ourselves to time-independent Wigner operators.[4] The condition $\hat{H}' = \hat{H}$ then implies $[\hat{H}, \hat{U}] = 0$ and, provided that the symmetry is not spontaneously broken, $[\hat{\rho}, \hat{U}] = 0$. Let us denote by $\{|n\rangle, \epsilon_n\}$ a complete set of eigenvectors of $\hat{H}$. The vectors $\hat{U}|n\rangle$ are also eigenvectors of $\hat{H}$, $\hat{H}\hat{U}|n\rangle = \epsilon_n\hat{U}|n\rangle$, and can be used to compute χ'',

$$\begin{aligned}\chi''_{A_iA_j}(t) &= \frac{1}{2}\sum_n \langle n|\hat{U}^\dagger\hat{\rho}[\hat{A}_i(t), \hat{A}_j]\hat{U}|n\rangle \\ &= \frac{1}{2}\sum_n \langle n|\hat{\rho}[\hat{U}^\dagger\hat{A}_i(t)\hat{U}, \hat{U}^\dagger\hat{A}_j\hat{U}]|n\rangle = \chi''_{U^\dagger A_iU, U^\dagger A_jU}(t)\end{aligned} \tag{3.19}$$

where we have used $[\hat{\rho}, \hat{U}] = 0$, $\hat{U}\hat{U}^\dagger = 1$, and $\hat{U}^\dagger\hat{A}_i(t)\hat{U} = e^{i\hat{H}t}\hat{U}^\dagger\hat{A}_i\hat{U}e^{-i\hat{H}t}$. The correlation function $\chi''_{A_iA_j}(t)$ is thus invariant under the transformation $\hat{A}_i \to \hat{U}^\dagger\hat{A}_i\hat{U}$ and $\hat{A}_j \to \hat{U}^\dagger\hat{A}_j\hat{U}$.[5]

As an example, let us consider a space translation, $\hat{U}^\dagger\hat{A}_i(\mathbf{r})\hat{U} = \hat{A}_i(\mathbf{r}-\mathbf{a})$, where $\mathbf{a}$ is an arbitrary vector (see Sec. 2.2.2). If the system is translation invariant, Eq. (3.19) implies $\chi''_{A_iA_j}(\mathbf{r}, \mathbf{r}', t) = \chi''_{A_iA_j}(\mathbf{r}-\mathbf{a}, \mathbf{r}'-\mathbf{a}, t)$, i.e.

$$\chi''_{A_iA_j}(\mathbf{r}, \mathbf{r}', t) = \chi''_{A_iA_j}(\mathbf{r}-\mathbf{r}', t). \tag{3.20}$$

Similarly, invariance under a parity transformation implies

$$\chi''_{A_iA_j}(\mathbf{r}, \mathbf{r}', t) = \epsilon^P_{A_i}\epsilon^P_{A_j}\chi''_{A_iA_j}(-\mathbf{r}, -\mathbf{r}', t) \tag{3.21}$$

for two operators with signatures $\epsilon^P_{A_i}$ and $\epsilon^P_{A_j}$: $\hat{U}^\dagger\hat{A}_i(\mathbf{r})\hat{U} = \epsilon^P_{A_i}\hat{A}_i(-\mathbf{r})$ and $\hat{U}^\dagger\hat{A}_j(\mathbf{r})\hat{U} = \epsilon^P_{A_j}\hat{A}_j(-\mathbf{r})$ (see Sec. 2.2.1).

In the case of time-reversal symmetry, the Wigner operator $\hat{U}(t)$ is antiunitary. χ'' can be evaluated using the time-reversed states $\hat{\Theta}|n\rangle$, where $\hat{\Theta} = \hat{U}(t)e^{-2i\hat{H}t}$ is the time-independent antiunitary operator introduced in Sec. 2.2.6. Time-reversal invariance implies $[\hat{H}, \hat{\Theta}] = [\hat{\rho}, \hat{\Theta}] = 0$. We then obtain[6]

$$\begin{aligned}\chi''_{A_iA_j}(t) &= \frac{1}{2}\sum_n (\langle n|\hat{\Theta}^\dagger)\hat{\rho}[\hat{A}_i(t), \hat{A}_j](\hat{\Theta}|n\rangle) = \frac{1}{2}\sum_n [\langle n|(\hat{\Theta}^\dagger\hat{\rho}[\hat{A}_i(t), \hat{A}_j]\hat{\Theta}|n\rangle)]^* \\ &= \frac{1}{2}\sum_n [\langle n|\hat{\rho}([\hat{\Theta}^\dagger\hat{A}_i(t)\hat{\Theta}, \hat{\Theta}^\dagger\hat{A}_j\hat{\Theta}]|n\rangle)]^* = [\chi''_{\Theta^\dagger A_i\Theta, \Theta^\dagger A_j\Theta}(-t)]^*\end{aligned}$$

[4] Time dependent symmetry transformations are more naturally handled in the functional integral formalism (see Sec. 3.2.7).

[5] In the language of Chap. 2, Eq. (3.19) means that the two observers $\mathcal{O}$ and $\mathcal{O}'$ measure the same correlation function $\chi''_{A_iA_j}$ in their respective reference frames when the system is invariant under the symmetry transformation.

[6] Recall that parentheses must be used to avoid the ambiguity of the Dirac notation when dealing with antilinear operators (Sec. 2.2.6).

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$$= \chi''_{\Theta^\dagger A_j^\dagger \Theta, \Theta^\dagger A_i^\dagger \Theta}(t) \tag{3.22}$$

i.e.

$$\chi''_{A_i A_j}(\omega) = \chi''_{\Theta^\dagger A_j^\dagger \Theta, \Theta^\dagger A_i^\dagger \Theta}(\omega). \tag{3.23}$$

We have used $\hat{\Theta}\hat{\Theta}^\dagger = 1$ and $\Theta^\dagger \hat{A}(t)\hat{\Theta} = e^{-i\hat{H}t}\hat{\Theta}^\dagger \hat{A}\hat{\Theta}e^{i\hat{H}t}$ (Chap. 2). For two operators with signatures $\epsilon^T_{A_i}$ and $\epsilon^T_{A_j}$ under time reversal symmetry ($\Theta^\dagger \hat{A}_i(t)\hat{\Theta} = \epsilon^T_{A_i}\hat{A}_i(-t)$ and $\Theta^\dagger \hat{A}_j(t)\hat{\Theta} = \epsilon^T_{A_j}\hat{A}_j(-t)$), Eqs. (3.22) and (3.23) give

$$\begin{aligned} \chi''_{A_i A_j}(t) &= \epsilon^T_{A_i}\epsilon^T_{A_j}[\chi''_{A_i A_j}(-t)]^*, \\ \chi''_{A_i A_j}(\omega) &= \epsilon^T_{A_i}\epsilon^T_{A_j}[\chi''_{A_i A_j}(\omega)]^* = \epsilon^T_{A_i}\epsilon^T_{A_j}\chi''_{A_j^\dagger A_i^\dagger}(\omega). \end{aligned} \tag{3.24}$$

From Eq. (3.24), we conclude that $\chi''_{A_i A_j}(\omega)$ is real if $\epsilon^T_{A_i}\epsilon^T_{A_j} = 1$ and imaginary if $\epsilon^T_{A_i}\epsilon^T_{A_j} = -1$. Properties of real- and imaginary-time correlation functions, similar to (3.22) and (3.23), were obtained in Sec. 2.2.6.

3.2.2 Dissipation

Another property of $\chi''_{A_i A_j}$ can be obtained by considering the energy dissipation of the system coupled to an external perturbation. If the system is stable, it can only absorb energy from the external field over a long time interval. The energy transferred to the system per unit time is given by

$$\begin{aligned} \frac{dW}{dt} &= \frac{d}{dt}\mathrm{Tr}\{\hat{\rho}(t)[\hat{H} + \hat{H}'(t)]\} \\ &= \mathrm{Tr}\left\{\hat{\rho}(t)\frac{d\hat{H}'(t)}{dt}\right\} + \mathrm{Tr}\left\{\frac{d\hat{\rho}(t)}{dt}\left[\hat{H} + \hat{H}'(t)\right]\right\}. \end{aligned} \tag{3.25}$$

Using Eq. (3.3), the last term in (3.25) is found to vanish, and

$$\frac{dW}{dt} = -\sum_i \mathrm{Tr}[\hat{\rho}(t)\hat{A}_i]\dot{h}_i(t) = -\sum_i \{\mathrm{Tr}[\hat{\rho}\hat{A}_i] + \mathrm{Tr}[\delta\hat{\rho}(t)\hat{A}_i]\}\dot{h}_i(t), \tag{3.26}$$

where $\dot{h}_i(t) = \partial_t h_i(t)$ denotes the time derivative of $h_i(t)$. Here $\mathrm{Tr}[\delta\hat{\rho}(t)\hat{A}_i] = \delta\langle\hat{A}_i(t)\rangle$ is the response of the system to the external fields.

Let us now consider a periodic perturbation of the form

$$h_i(t) = \frac{1}{2}\left[h_i(\omega)e^{-i\omega t+\eta t} + h_i(-\omega)e^{i\omega t+\eta t}\right], \tag{3.27}$$

with $h_{A_i^\dagger}(\omega) = h^*_{A_i}(-\omega)$ ($h_i(-\omega) = h_i^*(\omega)$ when $h_i(t)$ is real and $\hat{A}_i$ Hermitian). To lowest order in the field h_i, the mean power dissipated into the system reads

$$\begin{aligned} \overline{\frac{dW}{dt}} &= \frac{1}{T}\int_t^{t+T} dt\frac{dW}{dt} \\ &= -\frac{1}{4}\sum_{i,j}\left[\chi^R_{A_i A_j}(\omega)h_j(\omega)i\omega h_i(-\omega) - \chi^R_{A_i A_j}(-\omega)h_j(-\omega)i\omega h_i(\omega)\right] \end{aligned}$$

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Table 3.1: Symmetry properties of $\chi''_{A_iA_j}(\omega)$ and $\chi^{R,A}_{A_iA_j}(\omega)$. $\hat{A}_i$ and $\hat{A}_j$ are bosonic operators. ϵ^P_A and ϵ^T_A denote the signature of the operator $\hat{A}$ under parity and time reversal, respectively.

	$\chi''_{A_iA_j}(\omega)$	$\chi^{R,A}_{A_iA_j}(\omega)$
	$\chi''_{A_iA_j}(\omega) = -\chi''_{A_jA_i}(-\omega) = [\chi''_{A_j^\dagger A_i^\dagger}(\omega)]^*$	$\chi^R_{A_iA_j}(\omega) = [\chi^R_{A_i^\dagger A_j^\dagger}(-\omega)]^* = [\chi^A_{A_jA_i}(-\omega)]$
Space translation	$\chi''_{A_iA_j}(\mathbf{r},\mathbf{r}',\omega) = \chi''_{A_iA_j}(\mathbf{r}-\mathbf{r}',\omega)$	$\chi^R_{A_iA_j}(\mathbf{r},\mathbf{r}',\omega) = \chi^R_{A_iA_j}(\mathbf{r}-\mathbf{r}',\omega)$
Parity	$\chi''_{A_iA_j}(\mathbf{r},\mathbf{r}',\omega) = \epsilon^P_{A_i}\epsilon^P_{A_j}\chi''_{A_iA_j}(-\mathbf{r},-\mathbf{r}',\omega)$	$\chi^R_{A_iA_j}(\mathbf{r},\mathbf{r}',\omega) = \epsilon^P_{A_i}\epsilon^P_{A_j}\chi^R_{A_iA_j}(-\mathbf{r},-\mathbf{r}',\omega)$
Time reversal	$\epsilon^T_{A_i}\epsilon^T_{A_j} = 1$ $\chi''_{A_iA_j}(\omega) = [\chi''_{A_iA_j}(\omega)]^* = \Im[\chi^R_{A_iA_j}(\omega)]$	$\chi^R_{A_iA_j}(\omega) = \chi^R_{A_j^\dagger A_i^\dagger}(\omega) = [\chi^A_{A_iA_j}(\omega)]^*$
	$\epsilon^T_{A_i}\epsilon^T_{A_j} = -1$ $\chi''_{A_iA_j}(\omega) = -[\chi''_{A_iA_j}(\omega)]^* = -i\Re[\chi^R_{A_iA_j}(\omega)]$	$\chi^R_{A_iA_j}(\omega) = -\chi^R_{A_j^\dagger A_i^\dagger}(\omega) = -[\chi^A_{A_iA_j}(\omega)]^*$
$\hat{A}_i = \hat{A}_j^\dagger$	$\chi''_{A^\dagger A}(\omega) = \Im[\chi^R_{A^\dagger A}(\omega)]$	$\chi^R_{A^\dagger A}(\omega) = [\chi^A_{A^\dagger A}(\omega)]^*$
Stability	$\{\omega\chi''_{A_i^\dagger A_j}(\omega)\}$ positive matrix	$\{\chi^R_{A_i^\dagger A_j}(\omega=0)\}$ positive matrix
	$\mathrm{sgn}[\chi''_{A^\dagger A}(\omega)] = \mathrm{sgn}(\omega)$	$\chi^R_{A^\dagger A}(\omega=0) \geq 0$

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$$= -\frac{1}{4}\sum_{i,j} h_i(-\omega)\big[\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega)\big] i\omega h_j(\omega), \tag{3.28}$$

where $T = 2\pi/\omega$. From the definition of $\chi^R_{A_iA_j}$, we easily deduce

$$\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega) = 2i\chi''_{A_iA_j}(\omega), \tag{3.29}$$

and therefore

$$\overline{\frac{dW}{dt}} = \frac{1}{2}\sum_{i,j} h_i^*(\omega)\omega\chi''_{A_i^\dagger A_j}(\omega)h_j(\omega). \tag{3.30}$$

Here we have changed $\hat{A}_i \to \hat{A}_i^\dagger$ in the sum over i. Since the stability of the system requires $\overline{dW/dt} \geq 0$ regardless of the external perturbation, we conclude that $\omega\chi''_{A_i^\dagger A_j}(\omega)$ is a positive matrix for any set of operators $\hat{A}_i$. In particular, for the minimal set $\{\hat{A}, \hat{A}^\dagger\}$, this implies

$$\omega\chi''_{A^\dagger A}(\omega) \geq 0. \tag{3.31}$$

Using Eq. (3.44) below one then obtains the inequality $\chi^R_{A^\dagger A}(\omega = 0) \geq 0$ whose physical meaning will be discussed at the end of Sec. 3.2.7. Equation (3.31) can also be deduced from the expression of $\chi''_{A_iA_j}(\omega)$ given in (3.37) below.

3.2.3 Spectral representation

From the definition (3.16,3.17) of the Fourier transforms of the retarded and advanced response functions, we obtain

$$\begin{aligned}\chi^{R,A}_{A_iA_j}(\omega) &= \pm 2i\int_{-\infty}^{\infty} dt\, e^{i(\omega\pm i\eta)t}\Theta(\pm t)\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\chi''_{A_iA_j}(\omega')e^{-i\omega' t}\\ &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\chi''_{A_iA_j}(\omega')}{\omega' - (\omega \pm i\eta)}.\end{aligned} \tag{3.32}$$

Equation (3.32) allows one to generalize the definition of $\chi^{R,A}(\omega)$ to complex frequencies z by introducing

$$\chi_{A_iA_j}(z) = \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A_iA_j}(\omega)}{\omega - z}. \tag{3.33}$$

χ^R, χ^A and χ are related by

$$\begin{aligned}\chi^R_{A_iA_j}(\omega) &= \chi_{A_iA_j}(z = \omega + i\eta),\\ \chi^A_{A_iA_j}(\omega) &= \chi_{A_iA_j}(z = \omega - i\eta).\end{aligned} \tag{3.34}$$

Since

$$\chi^R_{A_iA_j}(\omega) - \chi^A_{A_iA_j}(\omega) = 2i\chi''_{A_iA_j}(\omega), \tag{3.35}$$

$\chi_{A_iA_j}(z)$ is discontinuous across the real axis wherever $\chi''_{A_iA_j}(\omega)$ does not vanish. Equation (3.33) is known as a spectral or Lehmann representation. It relates $\chi_{A_iA_j}(z)$ in the entire complex plane to $\chi''_{A_iA_j}(\omega)$ along the real axis.

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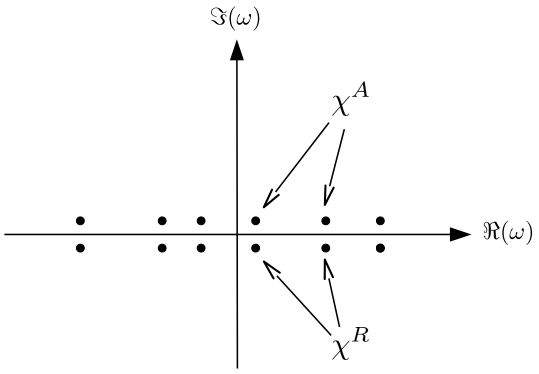


Figure 3.1: Poles of $\chi^R(\omega)$ and $\chi^A(\omega)$ in the complex ω plane.

A more explicit definition of $\chi_{A_iA_j}(z)$ can be obtained by expressing $\chi''_{A_iA_j}(\omega)$ in terms of a complete set of eigenvectors $\{|n\rangle, \epsilon_n\}$ of the Hamiltonian $\hat{H}$. Using the closure relation $\sum_n |n\rangle\langle n| = 1$, we obtain

$$\begin{aligned}\chi''_{A_iA_j}(t) &= \frac{1}{2Z}\mathrm{Tr}\left[e^{-\beta\hat{H}}\left(e^{i\hat{H}t}\hat{A}_i e^{-i\hat{H}t}\hat{A}_j - \hat{A}_j e^{i\hat{H}t}\hat{A}_i e^{-i\hat{H}t}\right)\right] \\ &= \frac{1}{2Z}\sum_{n,m} e^{-\beta\epsilon_n}\left(e^{i\epsilon_n t}A_i^{nm}e^{-i\epsilon_m t}A_j^{mn} - A_j^{nm}e^{i\epsilon_m t}A_i^{mn}e^{-i\epsilon_n t}\right), \end{aligned} \tag{3.36}$$

where $A_i^{nm} = \langle n|\hat{A}_i|m\rangle$. In frequency space, this gives

$$\chi''_{A_iA_j}(\omega) = \frac{\pi}{Z}\sum_{n,m}\left(e^{-\beta\epsilon_n} - e^{-\beta\epsilon_m}\right)A_i^{nm}A_j^{mn}\delta(\omega + \epsilon_n - \epsilon_m). \tag{3.37}$$

Inserting (3.37) into (3.33), we obtain an alternative form of the Lehmann representation, in terms of the exact eigenstates of the system,

$$\chi_{A_iA_j}(z) = \frac{1}{Z}\sum_{\substack{n,m \\ (\epsilon_n\neq\epsilon_m)}}\frac{e^{-\beta\epsilon_n} - e^{-\beta\epsilon_m}}{\epsilon_m - \epsilon_n - z}A_i^{nm}A_j^{mn}. \tag{3.38}$$

We have excluded of the sum the terms with $\epsilon_n = \epsilon_m$ which do not contribute to $\chi''_{A_iA_j}(\omega)$ [Eq. (3.37)]. Since $\chi''_{A_iA_j}(\omega)$ is a sum of delta peaks at the transition energies $\epsilon_m - \epsilon_n$, it gives information about the excitation spectrum of the system. For this reason, it is often referred to as the spectral function.

$\chi_{A_iA_j}(z)$ is an analytic function of z for $\Im(z) \neq 0$. It follows that $\chi^R_{A_iA_j}(\omega)$, considered as a function of the complex variable ω, is analytic in the upper-half complex plane $\Im(\omega) \geq 0$, whereas $\chi^A_{A_iA_j}(\omega)$ is analytic in the lower-half complex plane. In a finite system, the singularities of $\chi^R_{A_iA_j}(\omega)$ ($\chi^A_{A_iA_j}(\omega)$) always consist of discrete poles located infinitesimally below (above) the real axis (Fig. 3.1). The thermodynamic limit (large-size systems), whereby the sum over the state index n may be partially replaced by a continuous integral, qualitatively changes this picture. An infinite number of poles of vanishing strength can merge and form a branch cut corresponding to a continuous excitation spectrum. On the other hand, there can be a strong enhancement of the spectral function around some energy.

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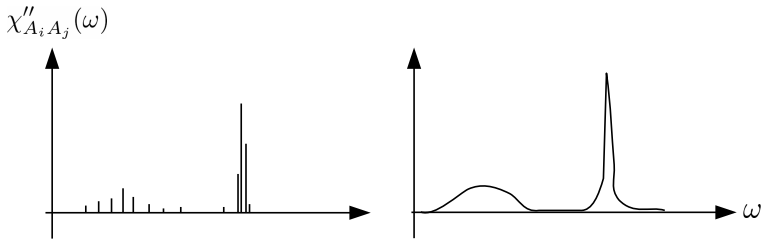


Figure 3.2: Schematic representation of the spectral function $\chi''_{A_iA_j}(\omega)$ – here assumed real – in a finite (left) and infinite (right) system.

Such an enhancement is often (approximately) described by an isolated pole located away from the real axis, i.e. at the complex frequency $\Re(\omega_0) + i\Im(\omega_0)$ with $\Im(\omega_0) < 0$ (> 0) for a pole of χ^R (χ^A). As will be seen from many examples, an isolated pole corresponds to a collective excitation (or collective mode) with an energy $\Re(\omega_0)$ and a lifetime $|\Im(\omega_0)|^{-1}$.[7] It shows up as a sharp peak in the spectral function $\chi''_{A_iA_j}(\omega)$ located at $\omega = \Re(\omega_0)$ with a width given by the inverse lifetime $|\Im(\omega_0)|$, whereas a branch cut gives rise to a structureless continuous excitation background (Fig. 3.2).

The spectral decomposition (3.32) of the retarded response function, which relates χ'' to χ^R and χ^A, can be written as

$$\chi^{R,A}_{A_iA_j}(\omega) = \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\omega')}{\omega' - \omega} \pm i\chi''_{A_iA_j}(\omega), \tag{3.39}$$

where $\mathcal{P}$ denotes the principal part. In a time-reversal-invariant system, $\chi''_{A_iA_j}(\omega)$ is real when the operators have the same signature ($\epsilon^T_{A_i} = \epsilon^T_{A_j}$). In the opposite case ($\epsilon^T_{A_i} = -\epsilon^T_{A_j}$), $\chi''_{A_iA_j}(\omega)$ is imaginary [Eq. (3.24)]. From (3.39), we then deduce

$$\begin{cases} \chi''_{A_iA_j}(\omega) = \Im[\chi^R_{A_iA_j}(\omega)] \\ \chi^A_{A_iA_j}(\omega) = [\chi^R_{A_iA_j}(\omega)]^* \end{cases} \quad \text{if} \quad \epsilon^T_{A_i} = \epsilon^T_{A_j}, \tag{3.40}$$

and

$$\begin{cases} \chi''_{A_iA_j}(\omega) = -i\Re[\chi^R_{A_iA_j}(\omega)] \\ \chi^A_{A_iA_j}(\omega) = -[\chi^R_{A_iA_j}(\omega)]^* \end{cases} \quad \text{if} \quad \epsilon^T_{A_i} = -\epsilon^T_{A_j}. \tag{3.41}$$

When $\hat{A}_i = \hat{A}_j^\dagger$, $\chi''_{A_iA_j}(\omega)$ is real and has the sign of ω, regardless of the behavior of $\hat{A}_i$ under time-reversal symmetry (see Eq. (3.37)), so that

$$\chi''_{A^\dagger A}(\omega) = \Im[\chi^R_{A^\dagger A}(\omega)] \quad \text{and} \quad \chi^A_{A^\dagger A}(\omega) = [\chi^R_{A^\dagger A}(\omega)]^*. \tag{3.42}$$

In practice, most cases of interest correspond to (3.40), (3.41) or (3.42).

3.2.3.1 The static limit

In general, $\lim_{\mathbf{q},\omega\to 0} \chi^R_{A_iA_j}(\mathbf{q},\omega)$ depends on the order of the limits $\mathbf{q} \to 0$ and $\omega \to 0$ (we write explicitly the $\mathbf{q}$ dependence and assume translation invariance). The static limit

[7] An isolated pole can also correspond to a single-particle excitation when $\chi^R_{A_iA_j}$ is the one-particle Green function: $\hat{A}_i = \hat{\psi}$ and $\hat{A}_j = \hat{\psi}^\dagger$ (see Sec. 3.5).

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$\omega \to 0$ determines the response to a time-independent external perturbation. In particular, the uniform susceptibility is obtained by taking $\omega \to 0$ and then $\mathbf{q} \to 0$, which amounts to taking the infinite volume (thermodynamic) limit ($\mathcal{V} \sim |\mathbf{q}|^{-3} \to \infty$) in the static case ($\omega = 0$),[8]

$$\chi_{A_iA_j} = \left.\frac{\partial \langle \hat{A}_i \rangle_h}{\partial h_j}\right|_{h=0} = \lim_{\mathbf{q}\to 0} \chi_{A_iA_j}(\mathbf{q}) \tag{3.43}$$

($\langle \hat{A}_i \rangle_h$ denotes the mean value of $\hat{A}_i$ in the presence of the external field h_j), where

$$\begin{aligned} \chi_{A_iA_j}(\mathbf{q}) &\equiv \chi^R_{A_iA_j}(\mathbf{q}, \omega = 0) \\ &= \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'} + i\chi''_{A_iA_j}(\mathbf{q},0) \\ &= \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\mathbf{q},\omega')}{\omega'} \equiv \chi_{A_iA_j}(\mathbf{q}, z = 0). \end{aligned} \tag{3.44}$$

Here we have used $\chi''_{A_iA_j}(\mathbf{q}, 0) = 0$ and the fact that the integral over ω' converges so that the principal part is not necessary.[9] The other limit, $\mathbf{q} = 0$ and $\omega \to 0$, describes transport properties as we shall see in Sec. 3.4.4.

Let us illustrate this point by considering the density-density response function χ_{nn}. The latter is introduced in Sec. 3.3 and will be encountered many times in the following chapters. For a propagating sound mode with velocity $c = 1/\sqrt{nm\kappa}$,

$$\begin{aligned} \chi_{nn}(\mathbf{q}, z) &= \frac{n}{m} \frac{\mathbf{q}^2}{c^2\mathbf{q}^2 - z^2}, \\ \chi''_{nn}(\mathbf{q}, \omega) &= \frac{\pi n}{2mc} |\mathbf{q}| [\delta(\omega - c|\mathbf{q}|) - \delta(\omega + c|\mathbf{q}|)], \end{aligned} \tag{3.45}$$

while for a diffusive mode with diffusion constant D [1, 2]

$$\begin{aligned} \chi_{nn}(\mathbf{q}, z) &= n^2\kappa \frac{D\mathbf{q}^2}{D\mathbf{q}^2 - iz\,\mathrm{sgn}(\Im z)}, \\ \chi''_{nn}(\mathbf{q}, \omega) &= n^2\kappa \frac{D\mathbf{q}^2\omega}{\omega^2 + D^2\mathbf{q}^4}, \end{aligned} \tag{3.46}$$

where κ is the compressibility (Sec. 3.3). It is straightforward to verify that in both cases

$$n^2\kappa = \lim_{\mathbf{q}\to 0} \chi_{nn}(\mathbf{q}) = \lim_{\mathbf{q}\to 0} \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q}\to 0} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} \tag{3.47}$$

but

$$n^2\kappa \neq \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \lim_{\mathbf{q}\to 0} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega}. \tag{3.48}$$

This last result shows that one must take the limit $\eta \to 0^+$ before $\mathbf{q} \to 0$. Physically this means that the adiabatic turning-on time $1/\eta$ must be longer than the characteristic time scale set by $\mathbf{q}$ to allow the density to relax towards equilibrium. We also notice that taking the limits $\mathbf{q} \to 0, \omega \to 0$ in reverse order does not yield the compressibility since $\chi_{nn}(0, z) = 0$ for $z \neq 0$, as follows from gauge invariance or particle number conservation (see Sec. 3.4.4).

[8] Whether $\chi_{A_iA_j}$ is the true thermodynamic susceptibility is discussed in Sec. 3.2.7.

[9] This can be seen from the fluctuation-dissipation theorem derived in Sec. 3.2.5. The structure factor $S_{A_iA_j}(t = 0) = \langle \hat{A}_i \hat{A}_j \rangle_c = \int_{-\infty}^{\infty} (d\omega/2\pi) S_{A_iA_j}(\omega)$ is finite. For $|\omega| \ll T$ the integral behaves as $\int d\omega (2T/\omega) \chi''_{A_iA_j}(\omega)$ so that $T \int_{-T}^{T} (d\omega/\omega) \chi''_{A_iA_j}(\omega) < \infty$.

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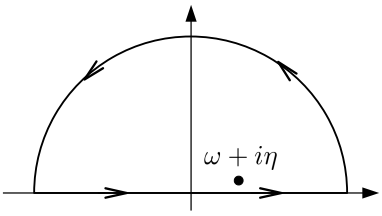


Figure 3.3: Integration contour $\mathcal{C}$ in Eq. (3.50).

3.2.4 Kramers-Kronig relations and causality

Kramers-Kronig relations are a consequence of the causality of the response function χ^R. The causality of

$$\chi^R(t)e^{-\eta t} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t}\chi^R(\omega) \tag{3.49}$$

is ensured by the analyticity of $\chi^R(\omega)$ in the upper-half complex plane. For $t < 0$, we can calculate $\chi^R(t)$ by closing the integration contour in the upper-half plane in Eq. (3.49). Since no pole or branch cut is enclosed, $\chi^R(t)$ vanishes for $t < 0$.

The Kramers-Kronig relations are derived by evaluating

$$\oint_{\mathcal{C}} \frac{d\omega'}{\pi} \frac{\chi^R(\omega')}{\omega' - \omega - i\eta} = 2i\chi^R(\omega + i\eta) = 2i\chi^R(\omega), \tag{3.50}$$

where $\mathcal{C}$ is the contour shown in Fig. 3.3. The result (3.50) relies only on the residue theorem and the analyticity of $\chi^R(\omega)$ in the upper-half complex plane. Assuming that $\chi^R(\omega') \to 0$ when $|\omega'| \to \infty$, there is no contribution from the part of the contour at infinity,[10] and Eq. (3.50) gives

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi^R(\omega')}{\omega' - \omega} = i\chi^R(\omega). \tag{3.51}$$

Taking the real and imaginary parts of (3.51), we obtain the Kramers-Kronig relations

$$\begin{aligned} \Re[\chi^R(\omega)] &= \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Im[\chi^R(\omega')]}{\omega' - \omega}, \\ \Im[\chi^R(\omega)] &= -\mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Re[\chi^R(\omega')]}{\omega' - \omega}. \end{aligned} \tag{3.52}$$

3.2.5 Fluctuation-dissipation theorem

Let us consider the structure factor $S_{A_iA_j}$ defined as the correlation function

$$S_{A_iA_j}(t) = \langle \delta\hat{A}_i(t)\delta\hat{A}_j\rangle = \langle \hat{A}_i(t)\hat{A}_j\rangle - \langle \hat{A}_i\rangle\langle \hat{A}_j\rangle, \tag{3.53}$$

where $\delta\hat{A}_i(t) = \hat{A}_i(t) - \langle \hat{A}_i\rangle$. In frequency space, we easily obtain

$$S_{A_iA_j}(\omega) = \frac{2\pi}{Z}\sum_{n,m} e^{-\beta\epsilon_n} A_i^{nm} A_j^{mn} \delta(\omega + \epsilon_n - \epsilon_m) - 2\pi\delta(\omega)\langle \hat{A}_i\rangle\langle \hat{A}_j\rangle, \tag{3.54}$$

[10] When $\lim_{\omega\to\infty} \chi^R(\omega) = \text{const}$, the Kramers-Kronig relations (3.52) hold for $\chi^R(\omega) - \chi^R(\omega \to \infty)$.

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where $\{|n\rangle, \epsilon_n\}$ is a complete set of eigenstates of the Hamiltonian $\hat{H}$. The real function $S_{AA^\dagger}(\omega)$ gives the spectral density – or power spectrum – of the spontaneous fluctuations of the variable $\hat{A}$. Changing ω into $-\omega$ in (3.54), we obtain the relation

$$S_{A_iA_j}(\omega) = e^{\beta\omega} S_{A_jA_i}(-\omega) \tag{3.55}$$

between the absorption ($\omega = \epsilon_m - \epsilon_n > 0$) and emission ($\omega < 0$) parts of the spectrum. The emission spectrum vanishes when $T \to 0$.

$\chi''_{A_iA_j}(t)$ and $S_{A_iA_j}(t)$ are related by

$$\chi''_{A_iA_j}(t) = \frac{1}{2}[S_{A_iA_j}(t) - S_{A_jA_i}(-t)]. \tag{3.56}$$

From (3.55) and (3.56), we deduce

$$\chi''_{A_iA_j}(\omega) = \frac{1}{2}\left(1 - e^{-\beta\omega}\right) S_{A_iA_j}(\omega). \tag{3.57}$$

The fluctuation-dissipation theorem is usually written as

$$S_{A_iA_j}(\omega) = 2[n_B(\omega) + 1]\chi''_{A_iA_j}(\omega). \tag{3.58}$$

It relates the spontaneous fluctuations in the system, whose return to equilibrium is described by $S_{A_iA_j}$, to the dissipation induced by an external perturbation.

If $|\omega| \ll T$, Eq. (3.57) gives

$$\chi''_{A_iA_j}(\omega) = \frac{\beta\omega}{2} S_{A_iA_j}(\omega). \tag{3.59}$$

At sufficiently high temperatures, the condition $|\omega| \ll T$ holds for all excitation energies of the system, i.e. for all ω such that $\chi''_{A_iA_j}(\omega)$ is nonzero. Integrating (3.59), we then obtain the classical limit of the fluctuation-dissipation theorem,[11]

$$\chi^R_{A_iA_j}(\omega = 0) = \beta S_{A_iA_j}(t = 0) = \beta\big[\langle \hat{A}_i\hat{A}_j\rangle - \langle \hat{A}_i\rangle\langle \hat{A}_j\rangle\big]. \tag{3.60}$$

3.2.6 Sum rules and high-frequency behavior

3.2.6.1 Thermodynamic sum rules

The static uniform susceptibility is given by (3.43),

$$\chi_{A_iA_j} \equiv \left.\frac{\partial\langle \hat{A}_i\rangle_h}{\partial h_j}\right|_{h=0} = \lim_{\mathbf{q}\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A_iA_j}(\mathbf{q},\omega)}{\omega}. \tag{3.61}$$

Equation (3.61) is a sum rule relating $\chi''_{A_iA_j}(\omega)$ to the susceptibility $\chi_{A_iA_j}$.

3.2.6.2 Other sum rules

Other sum rules are obtained by considering

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{A_iA_j}(\omega) = 2\big[(i\partial_t)^n\chi''_{A_iA_j}(t)\big]_{t=0} = \big[(i\partial_t)^n\langle[\hat{A}_i(t),\hat{A}_j]\rangle\big]_{t=0}. \tag{3.62}$$

Using $i\partial_t\hat{A}_i(t) = [\hat{A}_i(t),\hat{H}]$, we finally obtain

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{A_iA_j}(\omega) = \Big\langle\Big[[\hat{A}_i,\hat{H}],\hat{H}\big],\cdots,\hat{A}_j\Big]\Big\rangle. \tag{3.63}$$

[11] Note that the classical fluctuation-dissipation theorem is a direct consequence of linear response theory for a classical system.

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3.2.6.3 High-frequency behavior

These sum rules determine the asymptotic behavior of $\chi_{A_iA_j}(z)$ at high frequency. Noting that the spectral function $\chi''_{A_iA_j}(\omega)$ is expected to be bounded in frequency in many cases of interest – in particular when i stands for a momentum variable – the spectral representation gives

$$\chi_{A_iA_j}(z) = -\frac{1}{z}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\chi''_{A_iA_j}(\omega) - \frac{1}{z^2}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{A_iA_j}(\omega) + \mathcal{O}\left(\frac{1}{z^3}\right). \tag{3.64}$$

In many cases, the leading terms in (3.64) can be exactly calculated from their expression in terms of commutators [Eq. (3.63)]. Examples are discussed in Secs. 3.3 and 3.4.

3.2.7 Imaginary-time correlation function

So far we have discussed the retarded and advanced response functions χ^R and χ^A, as well as the structure factor S (related to χ'' by the fluctuation-dissipation theorem). In this section, we show how one can deduce these real-time correlation functions from the knowledge of their imaginary-time counterparts.

Let us first rephrase the results of Sec. 3.1 in the framework of the imaginary-time functional integral. In presence of an external field $h_i(\tau)$, the partition function reads

$$Z[h] = \int \mathcal{D}[\psi]\exp\Big\{-S[\psi] + \int_0^\beta d\tau \sum_i h_i(\tau)A_i(\tau)\Big\}. \tag{3.65}$$

As in the preceding sections, the space dependence of the fields is included in the index i. The advantage of the functional integral formulation is that the field A_i need not be bosonic. It can also be fermionic, in which case the external "field" (or source) h_i is a Grassmann variable. In order to calculate the linear response to the external perturbation, we integrate out the ψ field in (3.65),

$$\begin{aligned} Z[h] = Z[0]\exp\Big\{&\int_0^\beta d\tau \sum_i h_i(\tau)\langle A_i(\tau)\rangle \\ &+ \frac{1}{2}\int_0^\beta d\tau d\tau' \sum_{i,j} h_i(\tau)\langle A_i(\tau)A_j(\tau')\rangle_c h_j(\tau') + \mathcal{O}(h^3)\Big\}, \end{aligned} \tag{3.66}$$

where the averages $\langle\cdots\rangle$ are taken with the action $S[\psi]$ and $\langle A_i(\tau)A_j(\tau')\rangle_c$ denotes the cumulant $\langle A_i(\tau)A_j(\tau')\rangle - \langle A_i(\tau)\rangle\langle A_j(\tau')\rangle$. Recall that $\langle A_i(\tau)A_j(\tau')\rangle$ corresponds to the time-ordered correlation function $\langle T_\tau \hat{A}_i(\tau)\hat{A}_j(\tau')\rangle$ in the operator formalism (Chap. 1). The mean value of the field A_i is then given by

$$\begin{aligned} \langle A_i(\tau)\rangle_h &= \frac{\delta \ln Z[h]}{\delta h_i(\tau)} \\ &= \langle A_i(\tau)\rangle_{h=0} + \int_0^\beta d\tau' \sum_j \langle A_i(\tau)A_j(\tau')\rangle_c h_j(\tau') + \mathcal{O}(h^2). \end{aligned} \tag{3.67}$$

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The linear response to the field h is

$$\begin{aligned}\delta\langle A_i(\tau)\rangle &= \int_0^\beta d\tau' \sum_j \chi_{A_iA_j}(\tau,\tau')h_j(\tau'),\\ \chi_{A_iA_j}(\tau,\tau') &= \left.\frac{\delta^2 \ln Z[h]}{\delta h_i(\tau)\delta h_j(\tau')}\right|_{h=0} = \langle A_i(\tau)A_j(\tau')\rangle_c.\end{aligned} \tag{3.68}$$

The imaginary-time response function $\chi_{A_iA_j}(\tau,\tau')$ is given by a correlation function of the system at equilibrium ($h=0$). We shall show that it is related to the real-time correlation functions[12] (written here in operator form)

$$\begin{aligned}&\chi^{R,A}_{A_iA_j}(t) = \pm 2i\Theta(\pm t)\chi''_{A_iA_j}(t), \quad \chi''_{A_iA_j}(t) = \frac{1}{2}\langle[\hat{A}_i(t),\hat{A}_j]_{-\zeta}\rangle,\\ &\chi_{A_iA_j}(t) = i\langle T\hat{A}_i(t)\hat{A}_j\rangle.\end{aligned} \tag{3.69}$$

For bosonic operators ($\zeta=1$), χ^R and χ^A are the retarded and advanced response functions discussed in the preceding sections. For fermionic operators ($\zeta=-1$), the spectral function χ'' is defined by an anticommutator rather than a commutator. Equation (3.37) then takes the more general form

$$\chi''_{A_iA_j}(\omega) = \frac{\pi}{Z}\sum_{n,m} e^{-\beta\epsilon_n}\left(1-\zeta e^{-\beta\omega}\right) A_i^{nm}A_j^{mn}\delta(\omega+\epsilon_n-\epsilon_m), \tag{3.70}$$

but the spectral representation remains unchanged [Eqs. (3.32-3.34)]. The real function $\chi''_{A^\dagger A}(\omega)$ is positive for fermionic operators and has the sign of ω for bosonic operators.

3.2.7.1 Relation between $\chi_{A_iA_j}(i\omega_n)$ and $\chi^{R,A}_{A_iA_j}(\omega)$

Proceeding as for the derivation of (3.70), we obtain

$$\begin{aligned}\chi_{A_iA_j}(\tau) &= \langle T_\tau \hat{A}_i(\tau)\hat{A}_j\rangle - \langle\hat{A}_i\rangle\langle\hat{A}_j\rangle\\ &= \frac{1}{Z}\sum_{n,m} e^{-(\beta-\tau)\epsilon_n-\tau\epsilon_m}A_i^{nm}A_j^{mn} - \langle\hat{A}_i\rangle\langle\hat{A}_j\rangle \qquad (\tau>0).\end{aligned} \tag{3.71}$$

Discarding first the static case $i\omega_n=0$, we readily obtain

$$\begin{aligned}\chi_{A_iA_j}(i\omega_n) &= \int_0^\beta d\tau\, e^{i\omega_n\tau}\chi_{A_iA_j}(\tau) = \frac{1}{Z}\sum_{n,m} A_i^{nm}A_j^{mn}\frac{e^{-\beta\epsilon_n}-\zeta e^{-\epsilon_m}}{\epsilon_m-\epsilon_n-i\omega_n}\\ &= \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A_iA_j}(\omega)}{\omega-i\omega_n} \qquad (i\omega_n\neq 0),\end{aligned} \tag{3.72}$$

where ω_n is a bosonic ($\zeta=1$) or fermionic ($\zeta=-1$) Matsubara frequency. Comparing with (3.33), we see that $\chi_{A_iA_j}(i\omega_n)$ and $\chi_{A_iA_j}(z=i\omega_n)$ are identical for $i\omega_n\neq 0$.

The static limit $i\omega_n=0$ for boson operators requires some care. In that case, one should single out the terms with $\epsilon_n=\epsilon_m$ in (3.71), which yields

$$\chi_{A_iA_j}(i\omega_n=0) = \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A_iA_j}(\omega)}{\omega} + \frac{\beta}{Z}\sum_{\substack{n,m\\(\epsilon_n=\epsilon_m)}} e^{-\beta\epsilon_n}A_i^{nm}A_j^{mn} - \beta\langle\hat{A}_i\rangle\langle\hat{A}_j\rangle$$

[12] Note that although $\chi(\tau)$ and $\chi(t)$ are different functions, we use a unique symbol (χ) and distinguish them by their argument.

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$$= \chi_{A_iA_j}(z=0) + \beta\big[\langle \hat{A}_i^{(0)}\hat{A}_j^{(0)}\rangle - \langle \hat{A}_i^{(0)}\rangle\langle \hat{A}_j^{(0)}\rangle\big] \tag{3.73}$$

(recall that for $\zeta = 1$ we can omit the terms with $\epsilon_n = \epsilon_m$ in (3.70)). Here $\hat{A}_i^{(0)}$ denotes the energy diagonal part of $\hat{A}_i$: $A_i^{(0)nm} = A_i^{nm}$ if $\epsilon_n = \epsilon_m$ and $A_i^{(0)nm} = 0$ otherwise. Thus $\chi_{A_iA_j}(i\omega_n = 0)$ may differ from $\chi_{A_iA_j}(z=0) = \chi^R_{A_iA_j}(\omega = 0)$ as the last term in (3.73) does not necessarily vanish. $\chi_{A_iA_j}(i\omega_n = 0)$ and $\chi^R_{A_iA_j}(\omega = 0)$ carry different physical meanings. $\chi_{A_iA_j}(i\omega_n = 0)$ gives the static susceptibility as obtained from the equilibrium state of a system with the time-independent Hamiltonian $\hat{H} + \hat{H}'$. By contrast, $\chi^R_{A_iA_j}(\omega = 0)$ is obtained as the zero-frequency limit of the dynamic susceptibility calculated under the assumption of adiabatic evolution of the system subjected to the time-dependent Hamiltonian $\hat{H}'(t)$. That the occupation probabilities $p_n = e^{-\beta\epsilon_n}/Z$ remain constant in time as the external field is adiabatically switched on (unitary evolution) is guaranteed only when the system is isolated. For a system in thermal equilibrium with its environment, we do expect transitions between orthogonal states to occur when both the adiabatic switching time η^{-1} and the time scale $1/\omega$ of the perturbative field become longer and longer, thus allowing the system to reach the quasi-equilibrium state in which the density matrix takes the (grand) canonical form $e^{-\beta(\hat{H}+\hat{H}'(t))}/Z$.

Computing the static response function from the static limit $\chi^R(\omega = 0)$ of the dynamical susceptibility may therefore be dangerous. In Sec. 3.2.3, we argued that the static uniform susceptibility can be obtained from $\chi^R(\mathbf{q},\omega)$ in the limit $\omega = 0$ and $\mathbf{q} \to 0$. This turns out to be correct since $A^{(0)nm}(\mathbf{q})$ usually vanishes for a nonzero vector $\mathbf{q}$. In other words, one has $\chi_{A_iA_j}(\mathbf{q} = 0, i\omega_n = 0) = \lim_{\mathbf{q}\to 0}\chi^R_{A_iA_j}(\mathbf{q}, 0)$.

It is instructive to illustrate this point with the calculation of the density-density response function of a free electron gas. We have

$$\begin{aligned}\chi_{nn}(\mathbf{q}, i\omega_\nu) &= \langle n(\mathbf{q}, i\omega_\nu) n(-\mathbf{q}, -i\omega_\nu)\rangle \\ &= -\frac{2}{\beta\mathcal{V}}\sum_{\mathbf{k},\omega_n}(i\omega_n - \xi_{\mathbf{k}})^{-1}(i\omega_n + i\omega_\nu - \xi_{\mathbf{k}+\mathbf{q}})^{-1} \\ &= -2\int_{\mathbf{k}}\frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{i\omega_\nu + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}}\end{aligned} \tag{3.74}$$

(see Appendix 1.F), where $n(\mathbf{q}, i\omega_\nu)$ is the Fourier transform of $n(\mathbf{r},\tau) = \sum_\sigma \psi^*_\sigma(\mathbf{r},\tau)\psi_\sigma(\mathbf{r},\tau)$. Equation (3.74) gives

$$\chi^R_{nn}(\mathbf{q},\omega) = -2\int_{\mathbf{k}}\frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{\omega + i\eta + \xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}}. \tag{3.75}$$

Hence we find

$$\lim_{\mathbf{q}\to 0}\chi^R_{nn}(\mathbf{q}, 0) = -2\int d\xi\, N(\xi) n'_F(\xi) = \frac{\partial n}{\partial\mu}, \tag{3.76}$$

where $n = 2\int d\xi N(\xi) n_F(\xi)$ is the electron density and $N(\xi) = \int_{\mathbf{k}}\delta(\xi - \xi_{\mathbf{k}})$ the density of state per spin. χ^R_{nn} gives the response to a scalar potential. In the static and uniform limit, this potential is equivalent to a change in the chemical potential, so that the charge susceptibility should be equal to $\partial n/\partial\mu$ as obtained in (3.76). Taking first the limit $\mathbf{q} \to 0$, one obtains $\chi^R_{nn}(0,\omega) = 0$. As shown in Sec. 3.4.4, this result follows from particle number conservation (or gauge invariance).

Let us now compute the imaginary-time correlation function $\chi_{nn}(\mathbf{q}, i\omega_\nu)$ for $\mathbf{q} = \omega_\nu = 0$,

$$\chi_{nn}(\mathbf{q} = 0, i\omega_\nu = 0) = -\frac{2}{\beta\mathcal{V}}\sum_{\mathbf{k},\omega_n}(i\omega_n - \xi_{\mathbf{k}})^{-2}$$

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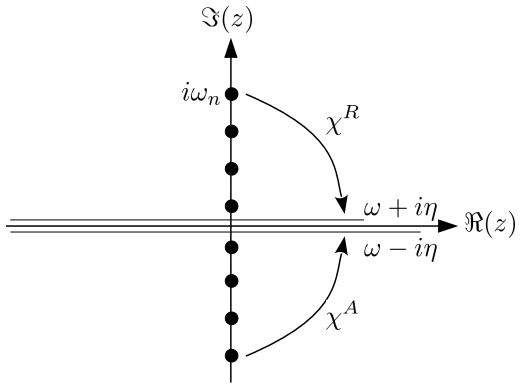


Figure 3.4: Analytic continuation of the function $\chi(z)$ from the imaginary axis ($z = i\omega_n$) to points infinitesimally above ($z = \omega + i\eta$) and below ($z = \omega - i\eta$) the real axis where it gives $\chi^R(\omega)$ and $\chi^A(\omega)$, respectively.

$$= \frac{i}{\pi}\sum_{n=0}^{\infty}\int d\xi\, N(\xi)\partial_\xi\left(\frac{1}{n+\frac{1}{2}+i\tilde{\xi}} - \text{c.c.}\right), \tag{3.77}$$

where $\tilde{\xi} = \xi/(2\pi T)$. Using $\sum_{n\geq 0}(n+\frac{1}{2}+ix)^{-1} - \text{c.c.} = -\Psi(\frac{1}{2}+ix) - \text{c.c.} = -i\pi\tanh(\pi x)$ (Ψ is the digamma function), we finally obtain

$$\begin{aligned}\chi_{nn}(\mathbf{q}=0, i\omega_\nu = 0) &= \int d\xi\, N(\xi)\partial_\xi \tanh\left(\frac{\xi}{2T}\right)\\ &= -2\int d\xi\, N(\xi) n_F'(\xi)\\ &= \frac{\partial n}{\partial \mu},\end{aligned} \tag{3.78}$$

in agreement with $\lim_{\mathbf{q}\to 0}\chi^R_{nn}(\mathbf{q}, 0)$. Note that if we take the limit $T \to 0$ before performing the Matsubara sum, we obtain

$$\chi_{nn}(\mathbf{q}=0, i\omega_\nu = 0) \to -2\int_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(i\omega - \xi_{\mathbf{k}})^{-2} = 0. \tag{3.79}$$

This shows that the limit $T \to 0$ must always be taken at the end of the calculation when computing static uniform response functions within the imaginary-time formalism.

Given that $\chi_{A_iA_j}(i\omega_n) = \chi_{A_iA_j}(z = i\omega_n)$ and $\chi_{A_iA_j}(z)$ is analytic everywhere in the complex plane except on the real axis, $\chi^{R,A}_{A_iA_j}(\omega) = \chi_{A_iA_j}(z = \omega \pm i\eta)$ can be obtained from $\chi_{A_iA_j}(i\omega_n)$ by analytic continuation (Fig. 3.4),

$$\begin{aligned}\chi^R_{A_iA_j}(\omega) &= \chi_{A_iA_j}(i\omega_n \to \omega + i\eta) \qquad (\omega_n > 0),\\ \chi^A_{A_iA_j}(\omega) &= \chi_{A_iA_j}(i\omega_n \to \omega - i\eta) \qquad (\omega_n < 0)\end{aligned} \tag{3.80}$$

(keeping in mind the possible difference between $\chi^R_{A_iA_j}(\omega = 0)$ and $\chi_{A_iA_j}(i\omega_n = 0)$ discussed above).

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In practical calculations, we do not make use of the expression (3.72) of $\chi_{A_iA_j}(i\omega_n)$ and the analytic continuation $i\omega_n \to z$ is not unambiguously defined. Suppose that we have (approximately) calculated $\chi_{A_iA_j}(i\omega_n)$, for example from perturbation theory. $\chi_{A_iA_j}(i\omega_n)$ is identical to an infinite number of analytic functions, e.g. $\chi_{A_iA_j}(i\omega_n)(1+\zeta e^{i\beta\omega_n})/2$. Which of these functions should be analytically continued to obtain $\chi_{A_iA_j}(z)$? We can pick up the correct function $\chi_{A_iA_j}(z)$ by verifying that its asymptotic behavior for $|z| \to \infty$ is in accordance with the spectral representation (3.33) (see Eq. (3.64)). To be more precise, we use the following result from the theory of complex functions. Let $\chi(z)$ and $\chi(i\omega_n \to z)$ be two analytic functions of the complex variable z in a certain domain of the complex plane. If

i) $\chi(z = i\omega_n) = \chi(i\omega_n)$ for all Matsubara frequencies ω_n,
ii) $\chi(z)$ and $\chi(i\omega_n \to z)$ exhibit the same asymptotic behavior for $|z| \to \infty$ and z in the analyticity domain,

then the functions $\chi(z)$ and $\chi(i\omega_n \to z)$ coincide in the domain of analyticity.

3.2.7.2 Relation between $\chi_{A_iA_j}(\omega)$ and $\chi^{R,A}_{A_iA_j}(\omega)$

Writing the real-time correlation function $\chi_{A_iA_j}(t) = i\langle T\hat{A}_i(t)\hat{A}_j\rangle$ as

$$\chi_{A_iA_j}(t) = \frac{i}{Z}\sum_{n,m} A_i^{nm}A_j^{mn}e^{i(\epsilon_n-\epsilon_m)t}[\Theta(t)e^{-\beta\epsilon_n} + \zeta\Theta(-t)e^{-\beta\epsilon_m}], \tag{3.81}$$

we obtain[13]

$$\chi_{A_iA_j}(\omega) = \frac{1}{Z}\sum_{n,m} A_i^{nm}A_j^{mn}\left(\frac{e^{-\beta\epsilon_n}}{\epsilon_m-\epsilon_n-\omega-i\eta} - \zeta\frac{e^{-\beta\epsilon_m}}{\epsilon_m-\epsilon_n-\omega+i\eta}\right). \tag{3.82}$$

When $\hat{A}_i$ and $\hat{A}_j$ have the same signature under time reversal, $\chi''_{A_iA_j}(\omega) = \Im[\chi^R_{A_iA_j}(\omega)]$ is real (see Sec. 3.2.3), we deduce

$$\begin{aligned}
\Re[\chi_{A_iA_j}(\omega)] &= \Re[\chi^R_{A_iA_j}(\omega)] = \mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\Im[\chi^R_{A_iA_j}(\omega')]}{\omega'-\omega},\\
\Im[\chi_{A_iA_j}(\omega)] &= \Im[\chi^R_{A_iA_j}(\omega)]\left[\tanh\left(\beta\frac{\omega}{2}\right)\right]^{-\zeta}.
\end{aligned} \tag{3.83}$$

When they have opposite signatures, $\chi''_{A_iA_j}(\omega) = -i\Re[\chi^R_{A_iA_j}(\omega)]$ is imaginary, and $\chi_{A_iA_j}(\omega)$ and $\chi^R_{A_iA_j}(\omega)$ are related by

$$\begin{aligned}
\Im[\chi_{A_iA_j}(\omega)] &= \Im[\chi^R_{A_iA_j}(\omega)] = -\mathcal{P}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\frac{\Re[\chi^R_{A_iA_j}(\omega')]}{\omega'-\omega},\\
\Re[\chi_{A_iA_j}(\omega)] &= \Re[\chi^R_{A_iA_j}(\omega)]\left[\tanh\left(\beta\frac{\omega}{2}\right)\right]^{-\zeta}.
\end{aligned} \tag{3.84}$$

[13] We use $\int_{-\infty}^{\infty} dt\, e^{i(\omega-\epsilon)t}\Theta(\pm t) = \pm\frac{i}{\omega\pm i\eta-\epsilon}$, which is easily deduced from the inverse relation $\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{\omega\pm i\eta-\epsilon} = \mp i\Theta(\pm t)e^{-i\epsilon t}$.

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Since $\chi^A_{A_iA_j}(\omega) = [\chi^R_{A_iA_j}(\omega)]^*$ in the first case ($\epsilon^T_{A_i} = \epsilon^T_{A_j}$) and $\chi^A_{A_iA_j}(\omega) = -[\chi^R_{A_iA_j}(\omega)]^*$ in the second one ($\epsilon^T_{A_i} = -\epsilon^T_{A_j}$), in both cases

$$\chi_{A_iA_j}(\omega) = [1 + \zeta n_\zeta(\omega)]\chi^R_{A_iA_j}(\omega) - \zeta n_\zeta(\omega)\chi^A_{A_iA_j}(\omega), \tag{3.85}$$

where $n_\zeta(\omega) = (e^{\beta\omega} - \zeta)^{-1}$ is the Bose-Einstein ($\zeta = 1$) or Fermi-Dirac ($\zeta = -1$) distribution function. At zero temperature one obtains

$$\chi_{A_iA_j}(\omega) = \Theta(\omega)\chi^R_{A_iA_j}(\omega) + \Theta(-\omega)\chi^A_{A_iA_j}(\omega) \qquad (T = 0), \tag{3.86}$$

showing that the poles of $\chi_{A_iA_j}(\omega)$ are in the upper-half (lower-half) complex plane if $\omega < 0$ ($\omega > 0$). It is easy to show that Eqs. (3.85) and (3.86) are verified when $\hat{A}_j = \hat{A}_i^\dagger$ regardless of the behavior of $\hat{A}_i$ under time reversal.

3.2.7.3 Relation between $\chi_{A_iA_j}(\tau)$ and $\chi_{A_iA_j}(t)$

It is possible to directly relate $\chi_{A_iA_j}(\tau)$ and $\chi_{A_iA_j}(t)$ without using the Fourier transforms. We write $\chi_{A_iA_j}(t)$ as

$$\begin{aligned}
\chi_{A_iA_j}(t) &= \Theta(t)\chi^>_{A_iA_j}(t) + \Theta(-t)\chi^<_{A_iA_j}(t), \\
\chi^>_{A_iA_j}(t) &= \frac{i}{Z}\mathrm{Tr}\left[e^{-(\beta - it)\hat{H}}\hat{A}_i e^{-i\hat{H}t}\hat{A}_j\right] = i\langle \hat{A}_i(t)\hat{A}_j\rangle, \\
\chi^<_{A_iA_j}(t) &= \zeta\frac{i}{Z}\mathrm{Tr}\left[e^{-(\beta + it)\hat{H}}\hat{A}_j e^{i\hat{H}t}\hat{A}_i\right] = i\zeta\langle \hat{A}_j(-t)\hat{A}_i\rangle,
\end{aligned} \tag{3.87}$$

and extend the definition of $\chi^>$ and $\chi^<$ to complex values of t. For the thermodynamic trace to converge in (3.87), the factors multiplying $\hat{H}$ in the exponentials must have negative real parts, since $\hat{H}$ must be positive for the partition function $Z = \mathrm{Tr}\, e^{-\beta\hat{H}}$ to exist.[14] Thus $\chi^>(t)$ can be analytically continued if $\Re(it - \beta) \leq 0$ and $\Re(it) \geq 0$, i.e. $-\beta \leq \Im(t) \leq 0$, while the analogous condition for $\chi^<(t)$ is $0 \leq \Im(t) \leq \beta$. $\chi(\tau)$ can then be obtained by analytically continuing $\chi^>(t)$ and $\chi^<(t)$ to the imaginary axis within their respective analyticity domains,

$$\begin{aligned}
\chi^>_{A_iA_j}(t = -i\tau) &= i\chi_{A_iA_j}(\tau) \qquad (0 \leq \tau \leq \beta), \\
\chi^<_{A_iA_j}(t = -i\tau) &= i\chi_{A_iA_j}(\tau) \qquad (-\beta \leq \tau \leq 0).
\end{aligned} \tag{3.88}$$

This result can be used to recover the relation between $\chi_{A_iA_j}(i\omega_n)$ and $\chi^{R,A}_{A_iA_j}(\omega)$. Consider

$$\chi_{A_iA_j}(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}\chi_{A_iA_j}(\tau) = -i\int_0^\beta d\tau\, e^{i\omega_n\tau}\chi^>_{A_iA_j}(t = -i\tau), \tag{3.89}$$

and allow ω_n to take any complex value with $\Re(\omega_n) > 0$. $\chi_{A_iA_j}(i\omega_n)$ can be calculated by deforming the integration contour into the analyticity domain of $\chi^>(t)$ as shown in Fig. 3.5,

$$\chi_{A_iA_j}(i\omega_n) = -i\int_{t=0}^{t=\infty} d(it)e^{-\omega_n t}\chi^>_{A_iA_j}(t) - i\int_{t=\infty}^{t=0} d(it)e^{-\omega_n(t - i\beta)}\chi^>_{A_iA_j}(t - i\beta). \tag{3.90}$$

[14] More precisely, we can always shift the energies, $\hat{H} \to \hat{H} + \mathrm{const}$, to make $\hat{H}$ positive.

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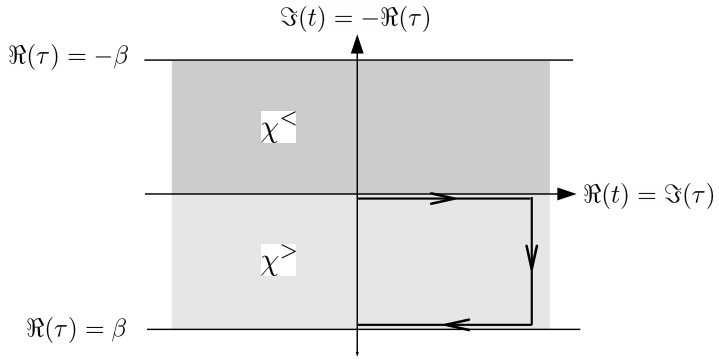


Figure 3.5: Analyticity domains of $\chi^>(t)$ and $\chi^<(t)$ in the complex t plane ($\tau = it$) and integration contour used in the calculation of $\chi(i\omega_n)$ [Eqs. (3.89-3.90)].

The condition $\Re(\omega_n) > 0$ ensures that the small vertical segment of the contour does not contribute ($e^{-\omega_n t} \to 0$ for $\Re(t) \to \infty$). Using $e^{i\beta\omega_n} = \zeta$ and $\chi^>_{A_iA_j}(t - i\beta) = i\langle \hat{A}_j \hat{A}_i(t)\rangle$, a consequence of the cyclic invariance of the trace, we obtain

$$\chi_{A_iA_j}(i\omega_n) = i\int_0^\infty dt\, e^{-\omega_n t}\langle \hat{A}_i(t)\hat{A}_j - \zeta \hat{A}_j\hat{A}_i(t)\rangle = \int_{-\infty}^\infty dt\, e^{-\omega_n t}\chi^R_{A_iA_j}(t). \tag{3.91}$$

This equation holds for any frequency ω_n satisfying $\Re(\omega_n) > 0$. For $i\omega_n = \omega + i\eta$, it yields $\chi_{A_iA_j}(i\omega_n = \omega + i\eta) = \chi^R_{A_iA_j}(\omega)$ as derived previously. Similarly, $\chi_{A_iA_j}(i\omega_n = \omega - i\eta) = \chi^A_{A_iA_j}(\omega)$ can be obtained by deforming the integration contour in the region $\Re(t) < 0$.

3.2.7.4 Stiffness and stability

Let us consider the Legendre transform

$$\Gamma[M] = -\ln Z[h] + \int_0^\beta d\tau \sum_i h_i(\tau) M_i(\tau). \tag{3.92}$$

where

$$M_i(\tau) = \langle A_i(\tau)\rangle_h = \frac{\delta \ln Z[h]}{\delta h_i(\tau)} \tag{3.93}$$

(A_i is a bosonic field in this section). In Eq. (3.92), $h \equiv h[M]$ is obtained by inverting (3.93). $\Gamma[M]$ satisfies the equation of motion

$$\frac{\delta\Gamma[M]}{\delta M_i(\tau)} = h_i(\tau) \tag{3.94}$$

and is therefore stationary at equilibrium ($h = 0$). Expanding about the stationary point $M = \bar{M}$, we obtain

$$\Gamma[M] = \Gamma[\bar{M}] + \frac{1}{2}\int_0^\beta d\tau d\tau' \sum_{i,j} \frac{\delta^2\Gamma[M]}{\delta M_i(\tau) M_j(\tau')}\bigg|_{M=\bar{M}} \delta M_i(\tau)\delta M_j(\tau')$$

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$$= \Gamma[\bar{M}] + \frac{1}{2}\int_0^\beta d\tau d\tau' \sum_{i,j} \chi^{-1}_{A_i A_j}(\tau - \tau')\delta M_i(\tau)\delta M_j(\tau'), \tag{3.95}$$

where $\delta M_i(\tau) = M_i(\tau) - \bar{M}_i$ and $\chi_{A_i A_j}(\tau)$ is the susceptibility defined in (3.68). The last line in (3.95) follows from the usual properties of Legendre transforms (Chap. 1). When $M_i(\tau)$ is time independent, $\beta^{-1}\Gamma[M]$ defines the Gibbs free energy

$$G[M] = G[\bar{M}] + \frac{1}{2}\sum_{i,j} \chi^{-1}_{A_i^\dagger A_j}(z=0)\delta M_i^* \delta M_j \tag{3.96}$$

(we have changed $A_i \to A_i^*$ in the sum over i), where $\chi(z=0)^{-1} = \chi^R(\omega=0)^{-1}$. Thus, the static response function $\chi^R_{A_i^\dagger A_j}(\omega=0)$ determines the stiffness (or rigidity) of the system with respect to a variation $\delta M_i = M_i - \bar{M}_i$ induced by a static external field $h_i = \delta G[M]/\delta M_i$. For the system to be stable, the stiffness matrix $\{\chi^R_{A_i^\dagger A_j}(\omega=0)^{-1}\}$ and its inverse $\{\chi^R_{A_i^\dagger A_j}(\omega=0)\}$ must be positive for any set of fields A_i. In particular

$$\chi^R_{A^\dagger A}(\omega=0) \geq 0. \tag{3.97}$$

As pointed out in Sec. 3.2.2, these results are a consequence of the positivity of the matrix $\omega\chi''_{A_i^\dagger A_j}(\omega)$.

3.3 Density-density response function

In this section, we consider an homogeneous and isotropic bosonic or fermionic system. An external potential $\phi(\mathbf{r},t)$ that couples to the density contributes to the Hamiltonian a term

$$\hat{H}'(t) = \int d^d r\, \phi(\mathbf{r},t)\hat{n}(\mathbf{r}) \tag{3.98}$$

and induces a density modulation

$$\delta\langle\hat{n}(\mathbf{r})\rangle(t) = -\int_{-\infty}^{\infty} dt' \int d^d r'\, \chi^R_{nn}(\mathbf{r}-\mathbf{r}', t-t')\phi(\mathbf{r}',t') \tag{3.99}$$

to linear order. The density-density response is defined by

$$\begin{aligned} \chi^R_{nn}(\mathbf{r},t) &= 2i\Theta(t)\chi''_{nn}(\mathbf{r},t), \\ \chi''_{nn}(\mathbf{r},t) &= \frac{1}{2}\langle[\hat{n}(\mathbf{r},t), \hat{n}(0,0)]\rangle. \end{aligned} \tag{3.100}$$

3.3.1 Symmetry properties

From parity invariance [Eq. (3.21)] and the general properties (3.18), one easily obtains

$$\chi''_{nn}(\mathbf{q},\omega) = [\chi''_{nn}(\mathbf{q},\omega)]^* = \chi''_{nn}(-\mathbf{q},\omega) = -\chi''_{nn}(\mathbf{q},-\omega). \tag{3.101}$$

$\chi''_{nn}(\mathbf{q},\omega)$ is real, odd in ω and even in $\mathbf{q}$. It follows that $\chi^R_{nn}(\mathbf{q},\omega)$ satisfies

$$\chi^R_{nn}(\mathbf{q},\omega) = \chi^R_{nn}(-\mathbf{q},\omega) = [\chi^R_{nn}(\mathbf{q},-\omega)]^*. \tag{3.102}$$

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3.3.2 High-frequency behavior and f-sum rule

$\chi''_{nn}(\mathbf{q},\omega)$ being odd in frequency, we obtain

$$\chi_{nn}(\mathbf{q},z) = -\frac{1}{z^2}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) + \mathcal{O}\left(\frac{1}{z^4}\right). \tag{3.103}$$

The coefficient of $1/z^2$ can be written as the mean value of an equal-time commutator (Sec. 3.2.6),

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) = \langle[i\partial_t\hat{n}(\mathbf{q},t),\hat{n}(-\mathbf{q},0)]\rangle_{t=0} = \mathbf{q}\cdot\langle[\hat{\mathbf{j}}(\mathbf{q}),\hat{n}(-\mathbf{q})]\rangle, \tag{3.104}$$

where the last result follows from the continuity equation $\partial_t\hat{n}(\mathbf{q},t) + i\mathbf{q}\cdot\hat{\mathbf{j}}(\mathbf{q},t) = 0$. By writing the operators $\hat{n}(\mathbf{q})$ and $\hat{\mathbf{j}}(\mathbf{q})$ in second-quantized form,[15] the equal-time commutator in (3.104) is easily calculated,

$$[\hat{\mathbf{j}}(\mathbf{q}),\hat{n}(-\mathbf{q})] = \frac{\mathbf{q}}{m\mathcal{V}}\hat{N}, \tag{3.105}$$

and we finally obtain

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\chi''_{nn}(\mathbf{q},\omega) = \frac{n\mathbf{q}^2}{m}, \tag{3.106}$$

where $n = \langle\hat{N}\rangle/\mathcal{V}$ is the mean density of particles. This result is known as the f-sum rule. It holds for both fermions and bosons.

3.3.3 Compressibility

The isothermal compressibility κ is defined as the volume variation induced by a change in pressure,

$$\kappa = -\frac{1}{\mathcal{V}}\frac{\partial\mathcal{V}}{\partial P}\bigg|_{T,N}. \tag{3.107}$$

The free energy $F(T,\mathcal{V},N) \equiv E - TS$ being an extensive quantity, it can be written as $F(T,\mathcal{V},N) = \mathcal{V}f(T,n)$ where $n = N/\mathcal{V}$ is the density. Since $P = -\partial F/\partial\mathcal{V}|_{T,N}$, we can express the compressibility as

$$\frac{1}{\kappa} = n\frac{\partial P}{\partial n}\bigg|_T = n^2\frac{\partial^2 f}{\partial n^2}\bigg|_T. \tag{3.108}$$

Using

$$\mu = \frac{\partial F}{\partial N}\bigg|_{T,\mathcal{V}} = \frac{\partial f}{\partial n}\bigg|_T, \tag{3.109}$$

κ can be related to the variation of the density induced by a change in the chemical potential,

$$\kappa = \frac{1}{n^2}\frac{\partial n}{\partial\mu}\bigg|_T. \tag{3.110}$$

[15] $\hat{n}(\mathbf{q}) = \frac{1}{\mathcal{V}^{1/2}}\sum_{\mathbf{k},\sigma}\hat{\psi}^\dagger_\sigma(\mathbf{k})\hat{\psi}_\sigma(\mathbf{k}+\mathbf{q})$ and $\hat{\mathbf{j}}(\mathbf{q}) = \frac{1}{\mathcal{V}^{1/2}m}\sum_{\mathbf{k},\sigma}(\mathbf{k}+\frac{\mathbf{q}}{2})\hat{\psi}^\dagger_\sigma(\mathbf{k})\hat{\psi}_\sigma(\mathbf{k}+\mathbf{q})$. This expression of the current assumes that there is no contribution from the interacting part of the Hamiltonian, as in the case of a density-density interaction.

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In the grand canonical ensemble, we can therefore obtain the compressibility from the response to a static uniform external potential $\phi \equiv \delta\mu$, i.e.

$$n^2\kappa = \frac{n}{mc_s^2} \equiv \left.\frac{\partial n}{\partial \mu}\right|_T = \lim_{\mathbf{q}\to 0} \chi^R_{nn}(\mathbf{q},0) = \lim_{\mathbf{q}\to 0} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega}. \tag{3.111}$$

The compressibility sum rule (3.111) is an example of a thermodynamic sum rule [Eq. (3.61)]. It is often expressed in terms of the macroscopic (first) sound velocity c_s. In the next section, we shall see how the compressibility sum rule must be modified when the particles interact *via* the long-range Coulomb interaction.

The relation (3.111) between the compressibility and the macroscopic sound velocity c_s can be obtained from simple hydrodynamic arguments. Let us consider an infinitesimal change $\delta\langle n(\mathbf{r},t)\rangle$ in density and assume the density oscillations to be sufficiently slow so that the system remains locally in thermodynamic equilibrium with pressure $P_{\rm eq} + \delta P(\mathbf{r},t)$. This requires the characteristic time τ of return to equilibrium to be much smaller than the period $2\pi/\omega$ of the density wave, i.e. $\omega\tau \ll 1$ (collisional or hydrodynamic regime). From the continuity equation

$$\partial_t \delta\langle n(\mathbf{r},t)\rangle = -n\boldsymbol{\nabla}\cdot\langle \mathbf{v}(\mathbf{r},t)\rangle \tag{3.112}$$

and the Euler equation

$$mn\partial_t \langle \mathbf{v}(\mathbf{r},t)\rangle = -\boldsymbol{\nabla}\delta P(\mathbf{r},t) \tag{3.113}$$

(Eqs. (3.112,3.113) are valid to lowest order in $\mathbf{v}$), we deduce

$$\partial_t^2 \delta\langle n(\mathbf{r},t)\rangle = m^{-1}\boldsymbol{\nabla}^2\delta P(\mathbf{r},t) = m^{-1}\left(\frac{\partial P}{\partial n}\right)_T \boldsymbol{\nabla}^2 \delta\langle n(\mathbf{r},t)\rangle. \tag{3.114}$$

Here we have used $P(\mathbf{r},t) = P(n+\delta\langle n(\mathbf{r},t)\rangle) \simeq P(n) + (\partial P/\partial n)\delta\langle n(\mathbf{r},t)\rangle$ for a system locally in equilibrium. This gives a density wave (first-sound mode) with linear dispersion $\omega = c_s|\mathbf{q}|$ and velocity $c_s^2 = m^{-1}(\partial P/\partial n)_T = 1/\kappa nm$. At finite temperature, a more correct hydrodynamic treatment would include the coupling between mass and energy density fluctuations. As a result, the sound velocity

$$c_s^2 = \frac{1}{m}\left(\frac{\partial P}{\partial n}\right)_S = \frac{1}{\kappa_S nm} \tag{3.115}$$

is related to the isentropic compressibility κ_S [1,2,5]. At low temperatures, the difference between the isothermal and isentropic sound velocities is in general weak and can be neglected.

3.4 Electromagnetic response function

In this section, we consider an homogeneous and isotropic electron system. The global electric neutrality is ensured by a uniform background of positive charge (jellium model, see Chap. 5). In the Coulomb gauge ($\boldsymbol{\nabla}\cdot\mathbf{A} = 0$), the action of the particles and the electromagnetic field reads (see Chap. 1)

$$\begin{aligned} S[\psi,\phi,\mathbf{A}] = \int_0^\beta d\tau \int d^dr \Big\{ \frac{\epsilon_0}{2}\Big[\big(\boldsymbol{\nabla}\phi(x)\big)^2 + \big(\partial_\tau \mathbf{A}_\perp(x)\big)^2 + c_l^2\big(\boldsymbol{\nabla}\times\mathbf{A}_\perp(x)\big)^2\Big] \\ + i\phi(x)\rho(x) - \mathbf{j}(x)\cdot\mathbf{A}_\perp(x) + \frac{e}{2m}\rho(x)\mathbf{A}_\perp^2(x)\Big\} + S'_m[\psi] \end{aligned} \tag{3.116}$$

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(c_l is the speed of light and $x = (\mathbf{r}, \tau)$), where $S'_m[\psi]$ is the action of the electrons without electromagnetic interactions. In the electron gas model (Chap. 5), it is nothing but the action of free electrons. In more realistic models of metals, it can include short-range (effective) interactions between electrons. $\rho(x) = en(x)$ is the charge density and $\mathbf{j}(x)$ the paramagnetic part of the current $\mathbf{J} = \mathbf{j} - (e/m)\rho\mathbf{A}_\perp$. The background of positive charge removes the $\mathbf{q} = 0$ component of the Coulomb interaction. This implies that the field $\phi(\mathbf{q}, \tau)$ is defined only for $\mathbf{q} \neq 0$.

Note that in the Euclidean formalism, $i\phi(x)$ plays the role of the scalar potential (Sec. 1.9.3). The mean values of the electric and magnetic fields are given by (1.636) and (1.637) and the propagators $D_{00}(q)$ and $D_{\mu\nu}(q)$ of the electromagnetic potentials are defined by (1.642). In the absence of coupling to the particles, they take the form (1.643).

In the following sections, we consider D_{00} and $D_{\mu\nu}$, as well as the longitudinal and transverse dielectric functions, when the electromagnetic potentials are coupled to the electron system.

3.4.1 Longitudinal dielectric function

To find the expression of the scalar potential propagator D_{00}, it is sufficient to consider the reduced action

$$S[\psi, \phi] = \int_0^\beta d\tau \int d^d r \left\{ \frac{\epsilon_0}{2} \big(\boldsymbol{\nabla}\phi(x)\big)^2 + [i\rho(x) - J(x)]\phi(x) \right\} + S'_m[\psi], \tag{3.117}$$

since the magnetic interactions can be neglected with respect to the Coulomb interaction in a non-relativistic system (Sec. 1.9.3). We have added an external source J to the action which allows us to obtain D_{00} from the functional derivatives of $\ln Z[J]$. Integrating out ϕ, we obtain

$$S[\psi] = -\frac{1}{2} \sum_q D_{00}^{(0)}(q)[J(-q)J(q) - 2iJ(-q)\rho(q)] + S_m[\psi], \tag{3.118}$$

where $D_{00}^{(0)}(q) = 1/\epsilon_0 \mathbf{q}^2$ and

$$S_m[\psi] = S'_m[\psi] + \frac{1}{2} \sum_q D_{00}^{(0)}(q)\rho(-q)\rho(q) \tag{3.119}$$

is the action of the electrons including the Coulomb interaction but not the magnetic interactions. Note that $S_m[\psi]$ is the usual action for non-relativistic charged particles. Integrating out the field ψ within a cumulant expansion, we finally obtain

$$\ln Z[J] = \frac{1}{2} \sum_q D_{00}^{(0)}(q)J(-q)J(q)[1 - D_{00}^{(0)}(q)\chi_{\rho\rho}(q)] + \mathcal{O}(J^3) \tag{3.120}$$

(the first-order cumulant $\sum_q D_{00}^{(0)}(q)J(-q)\langle\rho(q)\rangle = enD_{00}^{(0)}(q = 0)J(q = 0)$ vanishes), where

$$\chi_{\rho\rho}(q) = \langle\rho(q)\rho(-q)\rangle \tag{3.121}$$

is the density-density correlation function computed in the presence of the Coulomb interaction between particles, i.e. with the action $S_m[\psi]$. In the following, the expectation values $\langle\cdots\rangle$ will always be obtained with $S_m[\psi]$. From (3.120), we deduce

$$D_{00}(q) = \left.\frac{\delta^2 \ln Z[J]}{\delta J(-q)\delta J(q)}\right|_{J=0} = D_{00}^{(0)}(q)[1 - D_{00}^{(0)}(q)\chi_{\rho\rho}(q)]. \tag{3.122}$$

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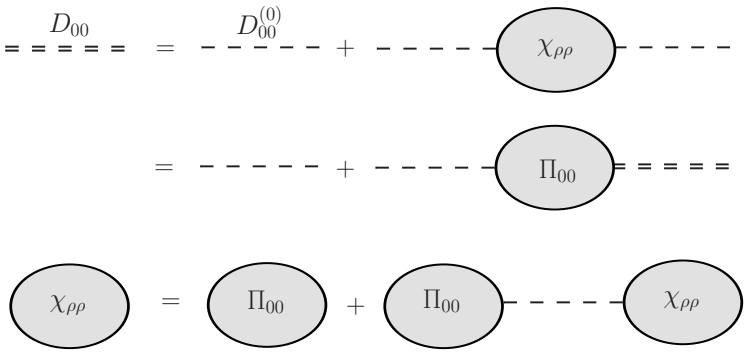


Figure 3.6: Diagrammatic representation of D_{00} and $\chi_{\rho\rho}$ in terms of the irreducible part Π_{00} of the density-density correlation function.

It is convenient to write $\chi_{\rho\rho}$ as

$$\chi_{\rho\rho}(q) = \frac{\Pi_{00}(q)}{1 + D_{00}^{(0)}(q)\Pi_{00}(q)}, \tag{3.123}$$

where Π_{00} is the "irreducible" part of $\chi_{\rho\rho}$, i.e. the part that cannot be split into two disconnected peaces by cutting a Coulomb line $D_{00}^{(0)}$. The relation (3.123) between $\chi_{\rho\rho}$ and Π_{00} follows from the diagrammatic rules discussed in Chap. 1. Equation (3.122) then gives

$$D_{00}^{-1}(q) = [D_{00}^{(0)}(q)]^{-1} + \Pi_{00}(q), \tag{3.124}$$

which shows that $\Pi_{00}(q)$ is the self-energy of the scalar potential. Equations (3.122-3.124) are shown diagrammatically in Fig. 3.6. In fact, one could have directly obtained D_{00} from its diagrammatic expansion. Note that the only approximation in (3.124) is the neglect of the magnetic interactions with respect to the Coulomb interaction in the irreducible density-density correlation function Π_{00}.

The longitudinal dielectric function $\epsilon_{\parallel}(q)$ is defined by

$$D_{00}(q) = \frac{1}{\epsilon_0 \epsilon_{\parallel}(q)\mathbf{q}^2}, \tag{3.125}$$

i.e.

$$\frac{1}{\epsilon_{\parallel}(q)} = 1 - \frac{\chi_{\rho\rho}(q)}{\epsilon_0 \mathbf{q}^2} \quad \text{or} \quad \epsilon_{\parallel}(q) = 1 + \frac{\Pi_{00}(q)}{\epsilon_0 \mathbf{q}^2}. \tag{3.126}$$

$D_{00}(q)$ can be seen as an effective (screened) Coulomb interaction between electrons, the screening being encoded in the dielectric function $\epsilon_{\parallel}(q)$ or, equivalently, the density-density correlation function $\chi_{\rho\rho}(q)$. This interpretation is particularly natural when one considers the diagrams contributing to D_{00} (Fig. 3.6). We shall show below that $\epsilon_{\parallel}$ also determines the screening of an external charge distribution. The zeros of $\epsilon_{\parallel}^R(\mathbf{q},\omega)$, i.e. the poles of $\chi_{\rho\rho}^R(\mathbf{q},\omega)$, describe charge oscillations of the electron system and in particular the collective density mode (plasmon) discussed below.

The determination of the longitudinal dielectric function $\epsilon_{\parallel}$ reduces to the calculation of the irreducible part Π_{00} of the density-density correlation function $\chi_{\rho\rho}$. The simplest

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approximation, known as the RPA, amounts to approximating Π_{00} by its non-interacting value and will be discussed in Chap. 5. In the following, we show that certain properties of $\epsilon_\parallel$ can be obtained without relying on an explicit calculation.

3.4.1.1 Analytic properties

It follows from the definition (3.126) that $\epsilon_\parallel^{-1}(\mathbf{q},z)-1=-\chi_{\rho\rho}(\mathbf{q},z)/\epsilon_0\mathbf{q}^2$ shares all the analytic properties of a genuine response function. In particular, it admits the spectral representation

$$\frac{1}{\epsilon_\parallel(\mathbf{q},z)}-1=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{1}{\omega-z}\Im\left[\frac{1}{\epsilon_\parallel^R(\mathbf{q},\omega)}\right], \tag{3.127}$$

and $1/\epsilon_\parallel^R(\mathbf{q},\omega)-1$ satisfies the Kramers-Kronig relations. Note that neither $\epsilon_\parallel(\mathbf{q},z)-1$ nor $\Pi_{00}(\mathbf{q},z)$ is *a priori* expected to satisfy these properties, since they do not describe the response of the system to an external probe.[16] However, the relation $\chi_{\rho\rho}^R(\mathbf{q},\omega)=\Pi_{00}^R(\mathbf{q},\omega)[1-\chi_{\rho\rho}^R(\mathbf{q},\omega)/(\epsilon_0\mathbf{q}^2)]$ together with the analytic properties of $\chi_{\rho\rho}^R(\mathbf{q},\omega)$ implies that a pole in $\Pi_{00}^R(\mathbf{q},\omega)$ at the complex frequency ω ($\Im(\omega)\geq 0$) is possible only if $\chi_{\rho\rho}^R(\mathbf{q},\omega)=\epsilon_0\mathbf{q}^2$ at the pole. We therefore expect $\Pi_{00}^R(\mathbf{q},\omega)$ and $\epsilon_\parallel^R(\mathbf{q},\omega)$ to be analytic in the upper-half complex plane in most cases. Possible non-analyticities of $\epsilon_\parallel^R(\mathbf{q},\omega)$ are discussed in Refs. [5,6].

3.4.1.2 Compressibility

In a charged system, the definitions (3.107) and (3.110) of the compressibility assume that the background of positive charge is compressed along with the electrons in order to maintain electric neutrality everywhere. By contrast χ_{nn}^R determines the response of the system to a change in chemical potential at fixed background of positive charge. Consequently the relation (3.111) between κ and χ_{nn}^R must be revised.

Let us consider the effect of a static longitudinal field $\langle\mathbf{D}_{\rm ext}(\mathbf{r})\rangle$ created by a distribution $\rho_{\rm ext}(\mathbf{r})$ of external charges.[17] The force $\langle\mathbf{F}(\mathbf{r})\rangle$ per unit volume due to the field induces a pressure variation $\delta P(\mathbf{r})$ such that

$$\boldsymbol{\nabla}\delta P(\mathbf{r})=\langle\mathbf{F}(\mathbf{r})\rangle. \tag{3.128}$$

In the long wavelength limit, the pressure distribution $\delta P(\mathbf{r})$ is related to the particle density $\delta\langle n(\mathbf{r})\rangle$ by

$$\delta\langle n(\mathbf{r})\rangle=\kappa n\delta P(\mathbf{r}). \tag{3.129}$$

This equation is a direct consequence of the definition of the compressibility, $\kappa^{-1}=n\partial P/\partial n|_T$ (Sec. 3.3). From (3.128) and (3.129), we deduce

$$\boldsymbol{\nabla}\delta\langle n(\mathbf{r})\rangle=\kappa n\langle\mathbf{F}(\mathbf{r})\rangle. \tag{3.130}$$

This result can be used to calculate κ provided that $\langle\mathbf{F}(\mathbf{r})\rangle$ is defined carefully [5]. The electrons respond to the external field $\langle\mathbf{D}_{\rm ext}(\mathbf{r})\rangle$ by producing a polarization field $\langle\mathbf{E}_P(\mathbf{r})\rangle$.

[16] $\epsilon_\parallel(\mathbf{q},z)-1$ and $\Pi_{00}(\mathbf{q},z)$ determine the response to the screened longitudinal field as can be seen from $\delta\langle\rho(\mathbf{q},\omega)\rangle=-\Pi_{00}^R(\mathbf{q},\omega)\langle\phi(\mathbf{q},\omega)\rangle=-\epsilon_0\mathbf{q}^2(\epsilon_\parallel^R(\mathbf{q},\omega)-1)\langle\phi(\mathbf{q},\omega)\rangle$ (compare with $\delta\langle\rho(\mathbf{q},\omega)\rangle=-\chi_{\rho\rho}^R(\mathbf{q},\omega)\phi_{\rm ext}(\mathbf{q},\omega)=\epsilon_0\mathbf{q}^2(1/\epsilon_\parallel^R(\mathbf{q},\omega)-1)\phi_{\rm ext}(\mathbf{q},\omega)$) (see Sec. 3.4.3).

[17] The charge distribution $\rho_{\rm ext}(\mathbf{r})$ is assumed classical (no fluctuations), but fluctuations of the electromagnetic field are taken into account (see Sec. 3.4.3).

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The background of positive charge adjusts itself to maintain electric neutrality and thus produces a field $-\langle \mathbf{E}_P(\mathbf{r})\rangle$. The total field felt by the electrons is then $\langle \mathbf{D}(\mathbf{r})\rangle = \langle \mathbf{D}_{\rm ext}(\mathbf{r})\rangle - \langle \mathbf{E}_P(\mathbf{r})\rangle$. When calculating the compressibility, we are interested in the forces that are external to the complete system consisting of the electrons and the background of positive charge, i.e. to the field $\langle \mathbf{D}_{\rm ext}\rangle$. But $\langle \mathbf{D}_{\rm ext}\rangle = \langle \mathbf{D}\rangle + \langle \mathbf{E}_P\rangle$ is nothing but the local electric field $-\boldsymbol{\nabla}\langle\phi(\mathbf{r})\rangle$, with $\phi(\mathbf{r})$ the scalar potential. We thus have $\langle \mathbf{F}(\mathbf{r})\rangle = -ne\boldsymbol{\nabla}\langle\phi(\mathbf{r})\rangle$ and

$$\boldsymbol{\nabla}\delta\langle n(\mathbf{r})\rangle = -e\kappa n^2 \boldsymbol{\nabla}\langle\phi(\mathbf{r})\rangle. \tag{3.131}$$

Using the relation between $\delta\langle n(\mathbf{r})\rangle$ and $\langle\phi(\mathbf{r})\rangle$ given below [Eq. (3.174)],

$$e\boldsymbol{\nabla}\delta\langle n(\mathbf{r})\rangle = -\lim_{\mathbf{q}\to 0}\Pi^R_{00}(\mathbf{q},0)\boldsymbol{\nabla}\langle\phi(\mathbf{r})\rangle = -\lim_{\mathbf{q}\to 0}\epsilon_0\mathbf{q}^2(\epsilon^R_\parallel(\mathbf{q},0)-1)\boldsymbol{\nabla}\langle\phi(\mathbf{r})\rangle, \tag{3.132}$$

we finally obtain

$$e^2n^2\kappa = \lim_{\mathbf{q}\to 0}\Pi^R_{00}(\mathbf{q},0) \tag{3.133}$$

or, equivalently,

$$\epsilon^R_\parallel(\mathbf{q},0) = 1 + \frac{n^2e^2\kappa}{\epsilon_0\mathbf{q}^2} = 1 + \frac{\omega_p^2}{c_s^2\mathbf{q}^2} \qquad (\mathbf{q}\to 0), \tag{3.134}$$

where $c_s = (1/\kappa nm)^{1/2}$ is the sound velocity (Sec. 3.3) and $\omega_p^2 = ne^2/\epsilon_0 m$ (the physical meaning of ω_p is discussed in Sec. 3.4.1.4).

In a charged system, the compressibility is determined by the irreducible part $\Pi^R_{00}(\mathbf{q},\omega)$ of the density-density correlation function $\chi^R_{\rho\rho}(\mathbf{q},\omega)$ [compare (3.111) and (3.133)]. It should be noted here that the compressibility κ given by (3.134) is not the true compressibility of the system. Indeed, we have assumed that the background of positive charge adjusts itself to maintain electric neutrality at no energy cost. Since we neglect the stiffness of the background, κ can be negative even for a stable system [3].

3.4.1.3 Sum rules and high-frequency behavior

The f-sum rule (3.106) can be rewritten in terms of the longitudinal dielectric function,

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega\Im\left[\frac{1}{\epsilon^R_\parallel(\mathbf{q},\omega)}\right] = -\omega_p^2 \qquad (\mathbf{q}\neq 0). \tag{3.135}$$

The high-frequency limit of the density-density response function (Sec. 3.3.2), which follows from the f-sum rule, implies

$$\epsilon^R_\parallel(\mathbf{q},\omega) = 1 - \frac{\omega_p^2}{\omega^2} \qquad (\omega\to\infty). \tag{3.136}$$

Another sum rule can be derived from

$$\lim_{\mathbf{q}\to 0}\frac{1}{\epsilon^R_\parallel(\mathbf{q},0)} = \lim_{\mathbf{q}\to 0}\frac{c_s^2\mathbf{q}^2}{\omega_p^2} = 0, \quad \text{i.e.} \quad \chi^R_{\rho\rho}(\mathbf{q},0) = \epsilon_0\mathbf{q}^2 \quad (\mathbf{q}\to 0). \tag{3.137}$$

Equation (3.137), which follows from (3.134), means that the screening becomes perfect in the static ($\omega = 0$) long-wavelength ($\mathbf{q}\to 0$) limit. Using the spectral representation of $1/\epsilon^R_\parallel(\mathbf{q},\omega) - 1$ or the Kramers-Kronig relations, we obtain the perfect-screening sum rule

$$\lim_{\mathbf{q}\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{1}{\omega}\Im\left[\frac{1}{\epsilon^R_\parallel(\mathbf{q},\omega)}\right] = -1. \tag{3.138}$$

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When $\epsilon_\parallel^R(\mathbf{q},\omega)$ is analytic in the upper-half complex plane, it satisfies the Kramers-Kronig relation

$$\Re[\epsilon_\parallel^R(\mathbf{q},\omega)] - 1 = \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Im[\epsilon_\parallel^R(\mathbf{q},\omega')]}{\omega' - \omega} \tag{3.139}$$

(note that $\lim_{\omega\to\infty} \epsilon_\parallel^R(\mathbf{q},\omega) - 1 = 0$). Taking the limit $\omega \to \infty$ and using the asymptotic behavior (3.136), we obtain

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \Im[\epsilon_\parallel^R(\mathbf{q},\omega)] = \omega_p^2. \tag{3.140}$$

Equation (3.140) can be rewritten as a sum rule for the longitudinal conductivity and is known as the longitudinal-conductivity sum rule (see Sec. 3.4.3). Finally, we can derive the compressibility sum rule from (3.134) and (3.139),

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\Im[\epsilon_\parallel^R(\mathbf{q},\omega)]}{\omega} = \frac{\omega_p^2}{c_s^2\mathbf{q}^2} = \frac{n^2e^2\kappa}{\epsilon_0\mathbf{q}^2} \qquad (\mathbf{q}\to 0). \tag{3.141}$$

3.4.1.4 Charge oscillations and plasmon mode

The zeros of $\epsilon_\parallel^R(\mathbf{q},\omega)$ are given by the poles of $\chi_{\rho\rho}^R(\mathbf{q},\omega)$. They describe charge oscillations of the electron system in the presence of the long-range Coulomb interaction. Besides the continuum of particle-hole pair excitations $\omega = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}$, we also expect a collective density mode showing up as an isolated zero of $\epsilon_\parallel^R(\mathbf{q},\omega)$, i.e. an isolated pole of $\chi_{\rho\rho}^R(\mathbf{q},\omega)$. In the absence of long-range interaction, the collective density mode of the electron system is the zero-sound mode (Chap. 4) or, in the collisional (hydrodynamic) regime, the first-sound mode (Sec. 3.3). Both these modes have a linear dispersion $\omega \propto |\mathbf{q}|$ at low energies. Because of the Coulomb interaction the collective density mode, known as the plasmon mode, is pushed up to high energies. To see this in a simple way, we consider the continuity equation

$$\partial_t \langle n(\mathbf{r},t)\rangle + \boldsymbol{\nabla}\cdot[\langle n(\mathbf{r},t)\rangle\langle \mathbf{v}(\mathbf{r},t)\rangle] = 0 \tag{3.142}$$

and Newton's equation of motion

$$m\frac{d}{dt}\langle \mathbf{v}(\mathbf{r},t)\rangle = m\partial_t\langle \mathbf{v}(\mathbf{r},t)\rangle + m(\langle \mathbf{v}(\mathbf{r},t)\rangle\cdot\boldsymbol{\nabla})\langle \mathbf{v}(\mathbf{r},t)\rangle = e\langle \mathbf{E}(\mathbf{r},t)\rangle. \tag{3.143}$$

Combining (3.142) and (3.143) with Poisson's equation

$$\boldsymbol{\nabla}\cdot\langle \mathbf{E}(\mathbf{r},t)\rangle = \epsilon_0^{-1} e[\langle n(\mathbf{r},t)\rangle - n], \tag{3.144}$$

we then obtain

$$\partial_t^2 \delta\langle n(\mathbf{r},t)\rangle = -\frac{ne}{m}\boldsymbol{\nabla}\cdot\langle \mathbf{E}(\mathbf{r},t)\rangle = -\frac{ne^2}{\epsilon_0 m}\delta\langle n(\mathbf{r},t)\rangle \tag{3.145}$$

to linear order in $\delta\langle n(\mathbf{r},t)\rangle = \langle n(\mathbf{r},t)\rangle - n$ and, after Fourier transformation,

$$(\omega^2 - \omega_p^2)\delta\langle n(\mathbf{q},\omega)\rangle = 0 \tag{3.146}$$

in a three-dimensional system. The plasmon frequency $\omega_p = (ne^2/m\epsilon_0)^{1/2}$ lies above the continuum of particle-hole pair excitations ($\omega = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}} \sim v_F|\mathbf{q}|$), which ensures that the

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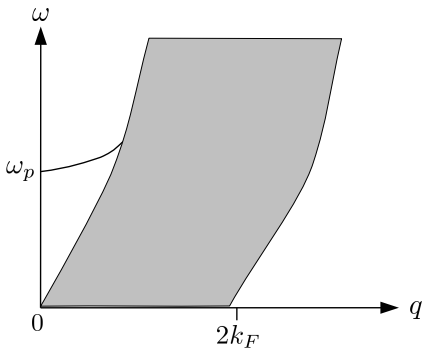


Figure 3.7: Plasmon mode in a three-dimensional electron system. The shaded area shows the continuum of particle-hole pair excitations $\omega = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}$.

plasmon mode remains undamped in the limit $\mathbf{q} \to 0$ (Fig. 3.7).[18] Note that in a typical metal, the plasmon energy is larger or of the order of the electronic bandwidth.

Let us assume that the particle-hole pair excitations do not contribute to $\Im[1/\epsilon_{\parallel}^R(\mathbf{q},\omega)]$ in the limit $\mathbf{q} \to 0$. This assumption can be verified within the RPA (Chap. 5) and more generally follows from phase space arguments (we now consider a three-dimensional system) [5]. We then expect

$$\lim_{\mathbf{q}\to 0} \Im\left[\frac{1}{\epsilon_{\parallel}^R(\mathbf{q},\omega)}\right] = A[\delta(\omega-\omega_0) - \delta(\omega+\omega_0)] \tag{3.147}$$

($\Im[1/\epsilon_{\parallel}^R(\mathbf{q},\omega)]$ is odd in frequency), where ω_0 is the frequency of the plasmon mode in the limit $\mathbf{q} \to 0$. The f-sum rule (3.135) and the perfect-screening sum rule (3.138) determine both A and ω_0: $A = -\omega_p\pi/2$ and $\omega_0 = \omega_p$. Thus ω_p is the exact value of the plasmon frequency in the $\mathbf{q} \to 0$ limit. Equivalently, Eq. (3.147) can be written as

$$\chi''_{\rho\rho}(\mathbf{q},\omega) = \frac{\pi}{2}\omega_p\epsilon_0\mathbf{q}^2[\delta(\omega-\omega_p) - \delta(\omega+\omega_p)] \qquad (\mathbf{q}\to 0). \tag{3.148}$$

Using the spectral representation of $1/\epsilon_{\parallel}^R(\mathbf{q},\omega) - 1$, we then obtain

$$\lim_{\mathbf{q}\to 0} \epsilon_{\parallel}^R(\mathbf{q},\omega) = 1 - \frac{\omega_p^2}{(\omega+i\eta)^2}. \tag{3.149}$$

3.4.2 Transverse dielectric function

To calculate the propagator of the vector potential, we first integrate out ϕ and obtain

$$S[\psi,\mathbf{A}_\perp] = S_m[\psi] + \int_0^\beta d\tau \int d^dr \Big\{ \frac{\epsilon_0}{2}\Big[\big(\partial_\tau \mathbf{A}_\perp(x)\big)^2 + c_l^2\big(\boldsymbol{\nabla}\times\mathbf{A}_\perp(x)\big)^2\Big] - \mathbf{j}(x)\cdot\mathbf{A}_\perp(x) + \frac{e}{2m}\rho(x)\mathbf{A}_\perp^2(x)\Big\}. \tag{3.150}$$

[18] For electrons confined to a two-dimensional plane (but interacting *via* the three-dimensional Coulomb interaction), one finds the plasmon dispersion $\omega = (|\mathbf{q}|ne^2/\epsilon_0 m)^{1/2}$. It vanishes for $\mathbf{q} \to 0$ but the (undamped) plasmon mode lies nevertheless above the particle-hole pair excitation spectrum.

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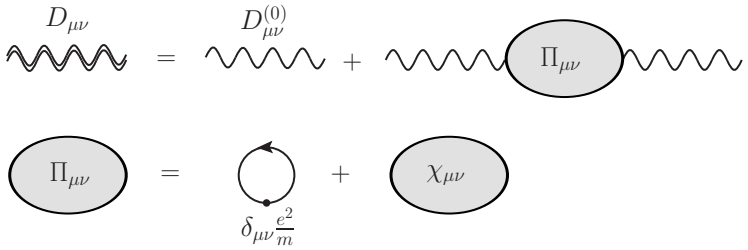


Figure 3.8: Diagrammatic representation of $D_{\mu\nu}$ and $\Pi_{\mu\nu}$.

The most direct way to determine $D_{\mu\nu}$ is to proceed diagrammatically as discussed in the preceding section. The Dyson equation satisfied by $D_{\mu\nu}$ is shown in Fig. 3.8. The self-energy $\Pi_{\mu\nu}$ is equal to

$$\Pi_{\mu\nu}(q) = \left(\delta_{\mu,\nu} - \frac{q_\mu q_\nu}{\mathbf{q}^2}\right)[-\epsilon_0\omega_p^2 + \chi_\perp(q)], \tag{3.151}$$

where $\chi_\perp(q)$ is the transverse part of the current-current correlation function

$$\chi_{j_\mu j_\nu}(q) = \langle j_\mu(q) j_\nu(-q)\rangle = \frac{q_\mu q_\nu}{\mathbf{q}^2}\chi_\parallel(q) + \left(\delta_{\mu,\nu} - \frac{q_\mu q_\nu}{\mathbf{q}^2}\right)\chi_\perp(q) \tag{3.152}$$

computed with the action $S_m[\psi]$. The first term in (3.151) comes from the diamagnetic term, while the second one is due to the coupling $\mathbf{j}\cdot\mathbf{A}_\perp = \mathbf{j}_\perp\cdot\mathbf{A}_\perp$ ($\mathbf{j}_\perp$ is the transverse component of the current density). If one ignores the magnetic interactions with respect to the Coulomb interaction, Eq. (3.151) is exact. It yields

$$D_\perp^{-1}(q) = [D_\perp^{(0)}(q)]^{-1} - \Pi_\perp(q) = [D_\perp^{(0)}(q)]^{-1} + \epsilon_0\omega_p^2 - \chi_\perp(q), \tag{3.153}$$

where $\chi_\perp$ is the transverse part of the current-current correlation function.

The transverse dielectric function $\epsilon_\perp(q)$ is defined by

$$D_\perp(q) = \frac{1}{\epsilon_0(\epsilon_\perp(q)\omega_n^2 + c_l^2\mathbf{q}^2)}, \tag{3.154}$$

i.e.

$$\epsilon_\perp(q) = 1 + \frac{\omega_p^2}{\omega_n^2} - \frac{\chi_\perp(q)}{\epsilon_0\omega_n^2}. \tag{3.155}$$

It determines the propagating modes of the electromagnetic field coupled to the transverse oscillations of the electron system, i.e. the "screening" of the electromagnetic field (Fig. 3.8).

3.4.2.1 Asymptotic behavior and analytic properties

Since $\lim_{|z|\to\infty}\chi_\perp(\mathbf{q},z) = 0$,

$$\epsilon_\perp^R(\mathbf{q},\omega) = 1 - \frac{\omega_p^2}{\omega^2} \qquad (\omega\to\infty). \tag{3.156}$$

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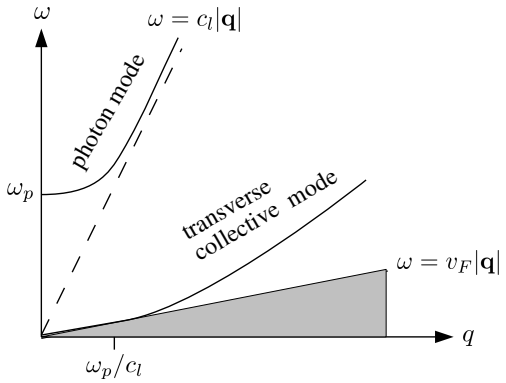


Figure 3.9: Transverse excitation spectrum of an electron system coupled to the electromagnetic field in the case of strong short-range interactions. For $c_l|\mathbf{q}| \lesssim \omega_p$, the transverse mode disappears in the continuum of particle-hole pair excitations (shaded area). (After Ref. [5].)

In a translation-invariant system where the total current $\hat{\mathbf{j}}(\mathbf{q}=0)$ is conserved, $\chi''_\perp(0,t)$ and $\chi^R_\perp(0,\omega)$ vanish,[19] and

$$\lim_{\mathbf{q}\to 0} \epsilon^R_\perp(\mathbf{q},\omega) = 1 - \frac{\omega_p^2}{(\omega+i\eta)^2}. \tag{3.157}$$

It readily follows from the definition (3.155) that $\epsilon^R_\perp(\mathbf{q},\omega)$ is analytic in the upper-half plane and satisfies the Kramers-Kronig relations. In particular,

$$\Re[\epsilon^R_\perp(\mathbf{q},\omega)] - 1 = \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Im[\epsilon^R_\perp(\mathbf{q},\omega')]}{\omega'-\omega}. \tag{3.158}$$

The analyticity properties of $\epsilon^R_\perp(\mathbf{q},\omega)$ also imply that the integral $\int_{\mathcal{C}} d\omega\, \omega \epsilon^R_\perp(\mathbf{q},\omega)$, where $\mathcal{C}$ is the contour defined by the real axis and the half circle of radius $R\to\infty$ located in the upper-half complex plane, must vanish. Because of (3.156), the contribution of the half circle is $-i\pi\omega_p^2$, so that

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \Im[\epsilon^R_\perp(\mathbf{q},\omega)] = \omega_p^2. \tag{3.159}$$

Equation (3.159) can be rewritten as a sum rule for the transverse conductivity (Sec. 3.4.4).

3.4.2.2 Photon mode and transverse collective mode

The dispersion of the transverse excitations of the electron system coupled to the electromagnetic field is obtained from the poles of $D^R_\perp(\mathbf{q},\omega)$,

$$\epsilon^R_\perp(\mathbf{q},\omega)\omega^2 = c_l^2\mathbf{q}^2. \tag{3.160}$$

Here we drop the infinitesimal $i\eta$ which does not play any role in the following discussion.

[19] The vanishing of $\chi''_{j_\mu j_\nu}(0,\omega)$ and $\chi^R_{j_\mu j_\nu}(0,\omega)$ is a direct consequence of the definition (3.12) of $\chi''_{j_\mu j_\nu}(\mathbf{q}=0,t)$ when $\hat{\mathbf{j}}(\mathbf{q}=0,t)$ is independent of t.

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Let us first look for a high-frequency solution $\omega \gtrsim \omega_p$. Using the asymptotic behavior (3.156), we obtain

$$\omega^2 \simeq \omega_p^2 + c_l^2 \mathbf{q}^2. \tag{3.161}$$

For $c_l|\mathbf{q}| \gg \omega_p$, the photon mode (3.161) is weakly coupled to the system and its frequency $\omega \simeq c_l|\mathbf{q}|$ is only slightly modified by the electrons. When $c_l|\mathbf{q}| \lesssim \omega_p$, the coupling between the electromagnetic field and the electrons is strong and leads to an enormous modification of the natural frequency $\omega \sim c_l|\mathbf{q}|$ of the field. Note that this strong coupling is due only to the diamagnetic term and does not involve the dynamics of the electrons.

Besides the photon mode (3.161), there are also low-energy excitations arising from genuine transverse fluctuations of the electron system, i.e. from the (isolated) poles of $\chi_\perp^R(\mathbf{q},\omega)$. Let us rewrite (3.160) as

$$\epsilon_0^{-1}\chi_\perp^R(\mathbf{q},\omega) = \omega_p^2 + c_l^2\mathbf{q}^2 - \omega^2. \tag{3.162}$$

Since transverse current fluctuations do not couple to the charge, $\chi_\perp^R$ does not contain the plasmon pole. The poles of $\chi_\perp^R(\mathbf{q},\omega)$ are therefore expected at low frequency $\omega \sim v_F|\mathbf{q}| \ll c_l|\mathbf{q}|$ in a metal. These poles satisfy (3.162), with only a slight shift due to the large but finite value of the rhs. These transverse excitations can exist only if they do not mix with the continuum of particle-hole pair excitations (the solutions of (3.160) would otherwise appear at complex frequencies). In Secs. 4.3.3 and 4.3.4, we shall study a transverse mode within a simple model based on Landau Fermi-liquid theory. The result suggests that a necessary condition for the propagation of transverse modes is that short-range interactions between electrons are sufficiently strong (thus making a transverse collective mode in real systems rather unlikely). When this condition is satisfied, one can show that the admixture of electromagnetic field into the transverse collective mode is negligible when $c_l|\mathbf{q}| \gg \omega_p$: The collective mode is essentially the same as in the neutral system. In the low-frequency regime $c_l|\mathbf{q}| \lesssim \omega_p$, the transverse collective mode is repelled by the photon mode (3.161) and disappears in the continuum of particle-hole pair excitations (Fig. 3.9) [5].

3.4.3 Linear response to external fields

In this section, we consider the effect of a field created by a charge (ρ_{ext}) and current ($\mathbf{j}_{\text{ext}}$) distribution external to the system. Fluctuations of ρ_{ext} and $\mathbf{j}_{\text{ext}}$ are neglected. In the Coulomb gauge, the coupling between the external field and the system is described by the action

$$S_{\text{ext}}[\phi, \mathbf{A}_\perp] = \int_0^\beta d\tau \int d^d r [i\phi(x)\rho_{\text{ext}}(x) - \mathbf{j}_{\text{ext}\perp}(x)\cdot\mathbf{A}_\perp(x)], \tag{3.163}$$

3.4.3.1 Screening of the external electromagnetic potentials

To linear order in the external perturbation, the mean value of the electromagnetic potentials is given by

$$\begin{aligned} \langle i\phi(q)\rangle &= -\langle i\phi(q) i\phi(-q)\rangle \rho_{\text{ext}}(q) = D_{00}(q)\rho_{\text{ext}}(q), \\ \langle \mathbf{A}_\perp(q)\rangle &= \langle \mathbf{A}_{\perp\mu}(q)\mathbf{A}_{\perp\mu}(-q)\rangle \mathbf{j}_{\text{ext}\perp}(q) = D_\perp(q)\mathbf{j}_{\text{ext}\perp}(q), \end{aligned} \tag{3.164}$$

where D_{00} and $D_\perp$ are the propagators in the absence of the external perturbation. These equations can be rewritten in terms of the dielectric functions,

$$\begin{aligned} \epsilon_0\epsilon_\parallel(q)\mathbf{q}^2\langle i\phi(q)\rangle &= \rho_{\text{ext}}(q), \\ \epsilon_0[\epsilon_\perp(q)\omega_n^2 + c_l^2\mathbf{q}^2]\langle \mathbf{A}_\perp(q)\rangle &= \mathbf{j}_{\text{ext}\perp}(q). \end{aligned} \tag{3.165}$$

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Real time equations are obtained from the analytic continuation $i\omega_n \to \omega + i\eta$ with $i\phi(q) \to \phi(\mathbf{q},\omega)$ and $\mathbf{A}_\perp(q) \to \mathbf{A}_\perp(\mathbf{q},\omega)$ so that $\phi(\mathbf{q},\omega)$ is the scalar potential according to the usual definition (see the discussion at the beginning of Sec. 3.4):

$$\begin{aligned} \epsilon_0 \epsilon_\parallel^R(\mathbf{q},\omega)\mathbf{q}^2\langle\phi(\mathbf{q},\omega)\rangle &= \rho_{\rm ext}(\mathbf{q},\omega), \\ \epsilon_0\left[-\epsilon_\perp^R(\mathbf{q},\omega)(\omega+i\eta)^2 + c_l^2\mathbf{q}^2\right]\langle\mathbf{A}_\perp(\mathbf{q},\omega)\rangle &= \mathbf{j}_{{\rm ext}\perp}(\mathbf{q},\omega). \end{aligned} \tag{3.166}$$

Thus we find that the average value of the electromagnetic field satisfies the Maxwell equations,

$$\begin{aligned} \boldsymbol{\nabla}\cdot\langle\mathbf{D}_\parallel(\mathbf{r},t)\rangle &= \rho_{\rm ext}(\mathbf{r},t), \\ \mu_0^{-1}\boldsymbol{\nabla}\times\langle\mathbf{B}(\mathbf{r},t)\rangle &= \frac{\partial\langle\mathbf{D}_\perp(\mathbf{r},t)\rangle}{\partial t} + \mathbf{j}_{{\rm ext}\perp}(\mathbf{r},t) \end{aligned} \tag{3.167}$$

(recall that $\epsilon_0\mu_0 c_l^2 = 1$), where

$$\begin{aligned} \langle\mathbf{D}_\parallel(\mathbf{q},\omega)\rangle &= \epsilon_0\epsilon_\parallel^R(\mathbf{q},\omega)\langle\mathbf{E}_\parallel(\mathbf{q},\omega)\rangle, \\ \langle\mathbf{D}_\perp(\mathbf{q},\omega)\rangle &= \epsilon_0\epsilon_\perp^R(\mathbf{q},\omega)\langle\mathbf{E}_\perp(\mathbf{q},\omega)\rangle \end{aligned} \tag{3.168}$$

is the displacement field. The dielectric functions that we defined from the propagator of the electromagnetic field correspond to those introduced in classical electromagnetism.

In the absence of coupling to the electrons, the external charge and current distribution create an electromagnetic potential defined by

$$\begin{aligned} [D_{00}^{(0)}(q)]^{-1} i\phi_{\rm ext}(q) &= \rho_{\rm ext}(q), \\ [D_\perp^{(0)}(q)]^{-1}\mathbf{A}_{{\rm ext}\perp}(q) &= \mathbf{j}_{{\rm ext}\perp}(q). \end{aligned} \tag{3.169}$$

Combining Eqs. (3.164), (3.165) and (3.169), we obtain the relation between the local $(\phi, \mathbf{A}_\perp)$ and external $(\phi_{\rm ext}, \mathbf{A}_{{\rm ext}\perp})$ potentials,

$$\begin{aligned} \langle\phi(\mathbf{q},\omega)\rangle &= \frac{D_{00}^R(\mathbf{q},\omega)}{D_{00}^{(0)R}(\mathbf{q},\omega)}\phi_{\rm ext}(\mathbf{q},\omega) = \frac{\phi_{\rm ext}(\mathbf{q},\omega)}{\epsilon_\parallel^R(\mathbf{q},\omega)}, \\ \langle\mathbf{A}_\perp(\mathbf{q},\omega)\rangle &= \frac{D_\perp^R(\mathbf{q},\omega)}{D_\perp^{(0)R}(\mathbf{q},\omega)}\mathbf{A}_{{\rm ext}\perp}(\mathbf{q},\omega) = \frac{(\omega+i\eta)^2 - c_l^2\mathbf{q}^2}{\epsilon_\perp^R(\mathbf{q},\omega)(\omega+i\eta)^2 - c_l^2\mathbf{q}^2}\mathbf{A}_{{\rm ext}\perp}(\mathbf{q},\omega), \end{aligned} \tag{3.170}$$

after analytic continuation $i\omega_n \to \omega + i\eta$. These equations enable to compute the local field as a function of the external field. In particular, the second one determines the screening of a static external magnetic field $\mathbf{B}_{{\rm ext}\perp}(\mathbf{q},0) = i\mathbf{q}\times\mathbf{A}_{{\rm ext}\perp}(\mathbf{q},0)$ and distinguishes between the weak orbital (Landau) diamagnetism of a normal metal and the perfect diamagnetism (Meissner effect) of a superconductor (Sec. 3.4.5).

3.4.3.2 Screening of the external charge and current densities

Similar relations can be obtained between the total and external charge and current densities. To linear order in the external perturbation

$$\delta\langle\rho(q)\rangle = -\langle\rho(q)i\phi(-q)\rangle\rho_{\rm ext}(q) = -\Pi_{00}(q)D_{00}(q)\rho_{\rm ext}(q) \tag{3.171}$$

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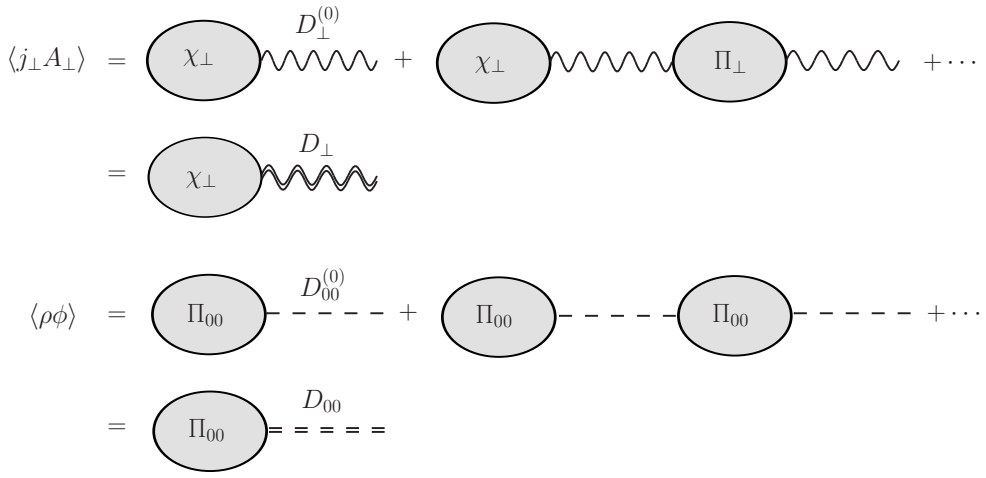


Figure 3.10: Diagrammatic representation of $\langle j_{\perp\mu}(q)A_{\perp\mu}(-q)\rangle$ and $\langle\rho(q)\phi(-q)\rangle$.

(see the relevant diagrams in Fig. 3.10), and

$$\begin{aligned}\langle\mathbf{J}_\perp(q)\rangle &= \langle\mathbf{j}_\perp(q)\rangle - \frac{ne^2}{m}\langle\mathbf{A}_\perp(q)\rangle,\\ &= \left[\langle j_{\perp\mu}(q)A_{\perp\mu}(-q)\rangle - \frac{ne^2}{m}D_\perp(q)\right]\mathbf{j}_{\mathrm{ext}\perp}(q)\\ &= \left[\chi_\perp(q) - \frac{ne^2}{m}\right]D_\perp(q)\mathbf{j}_{\mathrm{ext}\perp}(q).\end{aligned} \tag{3.172}$$

This yields

$$\begin{aligned}\delta\langle\rho(\mathbf{q},\omega)\rangle + \rho_{\mathrm{ext}}(\mathbf{q},\omega) &= \frac{\rho_{\mathrm{ext}}(\mathbf{q},\omega)}{\epsilon^R_\parallel(\mathbf{q},\omega)},\\ \langle\mathbf{J}_\perp(\mathbf{q},\omega)\rangle + \mathbf{j}_{\mathrm{ext}\perp}(\mathbf{q},\omega) &= \frac{(\omega+i\eta)^2 - c_l^2q^2}{\epsilon^R_\perp(\mathbf{q},\omega)(\omega+i\eta)^2 - c_l^2q^2}\mathbf{j}_{\mathrm{ext}\perp}(\mathbf{q},\omega).\end{aligned} \tag{3.173}$$

3.4.3.3 Conductivity

Finally, we can relate the current density to the electromagnetic field and obtain the conductivity. Equations (3.164) and (3.171) give

$$\delta\langle\rho(\mathbf{q},\omega)\rangle = -\Pi^R_{00}(\mathbf{q},\omega)\langle\phi(\mathbf{q},\omega)\rangle. \tag{3.174}$$

Using the continuity equation $(\omega+i\eta)\delta\langle\rho(\mathbf{q},\omega)\rangle = \mathbf{q}\cdot\langle\mathbf{J}(\mathbf{q},\omega)\rangle$, we deduce $\langle\mathbf{J}_\parallel(\mathbf{q},\omega)\rangle = \sigma_\parallel(\mathbf{q},\omega)\langle\mathbf{E}_\parallel(\mathbf{q},\omega)\rangle$ with[20]

$$\sigma_\parallel(\mathbf{q},\omega) = \frac{\omega+i\eta}{i\mathbf{q}^2}\Pi^R_{00}(\mathbf{q},\omega). \tag{3.175}$$

[20]The conductivity tensor can be written as $\sigma_{\mu\nu}(\mathbf{q},\omega) = (q_\mu q_\nu/\mathbf{q}^2)\sigma_\parallel(\mathbf{q},\omega) + (\delta_{\mu,\nu} - q_\mu q_\nu/\mathbf{q}^2)\sigma_\perp(\mathbf{q},\omega)$. This form follows from the homogeneity and isotropy of the system.

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From Eqs. (3.164,3.172), we obtain

$$\langle \mathbf{J}_\perp(\mathbf{q},\omega)\rangle = \left[\chi^R_\perp(\mathbf{q},\omega) - \frac{ne^2}{m}\right]\langle \mathbf{A}_\perp(\mathbf{q},\omega)\rangle \tag{3.176}$$

and

$$\sigma_\perp(\mathbf{q},\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_\perp(\mathbf{q},\omega) - \frac{ne^2}{m}\right]. \tag{3.177}$$

The conductivity is related to the dielectric function by

$$\epsilon^R_{\parallel,\perp}(\mathbf{q},\omega) = 1 + \frac{i}{\epsilon_0(\omega+i\eta)}\sigma_{\parallel,\perp}(\mathbf{q},\omega). \tag{3.178}$$

For each sum rule satisfied by $\epsilon^R_{\parallel,\perp}$, we can deduce a sum rule for $\sigma_{\parallel,\perp}$. Of particular interest are the longitudinal- and transverse-conductivity sum rules

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Re[\sigma_\parallel(\mathbf{q},\omega)] = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Re[\sigma_\perp(\mathbf{q},\omega)] = \frac{\epsilon_0}{2}\omega_p^2, \tag{3.179}$$

which follow from (3.140) and (3.159). Note that the longitudinal-conductivity sum rule assumes the analyticity of $\epsilon^R_\parallel(\mathbf{q},\omega)$ in the upper-half complex plane and may be violated. By contrast, $\epsilon^R_\perp(\mathbf{q},\omega)$ and $\sigma_\perp(\mathbf{q},\omega)$ are always analytic for $\Im(\omega)\geq 0$, and the transverse-conductivity sum rule is always valid.

3.4.4 Conductivity

The conductivity can also be calculated by considering the Hamiltonian

$$\hat{H} + \hat{H}'(t) = \hat{H} + \int d^dr\left[\phi(\mathbf{r},t)\hat{\rho}(\mathbf{r}) - \hat{\mathbf{j}}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r},t) + \frac{e}{2m}\hat{\rho}(\mathbf{r})\mathbf{A}^2(\mathbf{r},t)\right] \tag{3.180}$$

describing a system coupled to the electromagnetic potentials $(\phi,\mathbf{A})$. The Hamiltonian $\hat{H}$ includes the Coulomb interaction between particles but not the magnetic interactions. There is no necessity anymore to restrict ourselves to the Coulomb gauge (which was primarily dictated by the simple treatment of the electromagnetic field fluctuations, see Chap. 1.9).

The longitudinal potentials $(\phi,\mathbf{A}_\parallel)$ in (3.180) should be seen as external potentials. The polarization processes giving rise to screening will arise through a proper treatment of the Coulomb interaction included in the Hamiltonian (3.180). On the other hand $\mathbf{A}_\perp$ should be seen as a local potential since, in the absence of the electromagnetic part $\hat{H}_{\rm em}$ of the Hamiltonian (describing the dynamics of the electromagnetic field), the screening of the transverse field cannot be taken into account. The absence of $\hat{H}_{\rm em}$ in (3.180) also implies that the magnetic interactions between electrons are not included but they can be safely ignored in a non-relativistic system.[21] In the following, we shall therefore consider the transverse response to the local potential $\mathbf{A}_\perp$ and the longitudinal response to the external potentials $(\phi,\mathbf{A}_\parallel)$.

[21] See the discussion at the end of Sec. 1.9.3.

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3.4.4.1 Kubo's formulae

From Eq. (3.180), we readily obtain the linear response to the electromagnetic potentials,

$$\begin{aligned}\delta\langle\rho(\mathbf{q},\omega)\rangle &= -\chi^R_{\rho\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega) + \sum_\mu \chi^R_{\rho j_\mu}(\mathbf{q},\omega)A_\mu(\mathbf{q},\omega),\\ \langle\mathbf{J}_\mu(\mathbf{q},\omega)\rangle &= \sum_\nu \left[\chi^R_{j_\mu j_\nu}(\mathbf{q},\omega) - \frac{ne^2}{m}\delta_{\mu,\nu}\right] A_\nu(\mathbf{q},\omega) - \chi^R_{j_\mu\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega).\end{aligned} \tag{3.181}$$

Choosing the gauge $\phi = 0$, we deduce the expression of the conductivity tensor

$$\sigma_{\mu\nu}(\mathbf{q},\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{j_\mu j_\nu}(\mathbf{q},\omega) - \frac{ne^2}{m}\delta_{\mu,\nu}\right] \tag{3.182}$$

i.e.

$$\sigma_{\parallel,\perp}(\mathbf{q},\omega) = \frac{1}{i(\omega+i\eta)}\left[\chi^R_{\parallel,\perp}(\mathbf{q},\omega) - \frac{ne^2}{m}\right]. \tag{3.183}$$

Note that $\sigma_\parallel(\mathbf{q},\omega)$ differs from (3.175) which gives the response to the local field.[22] From now on, $\sigma_\parallel$ shall always denote the response to the external longitudinal electric field. We shall show below how Eq. (3.183) can be derived in an arbitrary gauge.

3.4.4.2 Gauge invariance and particle number conservation

When $\mathbf{A}_\parallel(\mathbf{r},t) = \boldsymbol{\nabla}\Lambda(\mathbf{r},t)$ and $\phi(\mathbf{r},t) = -\partial_t\Lambda(\mathbf{r},t)$ there is no longitudinal electric field, $\mathbf{E}_\parallel = -\boldsymbol{\nabla}\phi - \partial_t\mathbf{A}_\parallel = 0$, and the longitudinal response must therefore vanish for any function Λ. This gives

$$\begin{aligned}0 &= (\omega+i\eta)\chi^R_{\rho\rho}(\mathbf{q},\omega) - \sum_\mu q_\mu\chi^R_{\rho j_\mu}(\mathbf{q},\omega),\\ 0 &= \sum_\nu \left[\chi^R_{j_\mu j_\nu}(\mathbf{q},\omega) - \frac{ne^2}{m}\delta_{\mu,\nu}\right] q_\nu - (\omega+i\eta)\chi^R_{j_\mu\rho}(\mathbf{q},\omega).\end{aligned} \tag{3.184}$$

Multiplying the last equation by q_μ and summing over μ gives

$$\begin{aligned}0 =& \mathbf{q}^2\left[\chi^R_\parallel(\mathbf{q},\omega) - \frac{ne^2}{m}\right] - (\omega+i\eta)\sum_\mu q_\mu\chi^R_{j_\mu\rho}(\mathbf{q},\omega)\\ =& \mathbf{q}^2\left[\chi^R_\parallel(\mathbf{q},\omega) - \frac{ne^2}{m}\right] - (\omega+i\eta)^2\chi^R_{\rho\rho}(\mathbf{q},\omega).\end{aligned} \tag{3.185}$$

The last result is obtained using $\chi^R_{\rho j_\mu}(\mathbf{q},\omega) = \chi^R_{j_\mu\rho}(\mathbf{q},\omega)$. The equality of these two correlation functions is easily shown using (3.18), as well as parity and time-reversal invariance (see Table 3.1):

$$\chi''_{j_\mu\rho}(\mathbf{q},\omega) = [\chi''_{\rho j_\mu}(-\mathbf{q},\omega)]^* = \epsilon^T_\rho\epsilon^T_{j_\mu}\epsilon^P_\rho\epsilon^P_{j_\mu}\chi''_{\rho j_\mu}(\mathbf{q},\omega) = \chi''_{\rho j_\mu}(\mathbf{q},\omega) \tag{3.186}$$

($\epsilon^T_\rho = \epsilon^P_\rho = 1$ and $\epsilon^T_{j_\mu} = \epsilon^P_{j_\mu} = -1$), where ϵ^P_A and ϵ^T_A denote the signatures of the operator $\hat{A}$ under parity and time reversal (Chap. 2).

[22] The expression $\sigma_\parallel(\mathbf{q},\omega) = [(\omega+i\eta)/i\mathbf{q}^2]\chi^R_{\rho\rho}(\mathbf{q},\omega)$ derived below [Eq. (3.192)] can be deduced from (3.175) and the relation (3.170) between $\langle\phi(\mathbf{q},\omega)\rangle$ and $\phi_{\rm ext}(\mathbf{q},\omega)$.

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These results can also be derived from the continuity equation $(\omega + i\eta)\delta\langle\rho(\mathbf{q},\omega)\rangle - \mathbf{q}\cdot\langle\mathbf{J}_\parallel(\mathbf{q},\omega)\rangle = 0$, where $\delta\langle\rho(\mathbf{q},\omega)\rangle$ and $\langle\mathbf{J}_\parallel(\mathbf{q},\omega)\rangle$ are given by (3.181) to linear order in the electromagnetic potentials. Since the continuity equation must be satisfied for any value of $\mathbf{A}_\parallel$ and ϕ, we reproduce (3.184) except for the exchange $\chi^R_{\rho j_\mu}(\mathbf{q},\omega) \leftrightarrow \chi^R_{j_\mu\rho}(\mathbf{q},\omega)$.

Equations (3.184) and (3.185) can be used to derive the expression of $\sigma_\parallel(\mathbf{q},\omega)$ in an arbitrary gauge. It is convenient to introduce the longitudinal and transverse parts of the current,

$$\begin{aligned}\hat{\mathbf{J}}_\parallel(\mathbf{q}) &= \frac{\mathbf{q}}{\mathbf{q}^2}[\mathbf{q}\cdot\hat{\mathbf{J}}(\mathbf{q})] = \frac{\mathbf{q}}{|\mathbf{q}|}\hat{J}_\parallel(\mathbf{q}),\\ \hat{\mathbf{J}}_\perp(\mathbf{q}) &= \hat{\mathbf{J}}(\mathbf{q}) - \hat{\mathbf{J}}_\parallel(\mathbf{q})\end{aligned} \tag{3.187}$$

(similar expressions hold for the vector potential $\mathbf{A}$) and the correlation functions

$$\begin{aligned}\chi_\parallel(\mathbf{q},\omega) &= \sum_{\mu,\nu}\frac{q_\mu q_\nu}{\mathbf{q}^2}\chi_{j_\mu j_\nu}(\mathbf{q},\omega), \quad \chi_\perp(\mathbf{q},\omega) = \sum_{\mu,\nu}\left(\delta_{\mu,\nu} - \frac{q_\mu q_\nu}{\mathbf{q}^2}\right)\chi_{j_\mu j_\nu}(\mathbf{q},\omega),\\ \chi_{j_\parallel\rho}(\mathbf{q},\omega) &= \sum_\mu \frac{q_\mu}{|\mathbf{q}|}\chi_{j_\mu\rho}(\mathbf{q},\omega), \quad \chi_{\rho j_\parallel}(\mathbf{q},\omega) = \sum_\mu \chi_{\rho j_\mu}(\mathbf{q},\omega)\frac{q_\mu}{|\mathbf{q}|}.\end{aligned} \tag{3.188}$$

This allows us to rewrite Eqs. (3.181) as[23]

$$\begin{aligned}\delta\langle\rho(\mathbf{q},\omega)\rangle &= -\chi^R_{\rho\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega) + \chi^R_{\rho j_\parallel}(\mathbf{q},\omega)A_\parallel(\mathbf{q},\omega),\\ \langle J_\parallel(\mathbf{q},\omega)\rangle &= \left[\chi^R_\parallel(\mathbf{q},\omega) - \frac{ne^2}{m}\right]A_\parallel(\mathbf{q},\omega) - \chi^R_{j_\parallel\rho}(\mathbf{q},\omega)\phi(\mathbf{q},\omega)\end{aligned} \tag{3.189}$$

for the longitudinal part. Using Eqs. (3.184) and (3.185),

$$\begin{aligned}0 &= (\omega+i\eta)\chi^R_{\rho\rho}(\mathbf{q},\omega) - |\mathbf{q}|\chi^R_{\rho j_\parallel}(\mathbf{q},\omega),\\ 0 &= |\mathbf{q}|\left[\chi^R_\parallel(\mathbf{q},\omega) - \frac{ne^2}{m}\right] - (\omega+i\eta)\chi^R_{j_\parallel\rho}(\mathbf{q},\omega) = 0,\end{aligned} \tag{3.190}$$

we finally obtain

$$\begin{aligned}\delta\langle\rho(\mathbf{q},\omega)\rangle &= \frac{1}{i|\mathbf{q}|}\chi^R_{\rho\rho}(\mathbf{q},\omega)E_\parallel(\mathbf{q},\omega),\\ \langle J_\parallel(\mathbf{q},\omega)\rangle &= \frac{1}{i(\omega+i\eta)}\left[\chi^R_\parallel(\mathbf{q},\omega) - \frac{ne^2}{m}\right]E_\parallel(\mathbf{q},\omega),\end{aligned} \tag{3.191}$$

where $E_\parallel(\mathbf{q},\omega) = (\mathbf{q}/|\mathbf{q}|)\cdot\mathbf{E}_\parallel(\mathbf{q},\omega) = -i|\mathbf{q}|\phi(\mathbf{q},\omega) + i(\omega+i\eta)A_\parallel(\mathbf{q},\omega)$. Equations (3.191) and (3.190) give the (gauge-invariant) longitudinal conductivity

$$\begin{aligned}\sigma_\parallel(\mathbf{q},\omega) &= \frac{1}{i(\omega+i\eta)}\left[\chi^R_\parallel(\mathbf{q},\omega) - \frac{ne^2}{m}\right]\\ &= \frac{1}{i|\mathbf{q}|}\chi^R_{j_\parallel\rho}(\mathbf{q},\omega) = \frac{\omega+i\eta}{i\mathbf{q}^2}\chi^R_{\rho\rho}(\mathbf{q},\omega).\end{aligned} \tag{3.192}$$

Useful relations can be obtained from (3.184,3.185) or (3.190) by considering the two special cases $\omega = 0, \mathbf{q}\neq 0$ and $\omega\neq 0, \mathbf{q} = 0$:

$$\begin{aligned}\chi^R_\parallel(\mathbf{q},0) - \frac{ne^2}{m} = 0 \quad \text{and} \quad \sum_\mu \frac{q_\mu}{|\mathbf{q}|}\chi^R_{\rho j_\mu}(\mathbf{q},0) = \chi^R_{\rho j_\parallel}(\mathbf{q},0) = 0 \quad \text{for} \quad \mathbf{q}\neq 0,\\ \chi^R_{\rho\rho}(0,\omega) = 0 \quad \text{and} \quad \chi^R_{j_\mu\rho}(0,\omega) = 0 \quad \text{for} \quad \omega\neq 0.\end{aligned} \tag{3.193}$$

[23] For symmetry reasons, the charge density does not couple to the transverse part of the current density.

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The first of these equations gives

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi_{\parallel}''(\mathbf{q},\omega)}{\omega} = \frac{ne^2}{m} \qquad (\mathbf{q} \neq 0), \tag{3.194}$$

which is nothing but the f-sum rule as can be seen by inserting the continuity equation for the Heisenberg operators, $\omega\hat{\rho}(\mathbf{q},\omega) - \mathbf{q}\cdot\hat{\mathbf{j}}_{\parallel}(\mathbf{q},\omega) = 0$, into Eq. (3.106).

It is easy to see that the second of Eqs. (3.193) also holds for the Matsubara correlation functions, i.e.

$$\chi_{\rho\rho}(0, i\omega_n) = 0 \quad \text{and} \quad \chi_{j_\mu\rho}(0, i\omega_n) = \chi_{\rho j_\mu}(0, -i\omega_n) = 0 \quad \text{for} \quad \omega_n \neq 0. \tag{3.195}$$

This follows from $\chi_{\rho\rho}(\mathbf{q},\tau) = \langle T_\tau \hat{\rho}(\mathbf{q},\tau)\hat{\rho}(-\mathbf{q},0)\rangle$ and $\chi_{\rho j_\mu}(\mathbf{q},\tau) = \langle T_\tau \hat{\rho}(\mathbf{q},\tau)\hat{j}_\mu(-\mathbf{q},0)\rangle$ being independent of τ for $\mathbf{q} = 0$ since $\hat{\rho}(\mathbf{q}=0) = (e/\sqrt{\mathcal{V}})\hat{N}$ is nothing but the total particle number operator and therefore conserved: $[\hat{\rho}(\mathbf{q}=0), \hat{H}] = 0$ implies $\hat{\rho}(\mathbf{q}=0,\tau) = e^{\tau\hat{H}}\hat{\rho}(\mathbf{q}=0)e^{-\tau\hat{H}} = \hat{\rho}(\mathbf{q}=0)$.

3.4.4.3 Kubo's formulae from the functional integral formalism

It is instructive to derive the preceding results within the functional integral formalism, by considering the Euclidean action

$$S[\psi^*,\psi,A] = \int_0^\beta d\tau \int d^d r \sum_\sigma \psi_\sigma^* \Big[\partial_\tau - \mu - ieA_0 + \frac{1}{2m}(-i\boldsymbol{\nabla} - e\mathbf{A})^2\Big]\psi_\sigma + S_{\rm int}[\psi^*,\psi], \tag{3.196}$$

where $A_0 = -\phi$. The current density is defined by

$$J_\mu(x) = -\frac{\delta S}{\delta A_\mu(x)} \qquad (\mu = 0, x, \dots) \tag{3.197}$$

so that $J_0(x) = j_0(x) = i\rho(x)$ whereas $J_\mu(x)$ corresponds to the usual definition when $\mu \neq 0$. We thus have

$$\langle J_\mu(x)\rangle = -\frac{1}{Z[A]} \int \mathcal{D}[\psi^*,\psi] \frac{\delta S}{\delta A_\mu(x)} e^{-S} = \frac{\delta \ln Z[A]}{\delta A_\mu(x)}, \tag{3.198}$$

where $Z[A]$ is the partition function. The linear response to the gauge field is therefore given by

$$\langle J_\mu(x)\rangle = \langle J_\mu(x)\rangle_{A=0} + \int_0^\beta d\tau' \int d^d r' \sum_\nu K_{\mu\nu}(x,x') A_\nu(x') + \mathcal{O}(A^2), \tag{3.199}$$

where

$$K_{\mu\nu}(x,x') = \left.\frac{\delta^2 \ln Z[A]}{\delta A_\mu(x)\delta A_\nu(x')}\right|_{A=0}. \tag{3.200}$$

To obtain an explicit expression of the response function $K_{\mu\nu}$ we integrate out the field ψ in a cumulant expansion,

$$\begin{aligned} Z[A] &= \int \mathcal{D}[\psi^*,\psi]\, e^{-S[\psi^*,\psi,A=0] + \int_0^\beta d\tau \int d^d r \left(\sum_\mu j_\mu A_\mu + i\frac{ej_0}{2m}\mathbf{A}^2\right)} \\ &= Z[0]\, e^{\int_0^\beta d\tau \int d^d r \sum_\mu \langle j_\mu\rangle A_\mu + \frac{1}{2}\int_0^\beta d\tau d\tau' \int d^d r d^d r' \sum_{\mu,\nu} K_{\mu\nu}(x,x') A_\mu(x) A_\nu(x') + \mathcal{O}(A^3)}, \end{aligned} \tag{3.201}$$

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where $K_{\mu\nu}(x,x')$ is defined by its Fourier transform

$$K_{\mu\nu}(q) = \chi_{j_\mu j_\nu}(q) - \frac{ne^2}{m}\delta_{\mu,\nu}(1-\delta_{\mu,0}) \tag{3.202}$$

and all expectation values are now taken with the action $S[\psi^*,\psi,A=0]$. Performing the analytic continuation to real frequencies with $i\phi = -iA_0 \to \phi$, and noting that $\chi_{j_0 j_0} = -\chi_{\rho\rho}$ and $\chi_{j_0 j_\mu} = i\chi_{\rho j_\mu}$ $(\mu \neq 0)$, we reproduce (3.181).

Since the action (3.196) is invariant in the gauge transformation

$$\begin{gathered}\psi_\sigma(x) \to e^{ie\Lambda(x)}\psi_\sigma(x), \qquad \psi^*_\sigma(x) \to e^{-ie\Lambda(x)}\psi^*_\sigma(x), \\ A_\mu(x) \to A_\mu(x) + \partial_\mu\Lambda(x),\end{gathered} \tag{3.203}$$

the response to a pure gauge field $A_\mu = \partial_\mu\Lambda$ must vanish, i.e.

$$\begin{aligned}0 &= \int_0^\beta d\tau' \int d^d r' \sum_\nu K_{\mu\nu}(x,x')\partial_{x'_\nu}\Lambda(x') \\ &= -\int_0^\beta d\tau' \int d^d r' \sum_\nu \partial_{x'_\nu} K_{\mu\nu}(x,x')\Lambda(x'),\end{aligned} \tag{3.204}$$

which implies that the response function is transverse,

$$\sum_\nu \partial_{x'_\nu} K_{\mu\nu}(x,x') = 0. \tag{3.205}$$

In Fourier space this gives

$$0 = -\omega_n K_{\mu 0}(q) + \sum_{\nu\neq 0} q_\nu K_{\mu\nu}(q). \tag{3.206}$$

The analytic continuation of this equation yields Eqs. (3.184).

Finally we note that the continuity equation implies $\sum_\mu \partial_\mu \langle J_\mu(x)\rangle = 0$ and therefore

$$\sum_\mu \partial_\mu K_{\mu\nu}(x,x') = 0. \tag{3.207}$$

The equivalence between (3.205) and (3.207) follows from the property $K_{\mu\nu}(q) = K_{\nu\mu}(-q)$.

3.4.4.4 Longitudinal-conductivity sum rule

From Eq. (3.183), we deduce

$$\begin{aligned}\Re[\sigma_\parallel(\mathbf{q},\omega)] &= \Re\left[\mathcal{P}\frac{\chi^R_\parallel(\mathbf{q},\omega)}{i\omega}\right] - \pi\delta(\omega)\left\{\Re[\chi^R_\parallel(\mathbf{q},\omega)] - \frac{ne^2}{m}\right\} \\ &= \mathcal{P}\frac{\chi''_\parallel(\mathbf{q},\omega)}{\omega} - \pi\delta(\omega)\left\{\Re[\chi^R_\parallel(\mathbf{q},\omega)] - \frac{ne^2}{m}\right\},\end{aligned} \tag{3.208}$$

where we have used the spectral representation (3.32) and the fact that $\chi''_\parallel(\mathbf{q},\omega) = \Im[\chi^R_\parallel(\mathbf{q},\omega)]$ is real [Eq. (3.42)]. The term $\delta(\omega)\chi^R_\parallel(\mathbf{q},\omega)$ in Eq. (3.208) has a different meaning whether

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$\mathbf{q} \neq 0$ or $\mathbf{q} = 0$. In the former case, it reduces to $\delta(\omega)\chi_\parallel^R(\mathbf{q},0)$, whereas in the latter case it should be interpreted as $\delta(\omega)\lim_{\omega\to 0}\chi^R(0,\omega)$ – as follows from taking the limit $\mathbf{q} = 0$ before $\eta \to 0^+$.

Equation (3.208) implies

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Re[\sigma_\parallel(\mathbf{q},\omega)] = \frac{ne^2}{2m} = \frac{\epsilon_0}{2}\omega_p^2. \tag{3.209}$$

For $\mathbf{q} \neq 0$ we have used the relation (3.44) between $\chi_\parallel^R(\mathbf{q},0)$ and $\chi_\parallel''(\mathbf{q},\omega)$ whereas for $\mathbf{q} = 0$ we notice that $\chi_\parallel^R(0,\omega)$ and $\chi_\parallel''(0,\omega)$ vanish in a translation-invariant system where the total current $\hat{\mathbf{j}}(\mathbf{q} = 0)$ is conserved.[24] The longitudinal-conductivity sum rule (3.209), which involves the response to the external electric field, is identical to the sum rule (3.179) satisfied by the longitudinal response to the local field. However, the latter assumes the analyticity of $\epsilon_\parallel^R(\mathbf{q},\omega)$ in the upper-half complex plane, whereas the sum rule (3.209) is always valid.

3.4.4.5 Zero-frequency conductivity and Drude weight

For a uniform field ($\mathbf{q} = 0$), we cannot distinguish between longitudinal and transverse response functions, so that $\chi_\parallel^R(0,\omega) = \chi_\perp^R(0,\omega) \equiv \chi^R(0,\omega)$ and

$$\sigma_\parallel(0,\omega) = \sigma_\perp(0,\omega) \equiv \sigma(0,\omega). \tag{3.210}$$

The DC conductivity is defined by $\sigma_{\rm DC} = \lim_{\omega\to 0}\sigma(0,\omega)$. By taking the $\mathbf{q} \to 0$ limit first, we ensure that we are looking at an infinite volume, where energy levels can be arbitrarily close in energy, so that absorption remains possible even when $\omega \to 0$, a condition necessary to have a metallic (conducting) state. Recalling the definition of $\sigma_\parallel(\mathbf{q},\omega)$ and $\sigma_\perp(\mathbf{q},\omega)$ given at the beginning of Sec. 3.4.4, Eq. (3.210) implies that the local and external fields coincide, as expected when $\mathbf{q} = 0$.[25]

Equation (3.208) gives

$$\Re[\sigma(0,\omega)] = \mathcal{P}\frac{\chi''(0,\omega)}{\omega} + D\delta(\omega), \tag{3.211}$$

where the coefficient of the delta function,

$$D = \pi\lim_{\omega\to 0}\left\{\frac{ne^2}{m} - \Re[\chi^R(0,\omega)]\right\}, \tag{3.212}$$

is called the Drude weight. As pointed out above, $\chi^R(0,\omega)$ vanishes in translation-invariant systems and

$$\sigma(0,\omega) = \frac{D}{\pi}\frac{i}{\omega + i\eta} \quad \text{with} \quad D = \pi\frac{ne^2}{m}. \tag{3.213}$$

$\Re[\sigma(0,\omega)] = D\delta(\omega)$ and the Drude weight exhausts all the spectral weight in the conductivity sum rule (3.209) (perfect conductor). When translation invariance of the electron system

[24] See footnote 19 on page 248.

[25] The absence of screening of the longitudinal field, i.e. $\langle\phi(0,\omega)\rangle = \phi_{\rm ext}(0,\omega)$, comes from the vanishing of the $\mathbf{q} = 0$ component of the Coulomb interaction in the jellium model, so that $\epsilon_\parallel(0,\omega) = 1$ (note that $\epsilon_\parallel(0,\omega) \neq \lim_{\mathbf{q}\to 0}\epsilon_\parallel(\mathbf{q},\omega)$).

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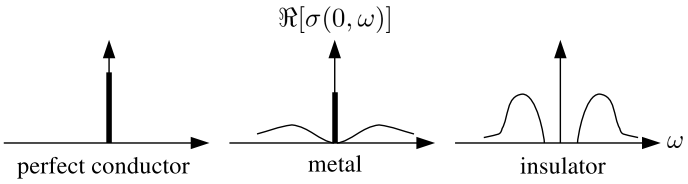


Figure 3.11: Schematic representation of $\Re[\sigma(0,\omega)]$ in a perfect conductor ($D = \pi ne^2/m$), a metal ($0 < D < \pi ne^2/m$) and an insulator ($D = 0$).

is broken, for instance by interactions with phonons or umklapp processes made possible by the crystal lattice, $\Re[\chi^R(0,\omega)]$ is finite and reduces the Drude weight. Part of the spectral weight is then pushed up to finite frequencies in agreement with the sum rule (3.209). A metal is defined by a finite Drude weight,[26] whereas an insulator corresponds to a vanishing Drude weight (Fig. 3.11), i.e.

$$\lim_{\omega\to 0} \Re[\chi^R(0,\omega)] = \frac{ne^2}{m}. \tag{3.214}$$

Together with the f-sum rule (3.193), this result means that

$$\lim_{\omega\to 0}\lim_{\mathbf{q}\to 0} \Re[\chi^R_\parallel(\mathbf{q},\omega)] = \lim_{\mathbf{q}\to 0}\lim_{\omega\to 0} \Re[\chi^R_\parallel(\mathbf{q},\omega)] \tag{3.215}$$

is independent of the order of the limits $\mathbf{q} \to 0$ and $\omega \to 0$. It is easy to show that a sufficient condition for (3.215) to hold is the presence of a gap in the longitudinal excitation spectrum, i.e. $\chi''_\parallel(\mathbf{q},\omega) = 0$ for $|\omega| < \Delta$ (regardless of the value of $\mathbf{q}$). From the Kramers-Kronig relations, we obtain

$$\Re[\chi^R_\parallel(\mathbf{q},\omega)] = \mathcal{P}\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_\parallel(\mathbf{q},\omega')}{\omega' - \omega}. \tag{3.216}$$

For $|\omega| < \Delta$, there is no singularity in this integral, and the limits $\omega \to 0$ and $\mathbf{q} \to 0$ are interchangeable,

$$\lim_{\omega\to 0}\lim_{\mathbf{q}\to 0} \Re[\chi^R_\parallel(\mathbf{q},\omega)] = \lim_{\mathbf{q}\to 0}\lim_{\omega\to 0} \Re[\chi^R_\parallel(\mathbf{q},\omega)] = 2\int_{\Delta}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_\parallel(0,\omega')}{\omega'}. \tag{3.217}$$

3.4.5 Superconductors

Superfluidity and superconductivity will be the subject of Chap. 7. Here we give a first introduction to superconductivity.

3.4.5.1 Landau diamagnetism in normal metals

While gauge invariance implies the f-sum rule $\chi^R_\parallel(\mathbf{q},0) = ne^2/m$, there is *a priori* no constraint on $\chi^R_\perp(\mathbf{q},0)$. However, if the current-current correlation function is short-range, i.e. if it decays fast enough in real space, the $\mathbf{q} \to 0$ limit should not be singular:

$$\lim_{\mathbf{q}\to 0} \chi^R_\perp(\mathbf{q},0) = \lim_{q_y\to 0}\lim_{q_x\to 0} \chi^R_{j_x j_x}(\mathbf{q},0) = \lim_{q_x\to 0}\lim_{q_y\to 0} \chi^R_{j_x j_x}(\mathbf{q},0) = \frac{ne^2}{m} \tag{3.218}$$

[26] In a disordered conductor, the Drude peak $D\delta(\omega)$ broadens into $D\frac{\tau_{\rm tr}}{1-i\omega\tau_{\rm tr}}$ where $\tau_{\rm tr}$ is the transport scattering time.

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($q_z, \cdots = 0$ in this equation), where the last result follows from the f-sum rule. In the long wavelength limit, we thus have $\epsilon_0^{-1}\chi_\perp^R(\mathbf{q},0) = \omega_p^2 - \alpha\mathbf{q}^2 + \mathcal{O}(|\mathbf{q}|^4)$. The screening of a slowly varying external static magnetic field is determined by (3.170),

$$\langle \mathbf{A}_\perp(\mathbf{q},0)\rangle = \frac{c_l^2\mathbf{q}^2}{c_l^2\mathbf{q}^2 + \omega_p^2 - \epsilon_0^{-1}\chi_\perp^R(\mathbf{q},0)}\mathbf{A}_{\text{ext}\perp}(\mathbf{q},0) \simeq \frac{c_l^2}{c_l^2+\alpha}\mathbf{A}_{\text{ext}\perp}(\mathbf{q},0). \tag{3.219}$$

The current $\langle \mathbf{J}_\perp\rangle$ produced by a static magnetic field is related to the orbital magnetization density $\langle \mathbf{M}\rangle$ by $\langle \mathbf{J}_\perp\rangle = \boldsymbol{\nabla}\times\langle\mathbf{M}\rangle$, i.e.

$$\left[\chi_\perp^R(\mathbf{q},0) - \frac{ne^2}{m}\right]\langle \mathbf{A}_\perp(\mathbf{q},0)\rangle = i\mathbf{q}\times\langle\mathbf{M}(\mathbf{q},0)\rangle. \tag{3.220}$$

Using (3.219) and taking the curl, one finds

$$\langle \mathbf{M}(\mathbf{q},0)\rangle = -\frac{\alpha\epsilon_0 c_l^2}{c_l^2+\alpha}\mathbf{B}_{\text{ext}}(\mathbf{q},0) \simeq -\alpha\epsilon_0\mathbf{B}_{\text{ext}}(\mathbf{q},0) \qquad (\mathbf{q}\to 0), \tag{3.221}$$

and the orbital susceptibility

$$\chi_{\text{orb}} = -\alpha\epsilon_0 = \lim_{\mathbf{q}\to 0}\frac{1}{\mathbf{q}^2}\left[\chi_\perp^R(\mathbf{q},0) - \frac{ne^2}{m}\right]. \tag{3.222}$$

In normal metals, χ_{orb} is negative (Landau diamagnetism).[27]

For free electrons, $\chi_\perp^R(\mathbf{q},0) = \chi_\perp(\mathbf{q}, i\omega_\nu = 0)$ is given by

$$\begin{aligned}\chi_\perp^R(\mathbf{q},0) &= \langle j_x(\mathbf{q}, i\omega_\nu = 0) j_x(-\mathbf{q}, i\omega_\nu = 0)\rangle \\ &= -\frac{2e^2}{\beta\mathcal{V}m^2}\sum_{\mathbf{k},\omega_n} k_x^2 (i\omega_n - \xi_{\mathbf{k}})^{-1}(i\omega_n - \xi_{\mathbf{k}+\mathbf{q}})^{-1} \\ &= -\frac{2e^2}{m^2}\int_{\mathbf{k}} k_x^2 \frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}}},\end{aligned} \tag{3.223}$$

where we have assumed $\mathbf{q}\perp\hat{\mathbf{x}}$ and used the expression of the current operator given in the footnote 15 on page 239. An elementary calculation gives

$$\chi_\perp^R(\mathbf{q},0) = \frac{ne^2}{m}\left(1 - \frac{\mathbf{q}^2}{4k_F^2}\right) + \mathcal{O}(\mathbf{q}^4), \tag{3.224}$$

for $T\to 0$ and $d = 3$, and

$$\chi_{\text{orb}} = -\frac{ne^2}{4mk_F^2} = -\frac{1}{3}\chi_P. \tag{3.225}$$

$\chi_P = (g\mu_B/2)^2 2N(0)$ is the (paramagnetic) Pauli susceptibility (with $g\simeq 2$) and $\mu_B = e/2m$ the Bohr magneton. The calculation of $\chi_P = (g\mu_B)^2\chi_{S^zS^z}(\mathbf{q}=0, i\omega_\nu = 0)$ is analogous to that of the charge susceptibility discussed in Sec. 3.2.7. ($S^z(\mathbf{r}) = \frac{1}{2}\sum_\sigma \psi_\sigma^*(\mathbf{r})\sigma\psi_\sigma(\mathbf{r})$ is the z-component of the spin density.)

[27] Note that a negative orbital susceptibility is not in contradiction with the stability of the system [6], which requires $\Re[\sigma_\perp(\mathbf{q},\omega)] \geq 0$ (see Sec. 3.4.5.3).

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3.4.5.2 Long-range current-current correlations and Meissner effect in superconductors

When the current-current correlations are long range, Eq. (3.218) can be violated, i.e.

$$\lim_{\mathbf{q}\to 0} \chi^R_\perp(\mathbf{q},0) = \frac{(n-n_s)e^2}{m}. \tag{3.226}$$

Equation (3.226) yields the London equation

$$\langle \mathbf{J}_\perp(\mathbf{q},0)\rangle = -\frac{n_s e^2}{m}\langle \mathbf{A}_\perp(\mathbf{q},0)\rangle \tag{3.227}$$

if we approximate $\chi^R_\perp(\mathbf{q},0)$ by its $\mathbf{q}\to 0$ limit. We shall see in Chap. 7 that the "superfluid density" n_s can be interpreted as the density of superfluid particles. We show below that $0 \leq n_s \leq n$.

The screening of a slowly varying static external magnetic field is then derived from[28]

$$\langle \mathbf{A}_\perp(\mathbf{q},0)\rangle = \frac{\mathbf{q}^2}{\mathbf{q}^2+\lambda_L^{-2}}\langle \mathbf{A}_{\perp\text{ext}}(\mathbf{q},0)\rangle \tag{3.228}$$

(see Eq. (3.170)), where

$$\lambda_L = c\left(\frac{\epsilon_0 m}{n_s e^2}\right)^{1/2} = \frac{c}{\omega_p}\sqrt{\frac{n}{n_s}} \tag{3.229}$$

is the London penetration depth. In real space, (3.228) becomes $\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\langle\mathbf{A}_\perp\rangle) + \lambda_L^{-2}\langle\mathbf{A}_\perp\rangle = \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\langle\mathbf{A}_{\perp\text{ext}}\rangle)$. Taking the curl and using $\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\times\langle\mathbf{B}\rangle) = -\boldsymbol{\nabla}^2\langle\mathbf{B}\rangle$, we finally obtain[29]

$$\boldsymbol{\nabla}^2\langle\mathbf{B}(\mathbf{r})\rangle = \lambda_L^{-2}\langle\mathbf{B}(\mathbf{r})\rangle \tag{3.230}$$

for a uniform external field $\mathbf{B}_{\text{ext}}$. Let us assume the superconductor to occupy the half space $z>0$ and the external field $\mathbf{B}_{\text{ext}}$ to be parallel to the interface between the superconductor and the vacuum. From (3.230) and the boundary condition $\langle\mathbf{B}(z=0)\rangle = \mathbf{B}_{\text{ext}}$ ($\langle\mathbf{B}\rangle = \langle\mathbf{B}_{\text{ext}}\rangle$ outside the superconductor), we find that the external field is screened in the superconductor ($z>0$) over a characteristic length λ_L,

$$\langle\mathbf{B}(z)\rangle = \mathbf{B}_{\text{ext}}\, e^{-z/\lambda_L}. \tag{3.231}$$

From Maxwell equation $\boldsymbol{\nabla}\times\langle\mathbf{B}\rangle = \mu_0\langle\mathbf{J}_\perp\rangle$, we deduce the existence of a current in a layer of width λ_L in the superconductor,

$$\langle\mathbf{J}_\perp(z)\rangle = -\frac{1}{\mu_0\lambda_L}\hat{\mathbf{z}}\times\mathbf{B}_{\text{ext}}\, e^{-z/\lambda_L}. \tag{3.232}$$

In the bulk of the superconductor ($z\gg\lambda_L$), the magnetic field is completely expelled. This perfect diamagnetism (Meissner effect) is the hallmark of a superconductor. We will see in Chap. 7 that long-range current-current correlations are at the root of superfluidity defined as the ability of a system to sustain a (dissipationless) superflow.

[28] Equation (3.228) is valid in the London limit where the superconducting coherence length ξ is much smaller than λ_L. In the (non local) Pippard limit $\xi\gg\lambda_L$, the $\mathbf{q}$ dependence of $\chi^R_\perp(\mathbf{q},0)$ cannot be neglected (Chap. 7).

[29] Equation (3.230) can also be obtained from the London equation (3.229) and the Maxwell equation $\boldsymbol{\nabla}\times\langle\mathbf{B}\rangle = \mu_0\langle\mathbf{J}_\perp\rangle$.

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Table 3.2: Drude weight D and superfluid weight D_s in a metal, an insulator and a superconductor.

	D	D_s
Metal	D	0
Insulator	0	0
Superconductor	D	D_s

3.4.5.3 Transverse conductivity and superfluid weight

The analog of (3.208) in the transverse case gives

$$\lim_{\mathbf{q}\to 0} \Re[\sigma_\perp(\mathbf{q},\omega)] = \lim_{\mathbf{q}\to 0} \mathcal{P}\frac{\chi''_\perp(\mathbf{q},\omega)}{\omega} + D_s\delta(\omega), \tag{3.233}$$

where

$$D_s = \pi \lim_{\mathbf{q}\to 0}\left[\frac{ne^2}{m} - \chi^R_\perp(\mathbf{q},0)\right] = \frac{\pi n_s e^2}{m} \tag{3.234}$$

is the superfluid weight. A superconductor is therefore characterized by a nonzero weight D_s of the zero-frequency delta peak in the transverse conductivity $\lim_{\mathbf{q}\to 0}\Re[\sigma_\perp(\mathbf{q},\omega)]$. Note the different order of the limits $\mathbf{q}\to 0$ and $\omega\to 0$ in the respective definitions of D and D_s. Equations (3.226) and (3.233) yield

$$\lim_{\mathbf{q}\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\Re[\sigma_\perp(\mathbf{q},\omega)] = \frac{1}{2}\lim_{\mathbf{q}\to 0}\chi^R_\perp(\mathbf{q},0) + \frac{D_s}{2\pi} = \frac{\epsilon_0}{2}\omega_p^2, \tag{3.235}$$

which is the $\mathbf{q}\to 0$ limit of the transverse-conductivity sum rule (3.179). The stability of the system implies $\Re[\sigma_\perp(\mathbf{q},\omega)]\geq 0$; the system can only absorb energy from the external field.[30] In particular, $D_s\geq 0$ and therefore $n_s\geq 0$. Furthermore the constraint $\chi^R_\perp(\mathbf{q},0)\geq 0$ together with the sum rule (3.235) gives $n_s\leq n$. In Chap. 7, we shall see that $n_s(T=0)=n$ in Galilean-invariant systems.

One can show that when there is a gap in the transverse excitation spectrum, D and D_s are equal. This is the case for instance in an s-wave superconductor where quasi-particle excitations are gapped while the Anderson-Bogoliubov mode appears in the longitudinal channel (Chap. 7). The same argument as that used to derive (3.217) gives

$$\lim_{\mathbf{q}\to 0}\lim_{\omega\to 0}\Re[\chi^R_\perp(\mathbf{q},\omega)] = \lim_{\omega\to 0}\lim_{\mathbf{q}\to 0}\Re[\chi^R_\perp(\mathbf{q},\omega)] = \lim_{\omega\to 0}\Re[\chi^R(0,\omega)] \tag{3.236}$$

and in turn $D_s = D$. The differences between a metal, an insulator and a superconductor are summarized in Table 3.2.

3.5 One-particle Green function

Apart from the correlation functions determining the linear response to external fields, such as the density-density or electromagnetic response functions discussed in Secs. 3.3 and 3.4,

[30] When the external perturbation is an electromagnetic field, the calculation of the dissipation in Sec. 3.2.2 must be modified to include the diamagnetic term (which is quadratic in the vector potential). It is not difficult to show that the dissipation is related to the real part of the conductivity and the stability of the system requires $\Re[\sigma_{\parallel,\perp}(\mathbf{q},\omega)]\geq 0$. On the other hand, the properties $\chi^R_{\parallel,\perp}(\mathbf{q},0)\geq 0$ follow from the definition of $\chi''_{\parallel,\perp}(\mathbf{q},\omega)$ (see Sec. 3.2.3).

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the one-particle Green function is the most important correlation function in a many-particle quantum system. On the one hand it is related to many observables (particle and current densities, mean kinetic energy, etc.). On the other hand it provides us with information about the propagation of an additional particle in the system and the possible existence of quasi-particle excitations, and can actually be measured in experiments where a single particle is injected into or extracted from the system. While the existence of quasi-particles in the case of fermions is discussed at length in Chap. 4 on Fermi-liquid theory, in the following we focus on the formal properties of the one-particle Green function.

3.5.1 Spectral function

The one-particle Green function is defined by

$$\begin{aligned} G_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau') &= -\langle T_\tau \hat{\psi}_\sigma(\mathbf{r},\tau)\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}',\tau')\rangle, \\ F_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau') &= -\langle T_\tau \hat{\psi}_\sigma(\mathbf{r},\tau)\hat{\psi}_{\sigma'}(\mathbf{r}',\tau')\rangle, \\ F^\dagger_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau') &= -\langle T_\tau \hat{\psi}^\dagger_\sigma(\mathbf{r},\tau)\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}',\tau')\rangle, \end{aligned} \tag{3.237}$$

where the anomalous Green functions F and $F^\dagger$ are nonzero if the global U(1) symmetry is broken, i.e. if the system is superfluid (Chap. 7). In the following we focus on the normal (non-superfluid) component G, assumed to be translation invariant and diagonal in the spin indices. We thus consider

$$G_\sigma(\mathbf{k}, i\omega_n) = \int_0^\beta d\tau \int d^d r\, e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_n\tau)} G_\sigma(\mathbf{r}-\mathbf{r}',\tau-\tau'). \tag{3.238}$$

The one-particle Green function $G_\sigma(\mathbf{k}, z)$, considered as a function of the complex frequency z, admits the spectral representation (3.33), i.e.

$$G_\sigma(\mathbf{k}, z) = \int_{-\infty}^{\infty} d\omega \frac{A_\sigma(\mathbf{k},\omega)}{z-\omega}, \tag{3.239}$$

where the spectral function is defined by

$$\begin{aligned} A_\sigma(\mathbf{k},t) &= \frac{1}{2\pi}\langle [\hat{\psi}_\sigma(\mathbf{k},t), \hat{\psi}^\dagger_\sigma(\mathbf{k},0)]_{-\zeta}\rangle, \\ A_\sigma(\mathbf{k},\omega) &= -\frac{1}{\pi}\Im[G^R_\sigma(\mathbf{k},\omega)]. \end{aligned} \tag{3.240}$$

The Matsubara Green function $G_\sigma(\mathbf{k}, i\omega_n)$ corresponds to $z = i\omega_n$ while the retarded and advanced correlation functions $G^{R,A}_\sigma(\mathbf{k},\omega)$ are obtained for $z = \omega \pm i\eta$ ($\eta \to 0^+$). The spectral function A_σ of the one-particle propagator is usually defined with a prefactor $-1/\pi$ as in (3.240) which explains why (3.239) slightly differs from (3.33). A_σ can be expressed in terms of a complete set $\{|n\rangle, \epsilon_n\}$ of eigenvectors of the (grand canonical) Hamiltonian (see, e.g., Eq. (3.37) or (3.70)),

$$A_\sigma(\mathbf{k},\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta\epsilon_n}(1-\zeta e^{-\beta\omega})|\langle n|\hat{\psi}_\sigma(\mathbf{k})|m\rangle|^2 \delta(\omega+\epsilon_n-\epsilon_m). \tag{3.241}$$

$A_\sigma(\mathbf{k},\omega)$ is positive for fermions ($\zeta=-1$) and has the sign of ω for bosons ($\zeta=1$).[31]

[31] The real-time Green function $G_\sigma(\mathbf{k},\omega) = -i\langle T\hat{\psi}_\sigma(\mathbf{k},t)\hat{\psi}^\dagger_\sigma(\mathbf{k},0)\rangle$ (that we do not discuss here) is given by $G_\sigma(\mathbf{k},\omega) = [1+\zeta n_\zeta(\omega)]G^R_\sigma(\mathbf{k},\omega) - \zeta n_\zeta(\omega) G^A(\mathbf{k},\omega)$ (see Sec. 3.2.7.2).

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For a non-interacting system, one simply has $G_0(\mathbf{k}, i\omega_n) = (i\omega_n - \xi_\mathbf{k})^{-1}$ (assuming the one-particle energy $\xi_\mathbf{k} = \epsilon_\mathbf{k} - \mu$ to be spin independent) and the spectral function $A_0(\mathbf{k}, \omega) = \delta(\omega - \xi_\mathbf{k})$ reduces to a Dirac function. In an interacting normal system, where the global U(1) symmetry is not broken ($F = F^\dagger = 0$), one usually expresses the Green function $G_\sigma(\mathbf{k}, z) = [z - \xi_\mathbf{k} - \Sigma_\sigma(\mathbf{k}, z)]^{-1}$ by introducing the self-energy $\Sigma_\sigma(\mathbf{k}, z)$ (Sec. 1.6.2) and the spectral function takes the form

$$A_\sigma(\mathbf{k}, \omega) = -\frac{1}{\pi} \frac{\Im[\Sigma^R_\sigma(\mathbf{k}, \omega)]}{(\omega - \xi_\mathbf{k} - \Re[\Sigma^R_\sigma(\mathbf{k}, \omega)])^2 + (\Im[\Sigma^R_\sigma(\mathbf{k}, \omega)])^2}, \tag{3.242}$$

where $\Sigma^R_\sigma(\mathbf{k}, \omega) = \Sigma_\sigma(\mathbf{k}, z = \omega + i\eta)$. The consequences of this equation for fermion systems are discussed at length in Chap. 4 in the context of Fermi-liquid theory. In superfluid systems, the self-energy has both normal and anomalous parts (see Eq. (3.252) below) and the expression of the spectral function is more complicated (Chaps. 7 and 13).

3.5.2 Analyticity properties

It follows from the spectral representation (3.239) that $G_\sigma(\mathbf{k}, z)$ is an analytic function of z when $\Im(z) \neq 0$ whereas $G^R_\sigma(\mathbf{k}, \omega)$ and $G^A_\sigma(\mathbf{k}, \omega)$ are analytic in the upper- and lower-half complex planes, respectively. $G^R_\sigma(\mathbf{k}, \omega)$ therefore satisfies the Kramers-Kronig relations (3.52). $G_\sigma(\mathbf{k}, z)$ is discontinuous across the real axis whenever the spectral function $A_\sigma(\mathbf{k}, \omega) = -[G_\sigma(\mathbf{k}, \omega + i\eta) - G_\sigma(\mathbf{k}, \omega - i\eta)]/(2i\pi)$ is nonzero.

The self-energy $\Sigma_\sigma(\mathbf{k}, z)$ inherits the analyticity properties of the Green function: It is analytic for $\Im(z) \neq 0$, the retarded part $\Sigma^R_\sigma(\mathbf{k}, \omega)$ is analytic in the upper-half complex plane and satisfies the Kramers-Kronig relations[32]

$$\begin{aligned} \Re[\Sigma^R_\sigma(\mathbf{k}, \omega) - \Sigma^R_\sigma(\mathbf{k}, \omega \to \infty)] &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Im[\Sigma^R_\sigma(\mathbf{k}, \omega')]}{\omega' - \omega}, \\ \Im[\Sigma^R_\sigma(\mathbf{k}, \omega)] &= -\mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\Re[\Sigma^R_\sigma(\mathbf{k}, \omega') - \Sigma^R_\sigma(\mathbf{k}, \omega \to \infty)]}{\omega' - \omega}. \end{aligned} \tag{3.243}$$

Furthermore the sign of the spectral function $A_\sigma(\mathbf{k}, \omega)$ implies $\Im[\Sigma^R_\sigma(\mathbf{k}, \omega)] \leq 0$ for fermions and $\operatorname{sgn}(\Im[\Sigma^R_\sigma(\mathbf{k}, \omega)]) = -\operatorname{sgn}(\omega)$ for bosons.

3.5.3 Sum rules and high-energy behavior

Sum rules are given by Eq. (3.63), i.e.

$$\int_{-\infty}^{\infty} d\omega\, \omega^n A_\sigma(\mathbf{k}, \omega) = \left\langle \Big[[\hat{\psi}_\sigma(\mathbf{k}), \hat{H}], \hat{H} \Big], \cdots, \hat{\psi}^\dagger_\sigma(\mathbf{k}) \Big]_{-\zeta} \right\rangle \tag{3.244}$$

($\hat{H}$ appears n times). For $n = 0$, one concludes that the spectral function is normalized to unity,

$$\int_{-\infty}^{\infty} d\omega\, A_\sigma(\mathbf{k}, \omega) = \langle [\hat{\psi}_\sigma(\mathbf{k}), \hat{\psi}^\dagger_\sigma(\mathbf{k})]_{-\zeta} \rangle = 1. \tag{3.245}$$

For $n = 1$, Eq. (3.244) gives

$$\int_{-\infty}^{\infty} d\omega\, \omega A_\sigma(\mathbf{k}, \omega) = \langle \big[[\hat{\psi}_\sigma(\mathbf{k}), \hat{H}], \hat{\psi}^\dagger_\sigma(\mathbf{k}) \big]_{-\zeta} \rangle. \tag{3.246}$$

[32] $\Sigma^R_\sigma(\mathbf{k}, \omega \to \infty)$ is real (see Sec. 3.5.3).

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We thus deduce the high-frequency behavior (see Eq. (3.64))

$$G_\sigma(\mathbf{k},z)=\frac{1}{z}+\frac{1}{z^2}\langle\big[[\hat\psi_\sigma(\mathbf{k}),\hat H],\hat\psi_\sigma^\dagger(\mathbf{k})\big]_{-\zeta}\rangle+\mathcal{O}\left(\frac{1}{z^3}\right). \tag{3.247}$$

For a normal (non-superfluid) system this leads in turn to the high-frequency limit of the self-energy,

$$\Sigma_\sigma(\mathbf{k},z)=-\xi_{\mathbf{k}}+\langle\big[[\hat\psi_\sigma(\mathbf{k}),\hat H],\hat\psi_\sigma^\dagger(\mathbf{k})\big]_{-\zeta}\rangle+\mathcal{O}\left(\frac{1}{z}\right). \tag{3.248}$$

As an example consider a spin-$\frac{1}{2}$ fermion system with Hamiltonian

$$\hat H=\sum_{\mathbf{k},\sigma}\xi_{\mathbf{k}}\hat\psi_\sigma^\dagger(\mathbf{k})\hat\psi_\sigma(\mathbf{k})+\frac{g}{2\mathcal{V}}\sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}}\hat\psi_\sigma^\dagger(\mathbf{k}+\mathbf{q})\hat\psi_{\sigma'}^\dagger(\mathbf{k}'-\mathbf{q})\hat\psi_{\sigma'}(\mathbf{k}')\hat\psi_\sigma(\mathbf{k}). \tag{3.249}$$

One easily obtains[33]

$$\lim_{|z|\to\infty}\Sigma_\sigma(\mathbf{k},z)=g\langle\hat\psi_{\bar\sigma}^\dagger(\mathbf{r})\hat\psi_{\bar\sigma}(\mathbf{r})\rangle=\frac{gn}{2} \tag{3.250}$$

(with the notation $\bar\sigma=-\sigma$), where the last result holds for a spin-rotation-invariant system (with n the mean particle density). For spin-zero bosons, one finds a similar expression,

$$\lim_{|z|\to\infty}\Sigma(\mathbf{k},z)=2g\langle\hat\psi^\dagger(\mathbf{r})\hat\psi(\mathbf{r})\rangle=2gn. \tag{3.251}$$

In both cases, spin-$\frac{1}{2}$ fermions and spin-zero bosons, the high-frequency limit of the self-energy is given by the Hartree-Fock result (i.e. the first-order self-consistent result). This result extends to the superfluid phase with broken global U(1) symmetry. For instance, for a superfluid boson system, the (connected) propagator is given by

$$\mathcal{G}^{-1}(\mathbf{k},i\omega_n)=\begin{pmatrix} i\omega+\mu-\epsilon_{\mathbf{k}}-\Sigma_{\rm n}(\mathbf{k},i\omega_n) & -\Sigma_{\rm an}(\mathbf{k},i\omega_n)\\ -\Sigma_{\rm an}^*(\mathbf{k},i\omega_n) & -i\omega+\mu-\epsilon_{\mathbf{k}}-\Sigma_{\rm n}(-\mathbf{k},-i\omega_n)\end{pmatrix}, \tag{3.252}$$

where $\mathcal{G}_{11}(\mathbf{k},i\omega_n)=-\langle\psi(\mathbf{k},i\omega_n)\psi^*(\mathbf{k},i\omega_n)\rangle_c$ and $\mathcal{G}_{12}(\mathbf{k},i\omega_n)=-\langle\psi(\mathbf{k},i\omega_n)\psi(-\mathbf{k},-i\omega_n)\rangle_c$ (Chap. 13). The high-frequency limit of the normal and anomalous self-energies $\Sigma_{\rm n}$ and $\Sigma_{\rm an}$ is given by [29]

$$\lim_{|z|\to\infty}\Sigma_{\rm n}(\mathbf{k},z)=2g\langle\hat\psi^\dagger(\mathbf{r})\hat\psi(\mathbf{r})\rangle,\qquad \lim_{|z|\to\infty}\Sigma_{\rm an}(\mathbf{k},z)=g\langle\hat\psi(\mathbf{r})^2\rangle. \tag{3.253}$$

3.5.4 Symmetry properties

The discussion of Sec. 3.2.1 about the symmetry properties of correlation functions applies to the one-particle Green function. As an example let us consider a s-wave superconductor (spin-$\frac{1}{2}$ fermion system) and the three Green functions defined in (3.237).

Invariance under parity implies

$$\begin{aligned} &G_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau';\Delta)=G_{\sigma\sigma'}(-\mathbf{r},\tau;-\mathbf{r}',\tau';\Delta),\\ \text{i.e.}\quad &G_{\sigma\sigma'}(\mathbf{k},i\omega_n;\Delta)=G_{\sigma\sigma'}(-\mathbf{k},i\omega_n;\Delta)\end{aligned} \tag{3.254}$$

in a translation-invariant system, and similar relations for F and $F^\dagger$. The notation emphasizes the fact that the Green function depends on the order parameter $\Delta\propto\langle\hat\psi_\downarrow(\mathbf{r})\hat\psi_\uparrow(\mathbf{r})\rangle$

[33] In the more general case of a momentum-dependent interaction $v(\mathbf{q})$: $\lim_{|z|\to\infty}\Sigma_\sigma(\mathbf{k},z)=v(\mathbf{q}=0)n-\int_{\mathbf{q}}v(\mathbf{q})\langle\hat\psi_\sigma^\dagger(\mathbf{k}+\mathbf{q})\hat\psi_\sigma(\mathbf{k}+\mathbf{q})\rangle$.

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(see Sec. 7.5.2), which is assumed here uniform and invariant under parity. Time-reversal invariance leads to (see Sec. 2.2.6)

$$\begin{aligned} G_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau';\Delta) &= \sigma\sigma' G_{\bar{\sigma}'\bar{\sigma}}(\mathbf{r}',-\tau';\mathbf{r},-\tau;\Delta^*), \\ F_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau';\Delta) &= \sigma\sigma' F^\dagger_{\bar{\sigma}'\bar{\sigma}}(\mathbf{r}',-\tau';\mathbf{r},-\tau;\Delta^*), \end{aligned} \tag{3.255}$$

i.e.

$$\begin{aligned} G_{\sigma\sigma'}(\mathbf{k},i\omega_n;\Delta) &= \sigma\sigma' G_{\bar{\sigma}'\bar{\sigma}}(-\mathbf{k},i\omega_n;\Delta^*), \\ F_{\sigma\sigma'}(\mathbf{k},i\omega_n;\Delta) &= \sigma\sigma' F^\dagger_{\bar{\sigma}'\bar{\sigma}}(-\mathbf{k},i\omega_n;\Delta^*). \end{aligned} \tag{3.256}$$

We have used the fact that $\Delta \to \Delta^*$ under time reversal.[34,35]

In systems that are spin-rotation invariant it is often convenient to write the one-particle Green function

$$\begin{aligned} G_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau') &= \frac{1}{2}\sigma^0_{\sigma\sigma'} G_{\rm ch}(\mathbf{r},\tau;\mathbf{r}',\tau') + \frac{1}{2}\boldsymbol{\sigma}_{\sigma\sigma'}\cdot\mathbf{G}_{\rm sp}(\mathbf{r},\tau;\mathbf{r}',\tau'), \\ F_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau') &= \frac{1}{2}(i\sigma^y)_{\sigma\sigma'} F_{\rm s}(\mathbf{r},\tau;\mathbf{r}',\tau') + \frac{1}{2}(i\boldsymbol{\sigma}\sigma^y)_{\sigma\sigma'}\cdot\mathbf{F}_{\rm t}(\mathbf{r},\tau;\mathbf{r}',\tau'), \\ F^\dagger_{\sigma\sigma'}(\mathbf{r},\tau;\mathbf{r}',\tau') &= \frac{1}{2}(i\sigma^y)^\dagger_{\sigma\sigma'} F^\dagger_{\rm s}(\mathbf{r},\tau;\mathbf{r}',\tau') + \frac{1}{2}(i\boldsymbol{\sigma}\sigma^y)^\dagger_{\sigma\sigma'}\cdot\mathbf{F}^\dagger_{\rm t}(\mathbf{r},\tau;\mathbf{r}',\tau') \end{aligned} \tag{3.257}$$

(σ^0 denotes the unit 2×2 matrix and $\boldsymbol{\sigma} = (\sigma^x,\sigma^y,\sigma^z)$ stands for the Pauli matrices) in terms of charge/spin and singlet/triplet components ($\mathbf{G}_{\rm sp} = (G^x_{\rm sp}, G^y_{\rm sp}, G^z_{\rm sp})$ and $\mathbf{F}^{(\dagger)}_{\rm t} = (F^{(\dagger)x}_{\rm t}, F^{(\dagger)y}_{\rm t}, F^{(\dagger)z}_{\rm t})$).

3.5.5 Relation to observables

Many physical observables can be related to the one-particle Green function.

3.5.5.1 One-body observable

Let us first consider a one-body operator

$$\hat{V}^{(1)} = \int d^d r \int d^d r' \sum_{\sigma,\sigma'} \langle \mathbf{r},\sigma|\hat{V}|\mathbf{r}',\sigma'\rangle \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_{\sigma'}(\mathbf{r}') \tag{3.258}$$

in second-quantized form (Sec. 1.2.2). Its expectation value can be written as

$$\begin{aligned} \langle\hat{V}^{(1)}\rangle &= -\zeta \int d^d r \int d^d r' \sum_{\sigma,\sigma'} \langle \mathbf{r},\sigma|\hat{V}|\mathbf{r}',\sigma'\rangle G_{\sigma'\sigma}(\mathbf{r}',\tau;\mathbf{r},\tau^+) \\ &= -\frac{\zeta}{\beta}\sum_{\omega_n} \int d^d r \int d^d r' \sum_{\sigma,\sigma'} \langle \mathbf{r},\sigma|\hat{V}|\mathbf{r}',\sigma'\rangle G_{\sigma'\sigma}(\mathbf{r}',\mathbf{r};i\omega_n) e^{i\omega_n\eta}. \end{aligned} \tag{3.259}$$

For the density operator

$$\hat{\jmath}^\nu_0(\mathbf{r}) = \sum_{\sigma,\sigma'} \hat{\psi}^\dagger_\sigma(\mathbf{r}) S^\nu_{\sigma\sigma'} \hat{\psi}_{\sigma'}(\mathbf{r}) \qquad (\nu = 0,x,y,\cdots), \tag{3.260}$$

[34] This follows from $(\langle\Psi|\hat{\Theta}^\dagger)\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})(\hat{\Theta}|\Psi\rangle) = \langle\Psi|\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})|\Psi\rangle^*$ for any ket $|\Psi\rangle$, where $\hat{\Theta}$ is the time-reversal operator introduced in Sec. 2.2.6.

[35] Equations (3.256) are satisfied by the Bardeen–Cooper–Shrieffer (BCS) correlation functions (7.244).

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one obtains

$$\langle \hat{j}_0^\nu(\mathbf{r})\rangle = -\zeta \sum_{\sigma,\sigma'} S^\nu_{\sigma\sigma'} G_{\sigma'\sigma}(\mathbf{r},\tau;\mathbf{r},\tau^+). \tag{3.261}$$

Here S^ν is the unit matrix if $\nu = 0$ and a spin matrix if $\nu \neq 0$ (e.g., for spin-$\frac{1}{2}$ fermions, $S^\nu = \frac{1}{2}\sigma^\nu$ with $\{\sigma^\nu\}$ the Pauli matrices). Similarly, for the current-density operator

$$\hat{j}_\mu^\nu(\mathbf{r}) = -\frac{i}{2m}\sum_{\sigma,\sigma'}[\hat{\psi}^\dagger_\sigma(\mathbf{r}) S^\nu_{\sigma\sigma'} \partial_\mu \hat{\psi}_{\sigma'}(\mathbf{r}) - \text{H.c.}] \qquad (\mu = x, y, \cdots), \tag{3.262}$$

one finds

$$\langle \hat{j}_\mu^\nu(\mathbf{r})\rangle = -\frac{\zeta}{m}\sum_{\sigma,\sigma'} S^\nu_{\sigma\sigma'} \lim_{\mathbf{r}'\to\mathbf{r}} \partial_\mu \Im[G_{\sigma'\sigma}(\mathbf{r},\tau;\mathbf{r}',\tau^+)]. \tag{3.263}$$

Finally the expectation value of the kinetic energy operator

$$\hat{T} = -\frac{1}{2m}\int d^d r \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r}) \boldsymbol{\nabla}^2 \hat{\psi}_\sigma(\mathbf{r}) \tag{3.264}$$

reads

$$\begin{aligned}\langle \hat{T}\rangle &= \frac{\zeta}{2m}\int d^d r \lim_{\mathbf{r}'\to\mathbf{r}} \sum_\sigma \boldsymbol{\nabla}^2 G_{\sigma\sigma}(\mathbf{r},\tau;\mathbf{r}',\tau^+) \\ &= -\frac{\zeta}{\beta\mathcal{V}} \sum_{\mathbf{k},\omega_n,\sigma} \epsilon_{\mathbf{k}} G_{\sigma\sigma}(\mathbf{k}, i\omega_n) e^{i\omega_n \eta},\end{aligned} \tag{3.265}$$

where $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m$.

3.5.5.2 Energy and thermodynamic potential

The expectation value of a two-body operator can be related to the two-particle Green function. In the case where the (grand canonical) Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ consists of the sum of $\hat{H}_0 = \hat{T} - \mu\hat{N}$ and a two-body interaction term,

$$\hat{V} = \frac{1}{2}\int d^d r \int d^d r' \sum_{\sigma_1\cdots\sigma_2'} v_{\sigma_1\sigma_2,\sigma_1'\sigma_2'}(\mathbf{r}-\mathbf{r}') \hat{\psi}^\dagger_{\sigma_1}(\mathbf{r}) \hat{\psi}^\dagger_{\sigma_2}(\mathbf{r}') \hat{\psi}_{\sigma_2'}(\mathbf{r}') \hat{\psi}_{\sigma_1'}(\mathbf{r}), \tag{3.266}$$

the expectation value $\langle \hat{V}\rangle$ can be expressed solely in terms of the one-particle Green function G. The equation of motion $\partial_\tau \hat{\psi}_\sigma(\mathbf{r},\tau) = [\hat{H}, \hat{\psi}_\sigma(\mathbf{r},\tau)]$ gives

$$\begin{aligned}\partial_\tau \hat{\psi}_\sigma(\mathbf{r},\tau) = &\left(\frac{\boldsymbol{\nabla}^2}{2m} + \mu\right)\hat{\psi}_\sigma(\mathbf{r},\tau) \\ &- \int d^d r'' \sum_{\sigma_1,\sigma_1',\sigma_2'} v_{\sigma_1\sigma,\sigma_1',\sigma_2'}(\mathbf{r}''-\mathbf{r}) \hat{\psi}^\dagger_{\sigma_1}(\mathbf{r}'',\tau) \hat{\psi}_{\sigma_1'}(\mathbf{r}'',\tau) \hat{\psi}_{\sigma_2'}(\mathbf{r},\tau).\end{aligned} \tag{3.267}$$

Multiplying from the left by $\hat{\psi}^\dagger_\sigma(\mathbf{r},\tau^+)$ and taking the expectation value, we obtain[36]

[36] We use $\langle \hat{\psi}^\dagger_\sigma(\mathbf{r}',\tau^+)\partial_\tau \hat{\psi}_\sigma(\mathbf{r},\tau)\rangle = -\zeta \lim_{\tau'\to\tau^+} \partial_\tau G_{\sigma\sigma}(\mathbf{r},\tau;\mathbf{r}',\tau')$, etc.

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$$\lim_{\substack{\mathbf{r}'\to\mathbf{r}\\ \tau'\to\tau^+}}\left(\partial_\tau-\mu-\frac{\boldsymbol{\nabla}^2}{2m}\right)G_{\sigma\sigma}(\mathbf{r},\tau;\mathbf{r}',\tau')=\zeta\int d^dr''\sum_{\sigma_1,\sigma_1',\sigma_2'}v_{\sigma_1\sigma,\sigma_1',\sigma_2'}(\mathbf{r}''-\mathbf{r})$$
$$\times\langle\hat\psi^\dagger_\sigma(\mathbf{r},\tau)\hat\psi^\dagger_{\sigma_1}(\mathbf{r}'',\tau)\hat\psi_{\sigma_1'}(\mathbf{r}'',\tau)\hat\psi_{\sigma_2'}(\mathbf{r},\tau)\rangle. \quad (3.268)$$

The last term in the rhs gives $2\zeta\langle\hat V\rangle$ (after summation over σ and $\mathbf{r}$) and we conclude that

$$\langle\hat V\rangle=\frac{\zeta}{2}\int d^dr\lim_{\substack{\mathbf{r}'\to\mathbf{r}\\ \tau'\to\tau^+}}\Big(\partial_\tau-\frac{\boldsymbol{\nabla}^2}{2m}-\mu\Big)\sum_\sigma G_{\sigma\sigma}(\mathbf{r},\tau;\mathbf{r}',\tau'). \quad (3.269)$$

The internal energy $E=\langle\hat T+\hat V\rangle=\langle\hat H_0+\mu\hat N+\hat V\rangle$ is therefore

$$E=\frac{\zeta}{2}\int d^dr\lim_{\substack{\mathbf{r}'\to\mathbf{r}\\ \tau'\to\tau^+}}\Big(\partial_\tau+\frac{\boldsymbol{\nabla}^2}{2m}-\mu\Big)\sum_\sigma G_{\sigma\sigma}(\mathbf{r},\tau;\mathbf{r}',\tau')$$
$$=-\frac{\zeta}{2\beta}\sum_{\mathbf{k},\omega_n}(i\omega_n+\mu+\epsilon_{\mathbf{k}})\sum_\sigma G_{\sigma\sigma}(\mathbf{k},i\omega_n)e^{i\omega_n\eta}. \quad (3.270)$$

The grand potential can now be obtained by means of an integration over a variable coupling constant considering the Hamiltonian

$$\hat H_\lambda=\hat H_0+\lambda\hat V. \quad (3.271)$$

To compute the thermodynamic potential $\Omega_\lambda=-\frac{1}{\beta}\ln Z_\lambda$, we consider the equation

$$\frac{\partial\Omega_\lambda}{\partial\lambda}=-\frac{1}{\beta Z_\lambda}\frac{\partial Z_\lambda}{\partial\lambda}\quad\text{where}\quad Z_\lambda=\mathrm{Tr}\big(e^{-\beta\hat H_\lambda}\big). \quad (3.272)$$

Using

$$\frac{\partial Z_\lambda}{\partial\lambda}=-\beta\mathrm{Tr}\bigg(e^{-\beta\hat H_\lambda}\frac{\hat H_\lambda}{\partial\lambda}\bigg), \quad (3.273)$$

one obtains the Hellmann-Feynman theorem (valid for any Hamiltonian $\hat H_\lambda$ depending on a continuous parameter λ),

$$\frac{\partial\Omega_\lambda}{\partial\lambda}=\left\langle\frac{\hat H_\lambda}{\partial\lambda}\right\rangle_\lambda, \quad (3.274)$$

where $\langle\cdots\rangle_\lambda$ denotes the ensemble average with $\hat H_\lambda$, which yields

$$\frac{\partial\Omega_\lambda}{\partial\lambda}=\langle\hat V\rangle_\lambda, \quad (3.275)$$

in the case of (3.271). Integrating (3.275) from $\lambda=0$ to $\lambda=1$ gives the thermodynamic potential $\Omega\equiv\Omega_{\lambda=1}$,

$$\Omega=\Omega_0+\int_0^1\frac{d\lambda}{\lambda}\langle\lambda\hat V\rangle_\lambda, \quad (3.276)$$

where Ω_0 is the thermodynamic potential for the Hamiltonian $\hat H_0$. From (3.269) we finally express

$$\Omega=\Omega_0+\frac{\zeta}{2}\int_0^1\frac{d\lambda}{\lambda}\int d^dr\lim_{\substack{\mathbf{r}'\to\mathbf{r}\\ \tau'\to\tau^+}}\Big(\partial_\tau-\frac{\boldsymbol{\nabla}^2}{2m}-\mu\Big)\sum_\sigma G^\lambda_{\sigma\sigma}(\mathbf{r},\tau;\mathbf{r}',\tau')$$

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$$= \Omega_0 - \frac{\zeta}{2}\int_0^1 \frac{d\lambda}{\lambda}\frac{1}{\beta}\sum_{\mathbf{k},\omega_n} G_0^{-1}(\mathbf{k},i\omega_n)\sum_\sigma G^\lambda_{\sigma\sigma}(\mathbf{k},i\omega_n)e^{i\omega_n\eta}, \tag{3.277}$$

in terms of the Green function $G^\lambda_{\sigma\sigma}$ of a system with Hamiltonian $\hat{H}_\lambda$.

3.6 Spontaneous symmetry breaking and Goldstone's theorem

Spontaneous symmetry breaking and the Goldstone theorem were discussed in Chap. 2. In this section, we reconsider these issues, but from a less formal point of view, using the general properties of correlation functions.[37] We first derive the Bogoliubov inequality which will be used in the subsequent sections.

3.6.1 The Bogoliubov inequality

We define the scalar product

$$\begin{aligned}\langle A|B\rangle = \chi_{A^\dagger B}(z=0) &= \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A^\dagger B}(\omega)}{\omega}\\ &= \frac{1}{Z}\sum_{\substack{n,m\\(\epsilon_n\neq\epsilon_m)}}\frac{e^{-\beta\epsilon_n}-e^{-\beta\epsilon_m}}{\epsilon_m-\epsilon_n}\langle n|\hat{A}^\dagger|m\rangle\langle m|\hat{B}|n\rangle\end{aligned} \tag{3.278}$$

for two operators $\hat{A}$ and $\hat{B}$ (not necessarily hermitian). The last line of (3.278) is the Lehmann representation (3.38) of $\chi_{A^\dagger B}(z=0)$. One readily verifies that this definition satisfies the basic properties of a scalar product: $\langle A|A\rangle \geq 0$, $\langle A|bB+cC\rangle = b\langle A|B\rangle + c\langle A|C\rangle$ (b, c complex numbers), and $\langle B|A\rangle = \langle A|B\rangle^*$. Therefore, the Schwarz inequality holds,

$$\langle A|A\rangle\langle B|B\rangle \geq |\langle A|B\rangle|^2. \tag{3.279}$$

More explicitly, Eq. (3.279) reads

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A^\dagger A}(\omega)}{\omega}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{B^\dagger B}(\omega)}{\omega} \geq \left|\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi''_{A^\dagger B}(\omega)}{\omega}\right|^2, \tag{3.280}$$

which is one form of the Bogoliubov inequality.

3.6.2 Spontaneous symmetry breaking

3.6.2.1 Example: the Heisenberg ferromagnet

Let us start with a simple example of broken symmetry, namely a three-dimensional isotropic Heisenberg ferromagnet with the Hamiltonian[38]

$$\hat{H} = -\frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} J_{\mathbf{r},\mathbf{r}'}\hat{\mathbf{S}}_\mathbf{r}\cdot\hat{\mathbf{S}}_{\mathbf{r}'}, \tag{3.281}$$

[37] Spontaneous symmetry breaking will also be discussed in Chap. 10.
[38] The Heisenberg (anti)ferromagnet is discussed in detail in Chap. 8.

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where $\mathbf{r}$ labels the sites of a lattice and $J_{\mathbf{r},\mathbf{r}'} \geq 0$ denotes the exchange interaction between spins located at sites $\mathbf{r}$ and $\mathbf{r}'$. The spin operators satisfy the commutation relations

$$[\hat{\mathbf{S}}^{\alpha}_{\mathbf{r}}, \hat{\mathbf{S}}^{\beta}_{\mathbf{r}'}] = i\delta_{\mathbf{r},\mathbf{r}'}\epsilon_{\alpha\beta\gamma}\hat{\mathbf{S}}^{\gamma}_{\mathbf{r}} \qquad (\alpha,\beta,\gamma = x,y,z). \tag{3.282}$$

The SU(2) spin-rotation invariance implies that the generator of spin rotations, $\hat{\mathbf{S}}_{\text{tot}} = \sum_{\mathbf{r}} \hat{\mathbf{S}}_{\mathbf{r}}$, commutes with the Hamiltonian: $[\hat{U}, \hat{H}] = 0$ where $\hat{U} = e^{-i\theta \hat{\mathbf{S}}_{\text{tot}}\cdot\mathbf{n}}$ with θ an arbitrary angle and $\mathbf{n}$ an arbitrary unit vector (see Sec. 2.2.3).

In the ferromagnetic state, spin-rotation invariance is spontaneously broken and the system exhibits a finite magnetization (assumed here to point in the z direction),

$$\langle \hat{\mathbf{S}}_{\text{tot}} \rangle = NM_0\hat{\mathbf{z}} \qquad (M_0 \neq 0), \tag{3.283}$$

where N is the number of lattice sites. Equation (3.283) implies that the density matrix cannot commute with $\hat{\mathbf{S}}_{\text{tot}}$. Indeed, using $[\hat{S}^x_{\text{tot}}, \hat{S}^y_{\text{tot}}] = i\hat{S}^z_{\text{tot}}$ and the cyclic invariance of the trace, we find

$$\langle \hat{S}^z_{\text{tot}} \rangle = -i\text{Tr}(\hat{\rho}[\hat{S}^x_{\text{tot}}, \hat{S}^y_{\text{tot}}]) = i\text{Tr}([\hat{\rho}, \hat{S}^y_{\text{tot}}]\hat{S}^x_{\text{tot}}) = -i\text{Tr}([\hat{\rho}, \hat{S}^x_{\text{tot}}]\hat{S}^y_{\text{tot}}), \tag{3.284}$$

and therefore

$$[\hat{\rho}, \hat{S}^x_{\text{tot}}] \neq 0, \qquad [\hat{\rho}, \hat{S}^y_{\text{tot}}] \neq 0 \tag{3.285}$$

when $\langle \hat{S}^z_{\text{tot}} \rangle \neq 0$. The canonical ensemble, where $\hat{\rho} \propto e^{-\beta\hat{H}}$, is no longer a good ensemble when the symmetry is spontaneously broken. This ensemble implies an average over all possible directions of the magnetization and inevitably gives $\langle \hat{\mathbf{S}}_{\text{tot}} \rangle = 0$, in contradiction with the assumption that the symmetry is spontaneously broken [Eq. (3.283)]. A possible way out of this difficulty is to assume the presence of an infinitesimal external magnetic field, i.e.

$$\hat{\rho}_h = \frac{e^{-\beta(\hat{H} - h\hat{S}^z_{\text{tot}})}}{\text{Tr}\, e^{-\beta(\hat{H} - h\hat{S}^z_{\text{tot}})}}. \tag{3.286}$$

In the ferromagnetic state, one then has

$$\lim_{h\to 0} \langle \hat{S}^z_{\text{tot}} \rangle = \lim_{h\to 0} \text{Tr}(\hat{\rho}_h \hat{S}^z_{\text{tot}}) \neq 0, \tag{3.287}$$

although $\text{Tr}(\hat{\rho}_{h=0}\hat{S}^z_{\text{tot}}) = 0$. As we shall see from many examples, it is rarely necessary to explicitly introduce a symmetry-breaking field. In general, the symmetry can be broken "by hand", e.g. by assuming a properly chosen operator to take a finite average value.

The expectation value $\langle \hat{\mathbf{S}}_{\text{tot}} \rangle$ (or, equivalently, $\langle \hat{\mathbf{S}}_{\mathbf{r}} \rangle$) allows to distinguish the ferromagnetic phase from the paramagnetic phase (where $\langle \hat{\mathbf{S}}_{\mathbf{r}} \rangle = 0$) and is referred to as the order parameter. A nonzero order parameter $\langle \hat{\mathbf{S}}_{\mathbf{r}} \rangle$ implies the existence of long-range order: The spin-spin correlation function

$$C(\mathbf{r},\mathbf{r}') = \langle \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'} \rangle \to \langle \hat{\mathbf{S}}_{\mathbf{r}} \rangle \cdot \langle \hat{\mathbf{S}}_{\mathbf{r}'} \rangle \neq 0 \tag{3.288}$$

does not vanish in the limit $|\mathbf{r} - \mathbf{r}'| \to \infty$. By contrast, in the paramagnetic phase, we expect the spin-spin correlation function $\langle \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'} \rangle \sim e^{-|\mathbf{r}-\mathbf{r}'|/\xi}$ to decay exponentially with distance (ξ is the correlation length).[39]

[39] In low-dimensional systems, it is possible for the correlation function to decay as a power law: $C(\mathbf{r},\mathbf{r}') \sim 1/|\mathbf{r} - \mathbf{r}'|^a$ with some exponent a. This is called algebraic long-range order or quasi-long-range order and is realized, for example, in the low-temperature phase of the two-dimensional XY model (Chap. 10).

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Let us now adiabatically apply a magnetic field in the x direction. This contributes to the Hamiltonian a term

$$\hat{H}'(t) = -\sum_{\mathbf{r}} h^x_{\mathbf{r}} \hat{S}^x_{\mathbf{r}} e^{\eta t} = -\sum_{\mathbf{q}} h^x_{-\mathbf{q}} \hat{S}^x_{\mathbf{q}} e^{\eta t} \qquad (\eta \to 0^+). \tag{3.289}$$

The magnetization is taken along the z axis for $t \to -\infty$. For a uniform field $h^x_{\mathbf{r}} = h^x$, we expect the magnetization $\langle \hat{\mathbf{S}}_{\rm tot} \rangle$ at time $t = 0$ to be in the x direction whatever the strength of the field, since all the ferromagnetic states with $|\langle \hat{\mathbf{S}}_{\rm tot} \rangle| = NM_0$ are degenerate. The linear response theory gives

$$\langle \hat{S}^x_{\mathbf{q}}(t=0) \rangle = \int_{-\infty}^{\infty} dt' \chi^R_{xx}(\mathbf{q}, -t') e^{\eta t'} h^x_{\mathbf{q}} = \chi_{xx}(\mathbf{q}) h^x_{\mathbf{q}}, \tag{3.290}$$

where $\chi_{xx}(\mathbf{q}) \equiv \chi_{S^x S^x}(\mathbf{q})$ is the static limit of the retarded response function [Eq. (3.44)]. Since $\lim_{\mathbf{q}\to 0} \langle \hat{S}^x_{\mathbf{q}}(t=0) \rangle = NM_0$ even when $h^x_{\mathbf{q}} \to 0$, (3.290) implies that the limit $\mathbf{q} \to 0$ of $\chi_{xx}(\mathbf{q})$ is singular,

$$\lim_{\mathbf{q}\to 0} \chi_{xx}(\mathbf{q}) = \infty. \tag{3.291}$$

A similar result holds for $\chi_{yy}(\mathbf{q})$. Both operators $\hat{S}^x$ and $\hat{S}^y$ being even under a parity transformation (Chap. 2), $\chi_{xx}(\mathbf{q})$ and $\chi_{yy}(\mathbf{q})$ are even in $\mathbf{q}$, and we expect $\chi_{xx}(\mathbf{q}), \chi_{yy}(\mathbf{q}) \sim 1/\mathbf{q}^2$ if we assume the divergence to be minimal.

The divergence of the transverse response functions $\chi_{xx}(\mathbf{q})$ and $\chi_{yy}(\mathbf{q})$ can also be derived using the Bogoliubov inequality. Taking the expectation value of $[\hat{S}^x_{\mathbf{r}}, \hat{S}^y_{\mathbf{r}'}] = i\delta_{\mathbf{r},\mathbf{r}'} \hat{S}^z_{\mathbf{r}}$ and summing over $\mathbf{r}$, we obtain

$$\chi''_{xy}(\mathbf{q} = 0, t = 0) = \frac{i}{2} M_0, \quad \text{i.e.} \quad \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \chi''_{xy}(\mathbf{q} = 0, \omega) = iM_0. \tag{3.292}$$

The Bogoliubov inequality (3.280) with $\hat{A}_{\mathbf{r}}(t) = \partial_t \hat{S}^x_{\mathbf{r}}(t)$ and $\hat{B}_{\mathbf{r}}(t) = \hat{S}^y_{\mathbf{r}}(t)$ gives

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{xx}(\mathbf{q}, \omega) \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\chi''_{yy}(\mathbf{q}, \omega)}{\omega} \geq \left| \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \chi''_{xy}(\mathbf{q}, \omega) \right|^2, \tag{3.293}$$

i.e.

$$\lim_{\mathbf{q}\to 0} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{xx}(\mathbf{q}, \omega) \chi_{yy}(\mathbf{q}) \geq M_0^2 \tag{3.294}$$

using (3.292). Since the total spin is conserved ($[\hat{\mathbf{S}}_{\rm tot}, \hat{H}] = 0$), the spin density obeys a continuity equation. In the long-wavelength limit, the lattice does not matter and the continuity equation takes the usual form

$$\partial_t \hat{S}^\nu_{\mathbf{r}}(t) + \boldsymbol{\nabla} \cdot \hat{\mathbf{j}}^\nu_{\mathbf{r}}(t) = 0 \tag{3.295}$$

(in the Heisenberg representation), where $\hat{\mathbf{j}}^\nu_{\mathbf{r}}$ is the spin current. From (3.295), we deduce

$$\omega^2 \chi''_{\nu\nu}(\mathbf{q}, \omega) = \sum_{\mu,\mu'} q_\mu q_{\mu'} \chi''_{j^\nu_\mu j^\nu_{\mu'}}(\mathbf{q}, \omega) = \mathcal{O}(\mathbf{q}^2), \tag{3.296}$$

and therefore

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{xx}(\mathbf{q}, \omega) = \mathcal{O}(\mathbf{q}^2). \tag{3.297}$$

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Equation (3.294) then implies that $\chi_{yy}(\mathbf{q})$ diverges at least as $1/\mathbf{q}^2$ in the limit $\mathbf{q} \to 0$. If we assume the divergence to be minimal, i.e. $\chi_{yy}(\mathbf{q}) \propto 1/\mathbf{q}^2$, we eventually obtain

$$\chi_{yy}(\mathbf{q}) = \chi_{xx}(\mathbf{q}) = \frac{M_0^2}{R\mathbf{q}^2} \qquad (\mathbf{q} \to 0), \tag{3.298}$$

where the "stiffness" (this terminology is explained below) R is bounded by

$$R \leq \lim_{\mathbf{q}\to 0} \frac{1}{\mathbf{q}^2} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{xx}(\mathbf{q}, \omega). \tag{3.299}$$

The bound in (3.299) can be shown to be finite if the exchange interactions are short-range, i.e. if $\sum_{\mathbf{r}'} J_{\mathbf{r},\mathbf{r}'} < \infty$ [19].

3.6.2.2 Spontaneous symmetry breaking

Although the ferromagnetic state exemplifies some aspects of spontaneous symmetry breaking – the existence of long-range order, the divergence of the transverse response function as well as the Goldstone theorem derived in Sec. 3.6.3 – it is a particular case to the extent where the order parameter operator $\hat{\mathbf{S}}_{\text{tot}} = \sum_{\mathbf{r}} \hat{\mathbf{S}}_{\mathbf{r}}$ commutes with the Hamiltonian. Any fully polarized state with all spins simultaneously pointing in the same direction is an eigenstate.[38] Even for a finite-size system, the ground state is therefore not unique. The actual ground state is selected by the infinitesimal applied field $\mathbf{h}$.

In the generic case however, the order parameter operator may not commute with the Hamiltonian and thus not be conserved. The ground state of a finite-size system is in general symmetric (i.e. does not break the symmetry) and unique. In the large-size limit, there are low-energy states that are symmetric and quasi-degenerate ($\Delta E \sim 1/\mathcal{V}$): They form a so-called tower of states. By taking a linear combination of these states, it is possible to construct non-symmetric states (i.e. exhibiting spontaneous symmetry breaking). For a finite volume $\mathcal{V}$, none of these non-symmetric states is an eigenstate of the Hamiltonian but their lifetimes diverge with $\mathcal{V}$. Thus in the thermodynamic limit the spontaneous-symmetry-breaking picture becomes valid.

The Heisenberg antiferromagnet falls in that category. It corresponds to the Hamiltonian (3.281) defined on a bipartite lattice with the exchange integrals $J_{\mathbf{r},\mathbf{r}'}$ being negative when $\mathbf{r}, \mathbf{r}'$ are nearest-neighbor sites and vanishing otherwise. The classical ground state is the Néel state with all spins on one sublattice pointing in a direction $\mathbf{n}$ and all spins on the other sublattice pointing in the opposite direction. The order parameter $\sum_{\mathbf{r}} (-1)^{\mathbf{r}} \langle \hat{\mathbf{S}}_{\mathbf{r}} \rangle$ corresponds to a staggered magnetization. Contrary to the ferromagnetic case, the classical state is not an eigenstate of the Hamiltonian.[38] Moreover, the ground state for an even finite number of sites N is unique and a spin singlet ($S_{\text{tot}} = 0$), i.e. rotationally invariant, which rules out symmetry breaking (Marshall's theorem). In the large-size limit, there is nevertheless a tower of symmetric states with $S_{\text{tot}} = 1, 2, ...$ The degeneracy of these states in the limit $N \to \infty$ can be used to construct a new set of eigenstates with a nonzero value of the staggered magnetization, and differing from one another by the direction of the latter.[40] As in the ferromagnetic case, the broken-symmetry picture requires a statistical ensemble where the density matrix does not commute with $\hat{\mathbf{S}}_{\text{tot}}$. Such a statistical ensemble can be defined by considering an infinitesimal staggered field $h_{\mathbf{r}} = (-1)^{\mathbf{r}} h$ (e.g. parallel to the z

[40] See also the discussion of spontaneous U(1) symmetry breaking in superfluids in Sec. 7.2.1.2.

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axis) that couples to the spins. Spontaneous symmetry breaking occurs if

$$\lim_{h\to 0}\lim_{N\to\infty}(-1)^{\mathbf{r}}\langle\hat{\mathbf{S}}_{\mathbf{r}}\rangle \neq 0. \tag{3.300}$$

We stress however that the classical Néel state is not the ground state because of quantum fluctuations that reduce the amplitude of the staggered magnetization.

As we shall see in the following chapters, spontaneous symmetry breaking includes many other examples: superfluids and superconductors, charge and magnetic instabilities in itinerant fermion systems, etc.

Long-range order without spontaneous symmetry breaking. In the thermodynamic limit, long-range order is a consequence of spontaneous symmetry breaking. In a finite system with a unique ground state, there cannot be spontaneous symmetry breaking for reasons discussed above but there can be long-range order, e.g.

$$\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty}\langle\hat{\mathbf{S}}_{\mathbf{r}}\cdot\hat{\mathbf{S}}_{\mathbf{r}'}\rangle \neq 0 \quad \text{and} \quad \langle\hat{\mathbf{S}}_{\mathbf{r}}\rangle = 0 \tag{3.301}$$

in the Heisenberg antiferromagnet. Such a state is however quite unnatural since it exhibits very large fluctuations of the Néel order parameter $\sum_{\mathbf{r}}(-1)^{\mathbf{r}}\langle\hat{\mathbf{S}}_{\mathbf{r}}\rangle$ (which is an extensive quantity) and therefore does not qualify as a macroscopic stable state. It also violates the cluster decomposition property which requires that

$$C_{ab}(\mathbf{r},\mathbf{r}') = \langle\hat{a}(\mathbf{r})\hat{b}(\mathbf{r}')\rangle - \langle\hat{a}(\mathbf{r})\rangle\langle\hat{b}(\mathbf{r}')\rangle \to 0 \quad \text{when} \quad |\mathbf{r}-\mathbf{r}'|\to\infty \tag{3.302}$$

for all local observables $\hat{a}(\mathbf{r})$ and $\hat{b}(\mathbf{r})$. In magnetic systems, states with long-range order without spontaneous symmetry breaking are never observed experimentally. A physically natural state with both long-range order and spontaneous symmetry breaking can be obtained, as explained above, from a linear combination of the quasi-degenerate states forming the low-energy tower of states. Although such a state is not an eigenstate of the Hamiltonian, it is expected to be stabilized by small symmetry-breaking perturbations that are inevitably present experimentally. This also explains why spontaneous symmetry breaking can occur in finite-size systems.

3.6.2.3 Classification of broken-symmetry states

A symmetry transformation g is represented by a unitary or antiunitary operator $\hat{U}(g)$ acting on the Hilbert space of state vectors (Chap. 2).[41] The set of all symmetry transformations forms a group G, e.g. the group SU(2) associated with spin rotations in the Heisenberg model. For simplicity we assume that $\hat{U}(g)$ is unitary and time independent and consider the zero-temperature limit.[42] Invariance of the system under the group G implies that $[\hat{H},\hat{U}(g)] = 0$ for all elements $g \in G$. Spontaneous symmetry breaking occurs when the ground state $|\psi\rangle$ of the system breaks some of the symmetries of the group G but is invariant under others: $|\psi\rangle$ and $\hat{U}(g)|\psi\rangle = e^{i\alpha}|\psi\rangle$ are equal (up to a phase) when g is unbroken but are distinct, inequivalent, states when g is broken. The set of all unbroken transformations forms a subgroup $H \subset G$ called the residual symmetry group.

Consider now the set of all states obtained from the ground state by applying the symmetry transformations of the group G. Two of these states, e.g. $\hat{U}(g_i)|\psi\rangle$ and $\hat{U}(g_j)|\psi\rangle$, are equivalent if there is an element h of H such that $g_i = g_j h$. Conversely, if $g_i \neq g_j h$ for all

[41] Note that we discuss here only global symmetries. Spontaneous breaking of a local symmetry is impossible (Elitzur's theorem [31]).

[42] We thus discard time-reversal symmetry and Galilean invariance.

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$h \in H$, $\hat{U}(g_i)|\psi\rangle$ and $\hat{U}(g_j)|\psi\rangle$ are distinct, inequivalent, states. This identifies the quotient set G/H as the set of inequivalent broken-symmetry states.

For the (anti)ferromagnetic Heisenberg model, the relevant symmetry transformations are spin rotations, i.e. $G = SU(2)$, and the residual symmetry group $H = U(1)$ corresponds to rotations about the axis $\mathbf{n}$ defining the direction of the (staggered) magnetization in the broken-symmetry state: $\hat{U}(\theta) = e^{-i\theta\hat{\mathbf{S}}\cdot\mathbf{n}}$. The quotient set $SU(2)/U(1)$ is isomorphic to the two-sphere S^2, which corresponds to the set of points on the surface of a sphere. These points indicate the direction of the residual rotation axis, i.e. the direction of the magnetization $\langle\mathbf{S}_\mathbf{r}\rangle$ (or $(-1)^\mathbf{r}\langle\mathbf{S}_\mathbf{r}\rangle$ in the antiferromagnetic case). A superfluid breaks the U(1) symmetry of the Hamiltonian and is characterized by a nonzero expectation value of the field operator $\hat{\psi}(\mathbf{r})$ (Chap. 7). Different ground states differ by the phase of the order parameter $\langle\hat{\psi}(\mathbf{r})\rangle$ but the modulus is the same. The residual symmetry group H is therefore the trivial group containing only the identity operator and the quotient space $G/H = U(1)$ is in one-to-one correspondence with the order parameter. These two examples exemplify a general result: Inequivalent broken-symmetry states can also be classified by the order parameter.[43]

For continuous groups, the symmetry operators $\hat{U}(g) = e^{i\sum_a \theta_a \hat{Q}_a}$ can be written in terms of the generators $\hat{Q}_a$. The system is invariant under the Lie group G if the Hamiltonian commutes with all generators: $[\hat{H}, \hat{Q}_a] = 0$. Symmetric states can be chosen to be also eigenstates of the generators. If the broken-symmetry state remains an eigenstate of $\hat{Q}_a$, it is invariant under the transformation $\hat{U}_a(\theta) = e^{i\theta\hat{Q}_a}$ and the generator is said to be unbroken. Generators that do not leave the state invariant are said to be broken. The dimension of the quotient space G/H is equal to the number of broken generators. In the (anti)ferromagnetic phase of the Heisenberg model one finds an unbroken generator, namely $\hat{S}^z_{\text{tot}}$ if the (staggered) magnetization points in the z direction, and two broken generators: $\hat{S}^x_{\text{tot}}$ and $\hat{S}^y_{\text{tot}}$.

3.6.3 Goldstone's theorem

Let us consider a system invariant under the transformations of a continuous group and denote by $\hat{Q}$ one of the generators with $\hat{\jmath}_0(\mathbf{r})$ the associated local density,

$$\hat{Q} = \int d^d r\, \hat{\jmath}_0(\mathbf{r}). \tag{3.303}$$

Since $\hat{Q}$ commutes with the Hamiltonian, the density $\hat{\jmath}_0(\mathbf{r}, t)$ in the Heisenberg representation satisfies a continuity equation,

$$\partial_t \hat{\jmath}_0(\mathbf{r}, t) + \boldsymbol{\nabla}\cdot\hat{\mathbf{j}}(\mathbf{r}, t) = 0. \tag{3.304}$$

Let us now suppose that we have identified two local observables[44] $\hat{A}(\mathbf{r})$ and $\hat{B}(\mathbf{r})$ such that $\hat{A}(\mathbf{r})$ transforms into $\hat{B}(\mathbf{r})$ under the symmetry transformation generated by $\hat{Q}$,[45]

$$\hat{B}(\mathbf{r}) = -i[\hat{Q}, \hat{A}(\mathbf{r})]. \tag{3.305}$$

[43] The order parameter does not necessarily distinguish between the different broken-symmetry states. There is however some freedom in its definition and it turns out that it is always possible to find an order parameter which is in one-to-one correspondence with the quotient space G/H.

[44] Although we now assume $\hat{A}(\mathbf{r})$ and $\hat{B}(\mathbf{r})$ to be Hermitian, this condition can easily be relaxed.

[45] Equation (3.305) simply follows from $\hat{A}(\mathbf{r}) \to \hat{U}^\dagger(\theta)\hat{A}(\mathbf{r})\hat{U}(\theta) = \hat{A}(\mathbf{r}) - i[\hat{Q}, \hat{A}(\mathbf{r})]\theta + \mathcal{O}(\theta^2)$ with $\hat{U}(\theta) = e^{i\theta\hat{Q}}$.

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This equation implies

$$\langle \hat{B}(\mathbf{r})\rangle = -i\mathrm{Tr}\{\hat{\rho}[\hat{Q},\hat{A}(\mathbf{r})]\} = -i\mathrm{Tr}\{[\hat{\rho},\hat{Q}]\hat{A}(\mathbf{r})\}. \tag{3.306}$$

If $\langle \hat{B}(\mathbf{r})\rangle \neq 0$ then $[\hat{\rho},\hat{Q}] \neq 0$: The symmetry is spontaneously broken and $\langle \hat{B}(\mathbf{r})\rangle$ is nothing but the order parameter. $\hat{A}(\mathbf{r})$ is referred to as the interpolating operator (or field) or the symmetry-restoring variable. From Eqs. (3.303) and (3.305), we then deduce

$$-i\int d^d r' \langle [\hat{\jmath}_0(\mathbf{r}',t),\hat{A}(\mathbf{r})]\rangle = \langle \hat{B}(\mathbf{r})\rangle \equiv \langle \hat{B}\rangle, \tag{3.307}$$

where for simplicity we assume that $\langle \hat{B}(\mathbf{r})\rangle \equiv \langle \hat{B}\rangle$ is uniform and does not break translation invariance.[46] The time t in (3.307) is arbitrary since $\hat{Q}(t) = \hat{Q}$ is conserved. We thus obtain

$$\chi''_{j_0 A}(\mathbf{q}=0,\omega) = i\pi\langle \hat{B}\rangle\delta(\omega). \tag{3.308}$$

The apparent conflict between (3.308) and the general property $\chi''_{A_i A_j}(\omega=0)=0$ derived in Sec. 3.2.3 is resolved by noting that the latter holds in the (grand) canonical ensemble which is incompatible with spontaneous symmetry breaking. In the example of the ferromagnet discussed above, the density matrix ρ_h would lead to an equation similar to (3.308) but with $\delta(\omega)$ replaced by $\delta(\omega-\omega_h)$ and ω_h vanishing for $h\to 0$.

The spectral decomposition (3.37) shows that χ'' is related to the density of excitation energies of the physical system. Equation (3.308) can then be understood as showing that there are $\mathbf{q}=\omega=0$ "excitations". But these "excitations" are just other equivalent (degenerate) states, so that it appears that (3.308) does not carry much information. However, if we assume that the $\mathbf{q}\to 0$ limit is regular, we obtain

$$\lim_{\mathbf{q}\to 0}\chi''_{j_0 A}(\mathbf{q},\omega) = i\pi\langle \hat{B}\rangle\delta(\omega), \tag{3.309}$$

which implies the existence of excitations with energies $\omega_{\mathbf{q}}$ satisfying $\lim_{\mathbf{q}\to 0}\omega_{\mathbf{q}}=0$. This is the Goldstone theorem, first encountered in Chap. 2: The spontaneous breaking of a continuous symmetry implies the existence of a collective mode (Goldstone mode) whose energy $\omega_{\mathbf{q}}$ goes to zero when $\mathbf{q}\to 0$.[47,48]

It is possible to show that Eqs. (3.308) and (3.309) are equivalent when the interactions are short-range. Equation (3.308) is equivalent to

$$\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{j_0 A}(\mathbf{q}=0,\omega) = i\langle \hat{B}\rangle\delta_{n,0} \quad \text{for} \quad n\geq 0, \tag{3.310}$$

so that what we need to show is

$$\lim_{\mathbf{q}\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{j_0 A}(\mathbf{q},\omega) = \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^n\chi''_{j_0 A}(\mathbf{q}=0,\omega) \quad \text{for} \quad n\geq 0. \tag{3.311}$$

When $\hat{\jmath}_0(\mathbf{r})$ and $\hat{A}(\mathbf{r})$ are local operators which depend on degrees of freedom located in the vicinity of $\mathbf{r}$, the commutator $[\hat{\jmath}_0(\mathbf{r}),\hat{A}(\mathbf{r}')]$ should vanish when $\mathbf{r}$ and $\mathbf{r}'$ are sufficiently

[46] This includes the case where the system is invariant under a set of discrete translations.

[47] In the antiferromagnet, where $\langle \hat{B}_{\mathbf{r}}\rangle \equiv \langle \hat{S}^z_{\mathbf{r}}\rangle$ is not uniform, the energy of the collective mode vanishes for $\mathbf{q}\to\pm\mathbf{Q}$ as well as $\mathbf{q}\to 0$ (see Chap. 8).

[48] In high-energy physics, a mode whose energy vanishes as $\mathbf{q}\to 0$ is referred to as a massless mode since it corresponds to a massless particle. In statistical physics, such a mode is sometimes referred to as a soft mode.

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far away. We then expect $\chi''_{j_0 A}(\mathbf{r}, t; \mathbf{r}', t)$ to rapidly decay as $|\mathbf{r} - \mathbf{r}'| \to \infty$ and its Fourier transform $\chi''_{j_0 A}(\mathbf{q}, t = 0)$ to be regular in the limit $\mathbf{q} \to 0$. This proves (3.311) for $n = 0$. For $n = 1$, we have

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{j_0 A}(\mathbf{r} - \mathbf{r}', \omega) = \big\langle \big[[\hat{\jmath}_0(\mathbf{r}), \hat{H}], \hat{A}(\mathbf{r}') \big] \big\rangle$$
$$= \int d^d r'' \big\langle \big[[\hat{\jmath}_0(\mathbf{r}), \hat{\mathcal{H}}(\mathbf{r}'')], \hat{A}(\mathbf{r}') \big] \big\rangle, \tag{3.312}$$

where we have written the Hamiltonian $\hat{H}$ in terms of an energy density operator $\hat{\mathcal{H}}(\mathbf{r})$. If all interactions are short-range, then $\hat{\mathcal{H}}(\mathbf{r})$ is a local operator and the rhs of (3.312) is expected to rapidly vanish as $|\mathbf{r} - \mathbf{r}'| \to \infty$. This ensures that Eq. (3.311) is satisfied for $n = 1$. This argument is easily extended to $n \geq 2$.

The Goldstone theorem breaks down when interactions are long-range. For instance, a ferromagnetic spin system with sufficiently long-range interactions $J_{\mathbf{r},\mathbf{r}'} \geq 0$ [Eq. (3.281)] would not exhibit a gapless spin-wave mode.[49] Another example is provided by a charged superfluid where the long-range Coulomb interaction obliterates the Goldstone mode (see Chap. 7).

3.6.3.1 Number of Goldstone modes

One could naively expect the number of Goldstone modes to be equal to the number of broken generators. The example of the ferromagnet discussed above shows that this is not the case. Although there are two broken generators (e.g. $\hat{S}^x_{\rm tot}$ and $\hat{S}^y_{\rm tot}$ if the magnetization points in the z direction), the Heisenberg ferromagnet is known to have a single Goldstone mode with a quadratic dispersion law $\omega \sim \mathbf{q}^2$ (Chap. 8). By contrast the Heisenberg antiferromagnet has two Goldstone modes with a linear dispersion $\omega \sim |\mathbf{q}|$. In condensed-matter physics the situation is therefore more diverse than in relativistic systems where the Lorentz invariance ensures the existence of a Goldstone mode with a linear dispersion for each broken generator.

In the general case, for internal symmetries,[50] the number of Goldstone modes is given by

$$n_G = n_{BG} - \frac{1}{2} \operatorname{rank} M \tag{3.313}$$

where

$$n_{BG} = \dim(G/H) = \dim(G) - \dim(H) \tag{3.314}$$

is the number of broken generators and

$$M_{ab} = -\frac{i}{\mathcal{V}} \langle [\hat{Q}_a, \hat{Q}_b] \rangle = \frac{1}{\mathcal{V}} \sum_c f_{abc} \langle \hat{Q}_c \rangle \tag{3.315}$$

is the Watanabe-Brauner matrix (f_{abc} denotes the structure constants of the Lie group G). Here a and b label all broken symmetry generators so that M is a $n_{BG} \times n_{BG}$ matrix. When the state of the system is translation invariant, the matrix element (3.315) can be written as[51]

$$M_{ab} = -i \langle [\hat{Q}_a, \hat{\jmath}_{b,0}(\mathbf{r})] \rangle, \tag{3.316}$$

[49] A thorough derivation of the Goldstone theorem for Heisenberg spins is given by Lange [19].
[50] We briefly comment on the case of spacetime symmetries below.
[51] Equation (3.316) does not hold for the antiferromagnet.

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where $\hat{\jmath}_{b,0}$ is the local density associated with the generator $\hat{Q}_b$. The real antisymmetric matrix M can always be diagonalized by an orthogonal matrix into the following form,

$$\begin{pmatrix} \bar{M}_1 & & & & & \\ & \ddots & & & & \\ & & \bar{M}_m & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix} \quad \text{with} \quad \bar{M}_i = \begin{pmatrix} 0 & \lambda_i \\ -\lambda_i & 0 \end{pmatrix}, \tag{3.317}$$

where all blank entries are zero and the λ_i's are nonzero. We thus get $\operatorname{rank} M = 2m$ and the rhs of (3.313) is an integer. The form (3.317) of the matrix M suggests that we can distinguish two types of Goldstone modes. To each pair $(\hat{Q}_{2l-1}, \hat{Q}_{2l})$ $(l = 1, 2, \cdots, m)$ of broken generators, we associate a type-B mode. The remaining broken generators correspond to type-A modes. Equation (3.313) is equivalent to

$$n_G = n_A + n_B \quad \text{with} \quad \begin{cases} n_B = \frac{1}{2} \operatorname{rank} M, \\ n_A = n_{BG} - 2n_B. \end{cases} \tag{3.318}$$

To understand why the pair $(\hat{Q}_{2l-1}, \hat{Q}_{2l})$ $(l = 1, 2, \cdots, m)$ leads to a single (type-B) Goldstone mode, let us consider the explicit form of the spectral function

$$\begin{aligned} \chi''_{j_{a,0}A}(\mathbf{q}, \omega) = \pi \sum_{n \neq 0} \big[& \langle \psi | \hat{\jmath}_{a,0}(\mathbf{q}) | n \rangle \langle n | \hat{A}(-\mathbf{q}) | \psi \rangle \delta(\omega + \epsilon_0 - \epsilon_n) \\ & - \langle \psi | \hat{A}(\mathbf{q}) | n \rangle \langle n | \hat{\jmath}_{a,0}(-\mathbf{q}) | \psi \rangle \delta(\omega + \epsilon_n - \epsilon_0) \big] \end{aligned} \tag{3.319}$$

in the zero-temperature limit, where $\{|n\rangle, \epsilon_n\}$ denotes a complete set of eigenstates of the Hamiltonian with $|0\rangle \equiv |\psi\rangle$ the ground state and $\hat{A}(\mathbf{r})$ is the interpolating operator. Since $\chi''_{j_{a,0}A}(\mathbf{q}, \omega) \sim \delta(\omega \pm \omega_{\mathbf{q}})$ with $\omega_{\mathbf{q}}$ the energy of the Goldstone mode, we see that the latter can be excited from the ground state by the operators $\hat{\jmath}_{a,0}$ or $\hat{A}$. A special case occurs when $\hat{A}(\mathbf{r})$ can be chosen as the density $\hat{\jmath}_{b,0}(\mathbf{r})$ associated with the broken generator $\hat{Q}_b$. Using (3.307) one then finds

$$-\frac{i}{\mathcal{V}} \langle [\hat{Q}_a, \hat{Q}_b] \rangle = -i \langle [\hat{Q}_a, \hat{\jmath}_{b,0}(\mathbf{r})] \rangle = \langle \hat{B} \rangle, \tag{3.320}$$

so that $\hat{Q}_a$ and $\hat{Q}_b$ form a pair of type-B generators. We therefore conclude that the pair $(\hat{Q}_{2l-1}, \hat{Q}_{2l})$ of generators excites the same (type-B) Goldstone mode, which leads to $n_B = m = \frac{1}{2} \operatorname{rank} M$.

A rigorous derivation of (3.313) is beyond the scope of our discussion but further insight can be gained by examining the most general action allowed by the symmetries in terms of the field $\Pi_a(\mathbf{r}, t)$ associated with the broken generators $\hat{Q}_a$.[52] To second order in a derivative expansion, the Lagrangian density reads

$$\mathcal{L}_{\text{eff}} = \sum_{a,b} \left\{ \frac{1}{2} m_{ab} (\Pi_a \partial_t \Pi_b - \Pi_b \partial_t \Pi_a) + \frac{1}{2} \bar{g}_{ab} \partial_t \Pi_a \partial_t \Pi_b - \frac{1}{2} g_{ab} \boldsymbol{\nabla} \Pi_a \cdot \boldsymbol{\nabla} \Pi_b \right\} \tag{3.321}$$

[52] The fields $\Pi_a(\mathbf{r}, t)$ can be defined by writing the Wigner operator of a global symmetry transformation as $\hat{U}(\{\Pi_a\}) = e^{i \sum_a \Pi_a \hat{Q}_a}$ and promoting the real variables Π_a to space- and time-dependent fields.

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assuming space to be isotropic (which forbids a linear terms in gradient). The key point of the derivation of (3.313) is that the coefficients m_{ab} coincide with the matrix elements M_{ab} of the Watanabe-Brauner matrix (3.315) [24]. It is now easy to find the collective modes from the equations of motion derived from $\mathcal{L}_{\rm eff}$. When $m_{ab} \neq 0$, the first-order time-derivative term in (3.321) dominates over the second-order one in the low-energy limit. The two fields Π_a and Π_b can then be considered as conjugate fields (in the low-energy sector) and describe the same degrees of freedom; as a result they produce a single (type-B) Goldstone mode with quadratic dispersion $\omega \sim \mathbf{q}^2$. When both m_{ab} and $\bar{g}_{ab}$ are nonzero, a gapped partner to the type-B Goldstone mode may exist with a mass of the order $m_{ab}/\sqrt{\bar{g}_{aa}\bar{g}_{bb}}$ (this conclusion may however be beyond the validity of the derivative expansion). The remaining $n_A = n_{BG} - n_B$ fields produce n_A modes with a linear dispersion $\omega \sim |\mathbf{q}|$.[53]

We thus reproduce the known results in the Heisenberg model mentioned above. In the ferromagnet, the two broken generators are $\hat{S}^x_{\rm tot}$ and $\hat{S}^y_{\rm tot}$. Since $\langle[\hat{S}^x_{\rm tot}, \hat{S}^y_{\rm tot}]\rangle = i\langle \hat{S}^z_{\rm tot}\rangle$, the off-diagonal elements of the 2×2 Watanabe-Brauner matrix do not vanish. There is a single, type-B, Goldstone mode with quadratic dispersion ($n_B = 1$ and $n_A = 0$). In the antiferromagnet, $\langle \hat{S}^z_{\rm tot}\rangle = 0$ and $M_{ab} = 0$, so that one has two type-A Goldstone modes with linear dispersion ($n_A = 2$ and $n_B = 0$).

In a superfluid, the generator of the U(1) symmetry is the number of particles $\hat{N} = \int d^d r\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$ and the field operator $\hat{\psi}(\mathbf{r})$ acts as the order parameter.[54] Since there is a single generator, one has a type-A Goldstone mode with linear dispersion. The interpolating operator is the field operator.[55] The Goldstone mode can be seen as a phase mode or a density mode (phonon mode) since phase and density are conjugate variables (Chap. 7).

A crystal in d dimensions breaks the symmetries of space. There are d generators for translation and $\frac{1}{2}d(d-1)$ generators for rotations. The translation group being Abelian, the associated Goldstone modes (phonons or sound waves) are all type-A. Local rotations and local translations are not independent so that broken rotations do not lead to independent Goldstone modes in the crystal [23, 25].

The apparent absence of Goldstone modes due to rotation symmetry breaking in a crystal is a particular case of a general result for spacetime symmetries. When the local densities $\hat{\jmath}_{a,0}(\mathbf{r})$ and $\hat{\jmath}_{b,0}(\mathbf{r})$ associated with the broken generators $\hat{Q}_a$ and $\hat{Q}_b$ are not independent, the gapless modes due these two broken generators are not independent either and Eq. (3.313) does not give the correct number of Goldstone modes [25]. This also explains why in a superfluid the Goldstone mode associated with the spontaneous breaking of Galilean symmetry is redundant with phonons.

3.6.3.2 Stiffness

It is straightforward to extend Eq. (3.298) to the general case by using (3.309), the continuity equation (3.304), and the Bogoliubov inequality with the operators $\hat{A}(\mathbf{r}, t)$ and $\partial_t \hat{\jmath}_0(\mathbf{r}, t)$. Assuming that the divergence of $\chi_{AA}(\mathbf{q})$ is minimal ($\propto 1/\mathbf{q}^2$), this gives

$$\chi_{AA}(\mathbf{q}) = \frac{\langle \hat{B}\rangle^2}{R\mathbf{q}^2} \quad (\mathbf{q} \to 0), \qquad R \leq \lim_{\mathbf{q}\to 0} \frac{1}{\mathbf{q}^2} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega \chi''_{j_0 j_0}(\mathbf{q}, \omega). \tag{3.322}$$

[53] If for some reason $g_{ab} = 0$, one must include fourth-order space-derivative terms in the effective Lagrangian. One then finds the dispersion $\omega \sim |\mathbf{q}|^4$ for type-B modes and $\omega \sim \mathbf{q}^2$ for type-A modes.

[54] A similar analysis holds for superconductors where the order parameter is $\langle \hat{\psi}_{\mathbf{r}\downarrow}\hat{\psi}_{\mathbf{r}\uparrow}\rangle$ (see Sec. 7.5).

[55] $[\hat{N}, \hat{\psi}(\mathbf{r})] = \int d^d r' [\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}'), \hat{\psi}(\mathbf{r})] = -\hat{\psi}(\mathbf{r})$.

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One can generally show that the bound (3.322) is finite for systems with sufficiently short-range interactions.

R measures the stiffness of the system with respect to spatial variation of the observable $\langle\hat{A}(\mathbf{r})\rangle$. To see this, let us consider the Gibbs free energy $G[\langle\hat{A}\rangle]$. Using the results of Sec. 3.2.7, its variation can be written as

$$\Delta G[\langle\hat{A}\rangle] = \frac{1}{2}\sum_{\mathbf{q}}\langle\hat{A}(-\mathbf{q})\rangle\chi_{AA}^{-1}(\mathbf{q})\langle\hat{A}(\mathbf{q})\rangle = \frac{R}{2\langle\hat{B}\rangle^2}\int d^dr[\boldsymbol{\nabla}\langle\hat{A}(\mathbf{r})\rangle]^2 \tag{3.323}$$

to lowest order in $\boldsymbol{\nabla}\langle\hat{A}(\mathbf{r})\rangle$. The external field required to create the configuration $\langle\hat{A}(\mathbf{r})\rangle$ is given by $\delta G[\langle\hat{A}\rangle]/\delta\langle\hat{A}(\mathbf{r})\rangle$. Local variations of the expectation value of the symmetry-restoring variable $\langle\hat{A}(\mathbf{r})\rangle$ yield an elastic contribution to the Gibbs free energy with a stiffness constant $R/\langle\hat{B}\rangle^2$.

It can also be argued in many cases that R determines the stiffness with respect to both external perturbations and spontaneous fluctuations. Suppose we are able to integrate out all degrees of freedom but those related to the symmetry-restoring field. The simplest effective action describing (small) fluctuations of A about its equilibrium value reads

$$S_{\text{eff}}[A] = \frac{\rho}{2}\int_0^\beta d\tau\int d^dr\left\{[\boldsymbol{\nabla}A(\mathbf{r},\tau)]^2 + \frac{[\partial_\tau A(\mathbf{r},\tau)]^2}{c^2}\right\}. \tag{3.324}$$

when A corresponds to a type-A Goldstone mode. This action gives the imaginary-time response function

$$\chi_{AA}(\mathbf{q},i\omega_n) = \frac{\rho^{-1}}{\mathbf{q}^2+\omega_n^2/c^2}, \tag{3.325}$$

from which we deduce the existence of a gapless mode $\omega = c|\mathbf{q}|$. The parameter ρ in (3.324) determines the stiffness of the system with respect to spontaneous fluctuations. Comparing $\chi_{AA}(\mathbf{q},i\omega_n)$ [Eq. (3.325)] with $\chi_{AA}(\mathbf{q}) = \chi_{AA}(\mathbf{q},i\omega_n=0)$ [Eq. (3.322)], we deduce $\rho = R/\langle\hat{B}\rangle^2$.

3.6.4 Mermin-Wagner theorem

The Mermin-Wagner theorem states that in one and two dimensions a continuous symmetry cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions. Let us consider the local fluctuations

$$\left\langle\left(\hat{A}(\mathbf{r}) - \langle\hat{A}(\mathbf{r})\rangle\right)^2\right\rangle = \int_{\mathbf{q}}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}S_{AA}(\mathbf{q},\omega) \tag{3.326}$$

of the symmetry-restoring variable $\hat{A}(\mathbf{r})$. $S_{AA}(\mathbf{q},\omega)$ is the structure factor defined in (3.53). Using the fluctuation-dissipation theorem, we obtain

$$\begin{aligned}\left\langle\left(\hat{A}(\mathbf{r}) - \langle\hat{A}(\mathbf{r})\rangle\right)^2\right\rangle &= \int_{\mathbf{q}}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\left[\coth\left(\frac{\beta\omega}{2}\right)+1\right]\chi''_{AA}(\mathbf{q},\omega)\\ &\geq 2T\int_{\mathbf{q}}\chi_{AA}(\mathbf{q}).\end{aligned} \tag{3.327}$$

The last inequality follows from $|x|\coth|x| \geq 1$ and $\chi''_{AA}(\mathbf{q},-\omega) = -\chi''_{AA}(\mathbf{q},\omega)$. Using Eq. (3.322) we see that the integral in (3.327) behaves as

$$\frac{\langle\hat{B}\rangle^2}{R}\int_0|\mathbf{q}|^{d-3}d|\mathbf{q}| \tag{3.328}$$

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for small $\mathbf{q}$. While the integral (3.328) is finite for $d > 2$, it diverges logarithmically when $d = 2$ and more strongly for $d < 2$. Since the fluctuations of $\hat{A}(\mathbf{r})$ are necessarily bounded, we conclude that we must have $\langle \hat{B} \rangle = 0$ for $d \leq 2$ and $T > 0$. This conclusion holds only if R is finite, which is the case for sufficiently short-range interactions.

This result can also be obtained from a classical model starting from the free energy functional $F[A] = \frac{\rho}{2} \int d^d r [\boldsymbol{\nabla} A(\mathbf{r})]^2 = \frac{\rho}{2} \sum_{\mathbf{q}} \mathbf{q}^2 A(-\mathbf{q}) A(\mathbf{q})$ describing energy fluctuations due to deviations from the perfectly ordered state. By the equipartition theorem $\rho \mathbf{q}^2 \langle A(-\mathbf{q}) A(\mathbf{q}) \rangle \sim T$, so that the local fluctuations

$$\langle A(\mathbf{r})^2 \rangle = \int_{\mathbf{q}} \langle A(-\mathbf{q}) A(\mathbf{q}) \rangle \sim \int_{\mathbf{q}} \frac{T}{\rho \mathbf{q}^2} \tag{3.329}$$

diverge in dimension $d \leq 2$.

3.6.5 Quantum disorder at zero temperature

The Mermin-Wagner theorem emphasizes the role of classical fluctuations at finite temperature. In this section we show that fluctuations can also suppress long-range order in the ground state of a quantum system in low dimensions. For two operators $\hat{A}$ and $\hat{B}$, we define the scalar product

$$\langle A | B \rangle = \langle 0 | [\hat{A}^\dagger, \hat{B}]_+ | 0 \rangle, \tag{3.330}$$

where $|0\rangle$ is the ground state (assumed unique) of the system. The Schwarz inequality implies

$$\langle 0 | [\hat{A}^\dagger, \hat{A}]_+ | 0 \rangle \langle 0 | [\hat{B}^\dagger, \hat{B}]_+ | 0 \rangle \geq |\langle 0 | [\hat{A}^\dagger, \hat{B}]_+ | 0 \rangle|^2. \tag{3.331}$$

We now introduce the auxiliary operator $\hat{\tilde{B}}$ defined by

$$\langle n | \hat{\tilde{B}} | 0 \rangle = \langle n | \hat{B} | 0 \rangle, \qquad \langle 0 | \hat{\tilde{B}} | n \rangle = -\langle 0 | \hat{B} | n \rangle, \tag{3.332}$$

and therefore

$$\langle n | \hat{\tilde{B}}^\dagger | 0 \rangle = -\langle n | \hat{B}^\dagger | 0 \rangle, \qquad \langle 0 | \hat{\tilde{B}}^\dagger | n \rangle = \langle 0 | \hat{B}^\dagger | n \rangle, \tag{3.333}$$

where $\{|n\rangle\}$ denotes a complete set of states. Using

$$\langle 0 | [\hat{A}^\dagger, \hat{B}]_+ | 0 \rangle = \sum_n \big(\langle 0 | \hat{A}^\dagger | n \rangle \langle n | \hat{B} | 0 \rangle + \langle 0 | \hat{B} | n \rangle \langle n | \hat{A}^\dagger | 0 \rangle \big), \tag{3.334}$$

one straightforwardly finds

$$\begin{aligned} \langle 0 | [\hat{A}^\dagger, \hat{\tilde{B}}]_+ | 0 \rangle &= \langle 0 | [\hat{A}^\dagger, \hat{B}] | 0 \rangle, \\ \langle 0 | [\hat{\tilde{B}}^\dagger, \hat{\tilde{B}}]_+ | 0 \rangle &= \langle 0 | [\hat{B}^\dagger, \hat{B}]_+ | 0 \rangle. \end{aligned} \tag{3.335}$$

Applying Eq. (3.331) to $\hat{A}$ and $\hat{\tilde{B}}$ (instead of $\hat{A}$ and $\hat{B}$) thus gives

$$\langle 0 | [\hat{A}^\dagger, \hat{A}]_+ | 0 \rangle \langle 0 | [\hat{B}^\dagger, \hat{B}]_+ | 0 \rangle \geq |\langle 0 | [\hat{A}^\dagger, \hat{B}] | 0 \rangle|^2 \tag{3.336}$$

(note the commutator, instead of the anticommutator, in the rhs). Equation (3.336) can be used to show the absence of long-range order in the ground state of some one-dimensional quantum systems.[56]

[56] The ground state of some one-dimensional systems may exhibit long-range order. For example, the non-interacting Bose gas exhibits BEC (see below) and the ground state of a one-dimensional Bose fluid with sufficiently long-range interactions is a Wigner crystal with spontaneously broken translation invariance [28].

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3.6.5.1 Bose superfluid

As an example let us consider an interacting boson system. In three and two dimensions, a superfluid ground state is characterized by broken U(1) invariance and a non-vanishing value of $\langle\hat{\psi}(\mathbf{r})\rangle$, where $\hat{\psi}(\mathbf{r})$ is the annihilation boson operator.[57] With the operators

$$\begin{aligned}\hat{A} &= \hat{\psi}^\dagger(\mathbf{q}),\\ \hat{B} &= \hat{n}(-\mathbf{q}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{q}'}\hat{\psi}^\dagger(\mathbf{q}')\hat{\psi}(\mathbf{q}'-\mathbf{q}),\end{aligned} \tag{3.337}$$

Eq. (3.336) gives

$$2(2n_\mathbf{q}+1)\mathcal{S}(\mathbf{q}) \geq n_0 \quad \text{i.e.} \quad n_\mathbf{q} \geq \frac{n_0}{4\mathcal{S}(\mathbf{q})} - \frac{1}{2}, \tag{3.338}$$

where $n_\mathbf{q} = \langle\hat{\psi}^\dagger(\mathbf{q})\hat{\psi}(\mathbf{q})\rangle$ is the mean number of bosons with momentum $\mathbf{q}$, $n_0 = |\langle\hat{\psi}(\mathbf{r})\rangle|^2$ the condensate density[57] and $\mathcal{S}(\mathbf{q}) = \langle\hat{n}(\mathbf{q})\hat{n}(-\mathbf{q})\rangle$ the equal-time density-density correlation function (structure factor).[58]

Now we note that

$$\mathcal{S}(\mathbf{q}) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\mathcal{S}(\mathbf{q},\omega) \leq \frac{1}{2\pi}\left[\int_0^\infty d\omega\,\omega\mathcal{S}(\mathbf{q},\omega)\int_0^\infty d\omega\frac{\mathcal{S}(\mathbf{q},\omega)}{\omega}\right]^{1/2}, \tag{3.339}$$

which follows from the fact that at zero temperature $\mathcal{S}(\mathbf{q},\omega)$ is nonzero only when $\omega \geq 0$ and is then positive.[59] The first integral in the rhs of (3.339) can be calculated using the fluctuation-dissipation theorem (3.58) and the f-sum rule (3.106),[60]

$$\int_0^\infty d\omega\,\omega\mathcal{S}(\mathbf{q},\omega) = \int_{-\infty}^\infty d\omega\,\omega\chi''_{nn}(\mathbf{q},\omega) = \frac{\pi n\mathbf{q}^2}{m}, \tag{3.340}$$

with n the density of bosons. As for the second integral we obtain

$$\int_0^\infty d\omega\frac{\mathcal{S}(\mathbf{q},\omega)}{\omega} = \int_{-\infty}^\infty d\omega\frac{\chi''_{nn}(\mathbf{q},\omega)}{\omega} \equiv \pi n^2\kappa(\mathbf{q}), \tag{3.341}$$

where $\lim_{\mathbf{q}\to 0}\kappa(\mathbf{q})$ is nothing but the compressibility $\kappa = 1/nmc_s^2$ with c_s the sound velocity [Eq. (3.111)]. Thus, in the limit $\mathbf{q}\to 0$, Eq. (3.338) becomes

$$n_\mathbf{q} \geq \frac{n_0 mc_s}{2n|\mathbf{q}|} \qquad (\mathbf{q}\to 0). \tag{3.342}$$

Since the integral $\int_\mathbf{q} n_\mathbf{q} = n$ must be convergent, we conclude that BEC, i.e. $n_0 \neq 0$, is not possible in a one-dimensional Bose fluid. This conclusion does not hold for the ideal Bose gas since in this case the compressibility is infinite and c_s vanishes. Superfluidity in an interacting one-dimensional Bose fluid is nevertheless possible but without BEC (see Sec. 7.2.2.1 and Chap. 13).

[57] See Chaps. 7 and 13 for a discussion of superfluidity.
[58] We have used $\langle[\hat{\psi}(\mathbf{q}),\hat{n}(-\mathbf{q})]\rangle = \frac{1}{\sqrt{L}}\langle\hat{\psi}(\mathbf{q}=0)\rangle = \langle\hat{\psi}(\mathbf{r})\rangle$.
[59] This can be deduced from (3.55) or (3.58).
[60] We use $\chi''_{nn}(\mathbf{q},-\omega) = -\chi''_{nn}(\mathbf{q},\omega)$ [Eq. (3.101)].

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3.6.5.2 Quantum antiferromagnet

As a second example we consider a quantum antiferromagnet defined on a d-dimensional hypercubic lattice with order parameter

$$M_0 = \frac{1}{N}\sum_{\mathbf{r}} e^{i\mathbf{Q}\cdot\mathbf{r}}\langle \hat{S}^z_{\mathbf{r}}\rangle, \tag{3.343}$$

where $\mathbf{Q} = (\pi, \cdots, \pi)$, N is the number of lattice sites, and $\hat{\mathbf{S}}^2_{\mathbf{r}} = S(S+1)$. We consider the inequality (3.336) with operators

$$\begin{aligned} \hat{A} &= \hat{S}^+_{\mathbf{q}+\mathbf{Q}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{-i(\mathbf{q}+\mathbf{Q})\cdot\mathbf{r}}\hat{S}^+_{\mathbf{r}}, \\ \hat{B} &= \hat{S}^+_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}}\hat{S}^+_{\mathbf{r}}, \end{aligned} \tag{3.344}$$

where $\hat{S}^\pm_{\mathbf{r}} = \hat{S}^x_{\mathbf{r}} \pm \hat{S}^y_{\mathbf{r}} = (\hat{S}^\mp_{\mathbf{r}})^\dagger$. Using

$$\begin{aligned} \langle[\hat{S}^-_{-\mathbf{q}-\mathbf{Q}}, \hat{S}^+_{\mathbf{q}}]\rangle &= \frac{1}{N}\sum_{\mathbf{r}} e^{i\mathbf{Q}\cdot\mathbf{r}}\langle[\hat{S}^-_{\mathbf{r}}, \hat{S}^+_{\mathbf{r}}\rangle = -2M_0, \\ \langle[\hat{S}^-_{-\mathbf{q}}, \hat{S}^+_{\mathbf{q}}]_+\rangle &= 2\langle \hat{S}^x_{-\mathbf{q}}, \hat{S}^x_{\mathbf{q}} + \hat{S}^y_{-\mathbf{q}}, \hat{S}^y_{\mathbf{q}}\rangle = 2\mathcal{S}_\perp(\mathbf{q}), \end{aligned} \tag{3.345}$$

we obtain

$$\mathcal{S}_\perp(\mathbf{q}+\mathbf{Q})\mathcal{S}_\perp(\mathbf{q}) \geq M_0^2, \tag{3.346}$$

where $\mathcal{S}_\perp(\mathbf{q})$ is the transverse (equal-time) structure factor.

We can now use (3.339) with

$$\begin{aligned} \int_0^\infty d\omega \frac{\mathcal{S}_\perp(\mathbf{q},\omega)}{\omega} &= \int_{-\infty}^\infty d\omega \frac{\chi''_\perp(\mathbf{q},\omega)}{\omega} = \pi\chi_\perp(\mathbf{q}), \\ \int_0^\infty d\omega\, \omega\mathcal{S}_\perp(\mathbf{q},\omega) &= c^2_{\text{eff}}(\mathbf{q})\mathbf{q}^2 \int_0^\infty d\omega \frac{\mathcal{S}_\perp(\mathbf{q},\omega)}{\omega}, \end{aligned} \tag{3.347}$$

where $c_{\text{eff}}(\mathbf{q})$ is an effective spin-wave velocity and $\chi_\perp$ the transverse spin susceptibility,[61] which leads to

$$\mathcal{S}_\perp(\mathbf{q}+\mathbf{Q}) \geq \frac{2M_0^2}{\chi_\perp(\mathbf{q})c_{\text{eff}}(\mathbf{q})|\mathbf{q}|}. \tag{3.348}$$

Since the integral ($N \to \infty$)

$$\int_{\mathbf{q}} \mathcal{S}_\perp(\mathbf{q}) \equiv \frac{1}{N}\sum_{\mathbf{q}} \mathcal{S}_\perp(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{r}} \langle \hat{S}^{x\,2}_{\mathbf{r}} + \hat{S}^{y\,2}_{\mathbf{r}}\rangle \leq S(S+1) \tag{3.349}$$

over the first Brillouin zone is finite, we conclude that long-range antiferromagnetic order, i.e. $M_0 \neq 0$, is not possible in one dimension if $\chi_\perp(\mathbf{q})$ and $c_{\text{eff}}(\mathbf{q})$ are finite in the limit $\mathbf{q} \to 0$. There is no reason for $\lim_{\mathbf{q}\to 0}\chi_\perp(\mathbf{q})$ to be infinite since a uniform transverse field is expected to produce a nonzero restoring force in an antiferromagnet. In the Heisenberg model, one can obtain an explicit expression of $\int_0^\infty d\omega\, \omega\mathcal{S}_\perp(\mathbf{q},\omega) = \pi\chi_\perp(\mathbf{q})c^2_{\text{eff}}(\mathbf{q})\mathbf{q}^2$, which leads to a finite value of $c_{\text{eff}}(\mathbf{q})$ in the limit $\mathbf{q} \to 0$ [27].

[61] For a system with a spin-wave mode (with velocity c) as sole transverse mode at low energies, one would have $\chi''_\perp(\mathbf{q},\omega) \propto \delta(\omega - c|\mathbf{q}|) - \delta(\omega + c|\mathbf{q}|)$ and therefore $c_{\text{eff}}(\mathbf{q}) = c$.

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Guide to the bibliography

- Linear response theory is discussed in many textbooks [1–4].
- For the electromagnetic response of fermion systems, see Refs. [3–9]
- Properties of the one-particle Green function are discussed in [3, 9, 10].
- Spontaneous symmetry breaking and its consequences (Goldstone's theorem [20–22], etc.) are reviewed in [1, 14, 15]. The Mermin-Wagner theorem, also known as the Mermin-Wagner-Hohenberg theorem [11] or the Coleman-Mermin-Wagner theorem [12], is proven in Ref. [13].
- For the counting of Goldstone modes, see Refs. [23–26].
- Quantum disorder at zero temperature in one-dimensional systems is discussed in Ref. [27].

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