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Chapter 10

Linear Response of Quantum Systems

10.1 Response and Resonance

10.1.1 Forced damped oscillator

Consider a damped harmonic oscillator subjected to a time-dependent forcing:

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = f(t) \quad , \tag{10.1}$$

where γ is the damping rate ($\gamma > 0$) and ω_0 is the natural frequency in the absence of damping[1]. We adopt the following convention for the Fourier transform of a function $H(t)$:

$$H(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \hat{H}(\omega)\, e^{-i\omega t} \qquad , \qquad \hat{H}(\omega) = \int\limits_{-\infty}^{\infty} dt\, H(t)\, e^{+i\omega t} \quad . \tag{10.2}$$

Note that if $H(t)$ is a real function, then $\hat{H}(-\omega) = \hat{H}^*(\omega)$. In Fourier space, then, eqn. (10.1) becomes

$$(\omega_0^2 - 2i\gamma\omega - \omega^2)\, \hat{x}(\omega) = \hat{f}(\omega) \quad , \tag{10.3}$$

with the solution

$$\hat{x}(\omega) = \frac{\hat{f}(\omega)}{\omega_0^2 - 2i\gamma\omega - \omega^2} \equiv \hat{\chi}(\omega)\, \hat{f}(\omega) \tag{10.4}$$

where $\hat{\chi}(\omega)$ is the *susceptibility function*:

$$\hat{\chi}(\omega) = \frac{1}{\omega_0^2 - 2i\gamma\omega - \omega^2} = \frac{-1}{(\omega - \omega_+)(\omega - \omega_-)} \quad , \tag{10.5}$$

[1]Note that $f(t)$ has dimensions of acceleration.

with

$$\omega_\pm = -i\gamma \pm \sqrt{\omega_0^2 - \gamma^2} \quad . \tag{10.6}$$

The complete solution to (10.1) is then

$$x(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \frac{\hat{f}(\omega)\, e^{-i\omega t}}{\omega_0^2 - 2i\gamma\omega - \omega^2} + x_{\rm h}(t) \tag{10.7}$$

where $x_{\rm h}(t)$ is the homogeneous solution,

$$x_{\rm h}(t) = A_+ e^{-i\omega_+ t} + A_- e^{-i\omega_- t} \quad . \tag{10.8}$$

Since $\mathsf{Im}\,(\omega_\pm) < 0$, $x_{\rm h}(t)$ is a *transient* which decays in time. The coefficients $A_\pm$ may be chosen to satisfy initial conditions on $x(0)$ and $\dot{x}(0)$, but the system 'loses its memory' of these initial conditions after a finite time, and in steady state all that is left is the inhomogeneous piece, which is completely determined by the forcing.

In the time domain, we can write

$$x(t) = \int\limits_{-\infty}^{\infty} dt'\; \chi(t-t')\, f(t') \qquad , \qquad \chi(s) \equiv \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\; \hat{\chi}(\omega)\, e^{-i\omega s} \quad , \tag{10.9}$$

which brings us to a very important and sensible result:

Claim: The response is *causal*, *i.e.* $\chi(t-t') = 0$ when $t < t'$, provided that $\hat{\chi}(\omega)$ is analytic in the upper half plane of the variable ω.

Proof: Consider eqn. (10.9). Of $\hat{\chi}(\omega)$ is analytic in the upper half plane, then closing in the UHP we obtain $\chi(s<0) = 0$.

For our example (10.5), we close in the LHP for $s > 0$ and obtain

$$\begin{aligned} \chi(s>0) &= (-2\pi i) \sum_{\omega\,\in\,\mathsf{LHP}} \mathsf{Res}\left\{ \frac{1}{2\pi}\, \hat{\chi}(\omega)\, e^{-i\omega s} \right\} \\ &= \frac{ie^{-i\omega_+ s}}{\omega_+ - \omega_-} + \frac{ie^{-i\omega_- s}}{\omega_- - \omega_+} \quad , \end{aligned} \tag{10.10}$$

i.e.

$$\chi(s) = \begin{cases} \frac{e^{-\gamma s}}{\sqrt{\omega_0^2 - \gamma^2}} \, \sin\left(\sqrt{\omega_0^2 - \gamma^2}\right) \Theta(s) & \text{if } \omega_0^2 > \gamma^2 \\ \frac{e^{-\gamma s}}{\sqrt{\gamma^2 - \omega_0^2}} \, \sinh\left(\sqrt{\gamma^2 - \omega_0^2}\right) \Theta(s) & \text{if } \omega_0^2 < \gamma^2 \quad , \end{cases} \tag{10.11}$$

where $\Theta(s)$ is the step function: $\Theta(s \geqslant 0) = 1$, $\Theta(s < 0) = 0$. Causality simply means that events occuring after the time t cannot influence the state of the system at t. Note that, in general, $\chi(t)$ describes the time-dependent response to a δ-function impulse at $t = 0$.

10.1.2 Energy dissipation

How much work is done by the force $f(t)$? Since the power applied is $P(t) = f(t)\,\dot{x}(t)$, we have

$$\begin{aligned} P(t) &= f(t)\,\frac{d}{dt}\int\limits_{-\infty}^{\infty}\!dt'\int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\;\hat{\chi}(\omega)\,e^{-i\omega(t-t')}f(t') \\ &= f(t)\int\limits_{-\infty}^{\infty}\!dt'\int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\;(-i\omega)\,\hat{\chi}(\omega)\,e^{-i\omega(t-t')}f(t') \\ \Delta E &= \int\limits_{-\infty}^{\infty}\!dt\,P(t) = \int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,(-i\omega)\,\hat{\chi}(\omega)\,\big|\hat{f}(\omega)\big|^2 \quad . \end{aligned} \tag{10.12}$$

Separating $\hat{\chi}(\omega)$ into real and imaginary parts,

$$\hat{\chi}(\omega) = \hat{\chi}'(\omega) + i\hat{\chi}''(\omega) \quad , \tag{10.13}$$

we find for our example

$$\begin{aligned} \hat{\chi}'(\omega) &= \frac{\omega_0^2-\omega^2}{(\omega_0^2-\omega^2)^2+4\gamma^2\omega^2} = +\hat{\chi}'(-\omega) \\ \hat{\chi}''(\omega) &= \frac{2\gamma\omega}{(\omega_0^2-\omega^2)^2+4\gamma^2\omega^2} = -\hat{\chi}''(-\omega) \quad . \end{aligned} \tag{10.14}$$

The energy dissipated may now be written

$$\Delta E = \int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\,\hat{\chi}''(\omega)\,\big|\hat{f}(\omega)\big|^2 \quad . \tag{10.15}$$

The even function $\hat{\chi}'(\omega)$ is called the *reactive* part of the susceptibility; the odd function $\hat{\chi}''(\omega)$ is the *dissipative* part. When experimentalists measure a *lineshape*, they usually are referring to features in $\omega\,\hat{\chi}''(\omega)$, which describes the absorption rate as a function of driving frequency.

10.1.3 Kramers-Kronig relations

Let $\hat{\chi}(z)$ be a complex function of the complex variable z which is analytic in the upper half plane. Then the following integral must vanish,

$$\oint\limits_{\mathcal{C}}\frac{dz}{2\pi i}\,\frac{\hat{\chi}(z)}{z-\zeta} = 0 \quad , \tag{10.16}$$

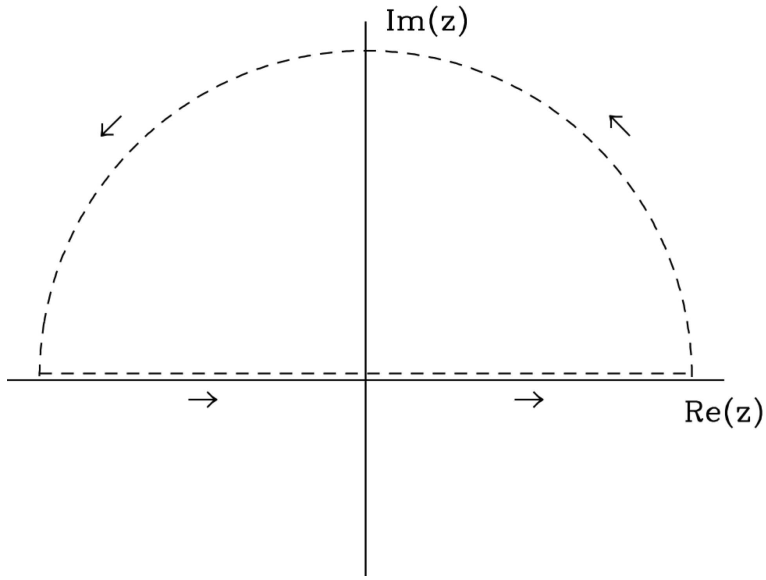

Figure 10.1: The complex integration contour $\mathcal{C}$.

whenever $\mathsf{Im}\,(\zeta) \leqslant 0$, where $\mathcal{C}$ is the contour depicted in fig. 10.1.

Now let $\omega \in \mathbb{R}$ be real, and define the complex function $\hat{\chi}(\omega)$ of the real variable ω by

$$\hat{\chi}(\omega) \equiv \lim_{\epsilon \to 0^+} \hat{\chi}(\omega + i\epsilon) \quad . \tag{10.17}$$

Assuming $\hat{\chi}(z)$ vanishes sufficiently rapidly that Jordan's lemma may be invoked (*i.e.* that the integral of $\hat{\chi}(z)$ along the arc of $\mathcal{C}$ vanishes), we have

$$\begin{aligned} 0 &= \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi i}\, \frac{\hat{\chi}(\nu)}{\nu - \omega + i\epsilon} \\ &= \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left[\hat{\chi}'(\nu) + i\hat{\chi}''(\nu)\right] \left[\frac{\mathcal{P}}{\nu - \omega} - i\pi\delta(\nu - \omega)\right] \end{aligned} \tag{10.18}$$

where $\mathcal{P}$ stands for 'principal part'. Taking the real and imaginary parts of this equation reveals the *Kramers-Kronig relations*:

$$\hat{\chi}'(\omega) = \mathcal{P}\!\int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi}\, \frac{\hat{\chi}''(\nu)}{\nu - \omega} \qquad , \qquad \hat{\chi}''(\omega) = -\mathcal{P}\!\int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi}\, \frac{\hat{\chi}'(\nu)}{\nu - \omega} \quad . \tag{10.19}$$

The Kramers-Kronig relations are valid for any function $\hat{\chi}(z)$ which is analytic in the upper half plane. If $\hat{\chi}(z)$ is analytic everywhere off the $\mathsf{Im}\,(z) = 0$ axis, we may write

$$\hat{\chi}(z) = \int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi}\, \frac{\hat{\chi}''(\nu)}{\nu - z} = -i\,\mathsf{sgn}(\mathsf{Im}\,z) \int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi}\, \frac{\hat{\chi}'(\nu)}{\nu - z} \quad . \tag{10.20}$$

This immediately yields the result

$$\lim_{\epsilon\to 0^+} \big[\hat{\chi}(\omega+i\epsilon) - \hat{\chi}(\omega-i\epsilon)\big] = 2i\,\hat{\chi}''(\omega) \quad . \tag{10.21}$$

As an example, consider the function

$$\hat{\chi}''(\omega) = \frac{\omega}{\omega^2+\gamma^2} \quad . \tag{10.22}$$

Then, choosing $\gamma > 0$,

$$\hat{\chi}(z) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{\pi}\,\frac{1}{\omega - z}\cdot\frac{\omega}{\omega^2+\gamma^2} = \begin{cases} +i/(z+i\gamma) & \text{if } \mathsf{Im}\,(z) > 0 \\ -i/(z-i\gamma) & \text{if } \mathsf{Im}\,(z) < 0 \end{cases} \quad . \tag{10.23}$$

Note that $\hat{\chi}(z)$ is separately analytic in the UHP and the LHP, but that there is a branch cut along the $\mathsf{Re}\,z$ axis, where $\hat{\chi}(\omega \pm i\epsilon) = \pm i/(\omega \pm i\gamma)$.

EXERCISE: Show that eqn. (10.21) is satisfied for $\hat{\chi}(\omega) = \omega/(\omega^2+\gamma^2)$.

If we *analytically continue* $\hat{\chi}(z)$ from the UHP into the LHP, we find a pole and no branch cut:

$$\tilde{\hat{\chi}}(z) = \frac{i}{z+i\gamma} \quad . \tag{10.24}$$

The pole lies in the LHP at $z = -i\gamma$.

10.2 Quantum Mechanical Response Functions

10.2.1 First order perturbation theory

Consider a time-dependent quantum system with Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1(t)$, where

$$\hat{H}_1(t) = -\sum_i \hat{Q}_i\,\phi_i(t) \quad , \tag{10.25}$$

where each $\hat{Q}_i$ is an operator labeled by an index i. In continuous systems, the operators may carry spatial labels as well, in which case we would write

$$\hat{H}(t) = \hat{H}_0 - \sum_i \int d^d x\,\hat{Q}_i(\boldsymbol{x})\,\phi_i(\boldsymbol{x},t) \quad . \tag{10.26}$$

The quantities $\phi_i(t)$ or $\phi_i(\boldsymbol{x},t)$ are spatiotemporally varying fields, such as a local scalar potential or local magnetic field. Some examples:

$$\hat{H}_1(t) = \begin{cases} -\hat{\boldsymbol{M}} \cdot \boldsymbol{B}(t) & \text{magnetic moment – magnetic field} \\ +\int d^3\!x\, \hat{\varrho}(\boldsymbol{x})\, \phi(\boldsymbol{x},t) & \text{charge density – scalar potential} \\ -\frac{1}{c} \int d^3\!x\, \hat{\boldsymbol{\jmath}}(\boldsymbol{x}) \cdot \boldsymbol{A}(\boldsymbol{x},t) & \text{electromagnetic current – vector potential} \end{cases} \tag{10.27}$$

Let's suppress for now the spatial label $\boldsymbol{x}$, which may be subsumed by the label i if we so desire. The time-dependent expectation value of the operator $\hat{Q}_i$ is given by

$$Q_i(t) \equiv \langle\, \Psi(t) \,|\, \hat{Q}_i \,|\, \Psi(t) \,\rangle \tag{10.28}$$

where $i\hbar\partial_t \,|\Psi(t)\rangle = \hat{H}(t)\,|\Psi(t)\rangle$. Without loss of generality, we may assume that the operators $\{\hat{Q}_i\}$ are each defined in such a way that $\langle \Psi_0 |\, \hat{Q}_i \,| \Psi_0 \rangle = 0$ for all i, where $|\Psi_0\rangle$ is the ground state of H_0, which itself is in general an interacting many-body Hamiltonian. We therefore expect that, to lowest nontrivial order in the fields $\{\phi_i\}$, that the observed response should be linear, *i.e.*

$$Q_i(t) = \int\limits_{-\infty}^{\infty} \!dt'\, \chi_{ij}(t-t')\, \phi_j(t') + \mathcal{O}(\phi^2) \quad . \tag{10.29}$$

The function $\chi_{ij}(t-t')$ is called a *response function*. It describes how the operator $\hat{Q}_i$ responds at time t to the imposition of a field ϕ_j at time t'. We presume that the responses are all causal, *i.e.* $\chi_{ij}(t-t') = 0$ for $t < t'$. To compute $\chi_{ij}(t-t')$, we will use first order perturbation theory to obtain $\big\langle \hat{Q}_i(t) \big\rangle$ and then functionally differentiate with respect to $\phi_j(t')$:

$$\chi_{ij}(t-t') = \frac{\delta \big\langle \hat{Q}_i(t) \big\rangle}{\delta \phi_j(t')} \bigg|_{\phi=0} \quad . \tag{10.30}$$

The first step is to establish the result,

$$|\, \Psi(t) \,\rangle = \hat{\mathcal{T}} \,\exp \left\{ -\frac{i}{\hbar} \int\limits_{t_0}^{t} \!dt' \,\Big[\hat{H}_0 + \hat{H}_1(t') \Big] \right\} |\, \Psi(t_0) \,\rangle \quad , \tag{10.31}$$

where $\hat{\mathcal{T}}$ is the *time ordering operator*, which places earlier times to the right. This is easily derived starting with the Schrödinger equation,

$$i\hbar \frac{d}{dt} \,|\, \Psi(t) \,\rangle = \hat{H}(t) |\, \Psi(t) \,\rangle \quad , \tag{10.32}$$

where $\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t)$. Integrating this equation from t to $t + \epsilon$ with infinitesimal ϵ gives

$$|\, \Psi(t+\epsilon) \,\rangle = \left(1 - \frac{i\epsilon}{\hbar}\, \hat{H}(t) \right) |\, \Psi(t) \,\rangle \quad . \tag{10.33}$$

Now let us integrate the Schrödinger equation from $t = t_1$ to $t = t_2$ where $t_1 < t_2$. We have

$$| \, \Psi(t_2) \, \rangle = \hat{U}(t_2, t_1) \, | \, \Psi(t_1) \, \rangle \tag{10.34}$$

where

$$\begin{aligned}\hat{U}(t_2, t_1) &= \lim_{N \to \infty} \bigg(1 - \frac{i\epsilon}{\hbar} \, \hat{H}\big(t_1 + (N-1)\epsilon\big)\bigg) \cdots \bigg(1 - \frac{i\epsilon}{\hbar} \, \hat{H}(t_1)\bigg) \\ &\equiv \hat{\mathcal{T}} \exp\Bigg\{ -\frac{i}{\hbar} \int\limits_{t_1}^{t_2} \! dt \, \hat{H}(t) \Bigg\} \quad ,\end{aligned} \tag{10.35}$$

where $\epsilon \equiv (t_2 - t_1)/N$. The operator $\hat{U}(t_2, t_1)$ is unitary operator (*i.e.* $\hat{U}^\dagger = \hat{U}^{-1}$), and is known as the *time evolution operator* between times t_1 and t_2.

EXERCISE: Show that, for $t_1 < t_2 < t_3$ that $\hat{U}(t_3, t_1) = \hat{U}(t_3, t_2) \, \hat{U}(t_2, t_1)$.

If $t_1 < t < t_2$, then differentiating $U(t_2, t_1)$ with respect to $\phi_i(t)$ yields

$$\frac{\delta \hat{U}(t_2, t_1)}{\delta \phi_j(t)} = \frac{i}{\hbar} \, \hat{U}(t_2, t) \, \hat{Q}_j \, \hat{U}(t, t_1) \quad , \tag{10.36}$$

since $\partial \hat{H}(t)/\partial \phi_j(t) = -\hat{Q}_j$. We may therefore write (assuming $t_0 < t, t'$)

$$\begin{aligned}\frac{\delta \, |\Psi(t)\rangle}{\delta \phi_j(t')}\bigg|_{\{\phi_i = 0\}} &= \frac{i}{\hbar} \, e^{-i\hat{H}_0 (t-t')/\hbar} \, \hat{Q}_j \, e^{-i\hat{H}_0 (t'-t_0)/\hbar} \, | \, \Psi(t_0) \, \rangle \, \Theta(t - t') \\ &= \frac{i}{\hbar} \, e^{-i\hat{H}_0 t/\hbar} \, \hat{Q}_j(t') \, e^{+i\hat{H}_0 \, t_0/\hbar} \, | \, \Psi(t_0) \, \rangle \, \Theta(t - t') \quad ,\end{aligned} \tag{10.37}$$

where

$$\hat{Q}_j(t) \equiv e^{i\hat{H}_0 t/\hbar} \, \hat{Q}_j \, e^{-i\hat{H}_0 t/\hbar} \tag{10.38}$$

is the operator Q_j in the time-dependent *interaction representation*. Finally, we have

$$\begin{aligned}\chi_{ij}(t - t') &= \frac{\delta}{\delta \phi_j(t')} \, \langle \, \Psi(t) \, | \, \hat{Q}_i \, | \, \Psi(t) \, \rangle = \frac{\delta \langle \Psi(t) |}{\delta \phi_j(t')} \, \hat{Q}_i \, |\Psi(t)\rangle + \langle \Psi(t) | \, \hat{Q}_i \, \frac{\delta |\Psi(t)\rangle}{\delta \phi_j(t')} \\ &= \bigg\{ -\frac{i}{\hbar} \, \langle \, \Psi(t_0) \, | \, e^{-i\hat{H}_0 \, t_0/\hbar} \, \hat{Q}_j(t') \, e^{+i\hat{H}_0 \, t/\hbar} \, \hat{Q}_i \, | \, \Psi(t) \, \rangle \\ &\qquad\qquad + \frac{i}{\hbar} \, \langle \, \Psi(t) \, | \, \hat{Q}_i \, e^{-i\hat{H}_0 \, t/\hbar} \, \hat{Q}_j(t') \, e^{+i\hat{H}_0 \, t_0/\hbar} \, | \, \Psi(t_0) \, \rangle \bigg\} \, \Theta(t - t') \\ &= \frac{i}{\hbar} \, \big\langle \big[\hat{Q}_i(t), \hat{Q}_j(t') \big] \big\rangle \, \Theta(t - t') \quad ,\end{aligned} \tag{10.39}$$

were averages are with respect to the wavefunction $|\,\widetilde{\Psi}_0\,\rangle \equiv \exp(i\hat{H}_0\,t_0/\hbar)\,|\,\Psi(t_0)\,\rangle$, where we take $t_0 \to -\infty$, or, at finite temperature, with respect to a Boltzmann-weighted distribution of such states. To reiterate,

$$\chi_{ij}(t-t') = \frac{i}{\hbar}\,\big\langle\big[\hat{Q}_i(t), \hat{Q}_j(t')\big]\big\rangle\,\Theta(t-t') \quad . \tag{10.40}$$

This is sometimes known as the *retarded* response function.

10.2.2 Spectral representation

We now derive an expression for the response functions in terms of the spectral properties of the Hamiltonian $\hat{H}_0$, which may describe a fully interacting system. Write $\hat{H}_0\,|\,n\,\rangle = E_n\,|\,n\,\rangle$, in which case[2]

$$\begin{aligned}\hat{\chi}_{ij}(\omega) &= \frac{i}{\hbar}\int\limits_0^\infty\! dt\; e^{i\omega t}\,\big\langle\big[\hat{Q}_i(t), \hat{Q}_j(0)\big]\big\rangle \\ &= \frac{i}{\hbar}\int\limits_0^\infty\! dt\; e^{i\omega t}\sum_{m,n} P_m\,\Big\{\langle\, m\,|\,\hat{Q}_i\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_j\,|\,m\,\rangle\, e^{+i(\omega_m-\omega_n)t} \\ &\qquad\qquad\qquad - \langle\, m\,|\,\hat{Q}_j\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_i\,|\,m\,\rangle\, e^{+i(\omega_n-\omega_m)t}\Big\} \quad ,\end{aligned} \tag{10.41}$$

where $\beta = 1/k_{\rm B}T$, $P_m = Z^{-1}\exp(-\beta E_m)$ the Boltzmann weight, with $Z = \mathsf{Tr}\,\exp(-\beta\hat{H}_0)$ the partition function, and the excitation frequencies are defined as $\omega_m \equiv (E_m - E_0)/\hbar$ where E_0 is the ground state energy of $\hat{H}_0$, which, recall, is the Hamiltonian of a fully interacting system. Regularizing the integrals at $t\to\infty$ with $\exp(-\epsilon t)$ with $\epsilon = 0^+$, we use

$$\int\limits_0^\infty\! dt\; e^{i(\omega-\Omega+i\epsilon)t} = \frac{i}{\omega - \Omega + i\epsilon} \tag{10.42}$$

to obtain the *spectral representation* of the (retarded) response function[3],

$$\hat{\chi}_{ij}(\omega+i\epsilon) = \frac{1}{\hbar}\sum_{m,n} P_m\,\left\{\frac{\langle\, m\,|\,\hat{Q}_j\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_i\,|\,m\,\rangle}{\omega - \omega_m + \omega_n + i\epsilon} - \frac{\langle\, m\,|\,\hat{Q}_i\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_j\,|\,m\,\rangle}{\omega + \omega_m - \omega_n + i\epsilon}\right\} \quad . \tag{10.43}$$

We will refer to this as $\hat{\chi}_{ij}(\omega)$, although formally $\hat{\chi}_{ij}(\omega)$ has poles or a branch cut (for continuous spectra) along the $\mathsf{Re}\,(\omega)$ axis. Note that $\hat{\chi}^*_{ij}(\omega) = \hat{\chi}_{ij}(-\omega)$, which also follows from the fact that

[2]Note that we are using hats to denote operators such as $\hat{H}$ and $\hat{\mathcal{T}}$ as well as Fourier transforms such as $\hat{\chi}_{ij}(\omega)$. Be alert and understand what all the hatted symbols mean!

[3]The spectral representation is sometimes known as the *Lehmann representation*.

$\chi_{ij}(t-t') \in \mathbb{R}$ is a real function of its argument. Diagrammatic perturbation theory does not give us $\hat{\chi}_{ij}(\omega)$, but rather the *time-ordered* response function,

$$\begin{aligned}\chi^{\mathrm{T}}_{ij}(t-t') &\equiv \frac{i}{\hbar}\,\big\langle \hat{\mathcal{T}}\,\hat{Q}_i(t)\,\hat{Q}_j(t')\big\rangle \\ &= \frac{i}{\hbar}\,\big\langle \hat{Q}_i(t)\,\hat{Q}_j(t')\big\rangle\,\Theta(t-t') + \frac{i}{\hbar}\,\big\langle \hat{Q}_j(t')\,\hat{Q}_i(t)\big\rangle\,\Theta(t'-t) \quad .\end{aligned}$$

The spectral representation of $\hat{\chi}^{\mathrm{T}}_{ij}(\omega)$ is

$$\hat{\chi}^{\mathrm{T}}_{ij}(\omega+i\epsilon) = \frac{1}{\hbar}\sum_{m,n} P_m \left\{ \frac{\langle\, m\,|\,\hat{Q}_j\,|\,n\,\rangle\langle\, n\,|\,\hat{Q}_i\,|\,m\,\rangle}{\omega-\omega_m+\omega_n-i\epsilon} - \frac{\langle\, m\,|\,\hat{Q}_i\,|\,n\,\rangle\langle\, n\,|\,\hat{Q}_j\,|\,m\,\rangle}{\omega+\omega_m-\omega_n+i\epsilon} \right\} \quad . \tag{10.44}$$

The difference between $\hat{\chi}_{ij}(\omega)$ and $\hat{\chi}^{\mathrm{T}}_{ij}(\omega)$ is thus only in the sign of the infinitesimal $\pm i\epsilon$ term in one of the denominators.

Let us now define the real and imaginary parts of the product of expectations values encountered above:

$$\langle\, m\,|\,\hat{Q}_i\,|\,n\,\rangle\langle\, n\,|\,\hat{Q}_j\,|\,m\,\rangle \equiv A_{mn}(ij) + iB_{mn}(ij) \quad . \tag{10.45}$$

That is[4],

$$\begin{aligned} A_{mn}(ij) &= \frac{1}{2}\,\langle\, m\,|\,\hat{Q}_i\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_j\,|\,m\,\rangle + \frac{1}{2}\,\langle\, m\,|\,\hat{Q}_j\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_i\,|\,m\,\rangle \\ B_{mn}(ij) &= \frac{1}{2i}\langle\, m\,|\,\hat{Q}_i\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_j\,|\,m\,\rangle - \frac{1}{2i}\langle\, m\,|\,\hat{Q}_j\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_i\,|\,m\,\rangle. \end{aligned} \tag{10.46}$$

Note that $A_{mn}(ij)$ is separately symmetric under interchange of either m and n, or of i and j, whereas $B_{mn}(ij)$ is separately antisymmetric under these operations:

$$\begin{aligned} A_{mn}(ij) &= +A_{nm}(ij) = A_{nm}(ji) = +A_{mn}(ji) \\ B_{mn}(ij) &= -B_{nm}(ij) = B_{nm}(ji) = -B_{mn}(ji) \quad . \end{aligned} \tag{10.47}$$

We define the *spectral densities*

$$\begin{Bmatrix} \varrho^{A}_{ij}(\omega) \\ \varrho^{B}_{ij}(\omega) \end{Bmatrix} \equiv \hbar^{-1}\sum_{m,n} P_m \begin{Bmatrix} A_{mn}(ij) \\ B_{mn}(ij) \end{Bmatrix} \delta(\omega-\omega_n+\omega_m) \quad , \tag{10.48}$$

which satisfy

$$\begin{aligned} \varrho^{A}_{ij}(\omega) &= +\varrho^{A}_{ji}(\omega) \quad , \quad \varrho^{A}_{ij}(-\omega) = +e^{-\beta\hbar\omega}\,\varrho^{A}_{ij}(\omega) \\ \varrho^{B}_{ij}(\omega) &= -\varrho^{B}_{ji}(\omega) \quad , \quad \varrho^{B}_{ij}(-\omega) = -e^{-\beta\hbar\omega}\,\varrho^{B}_{ij}(\omega) \quad . \end{aligned} \tag{10.49}$$

[4]We assume all the $\hat{Q}_i$ are Hermitian, *i.e.* $\hat{Q}_i = \hat{Q}_i^{\dagger}$.

In terms of these spectral densities,

$$\begin{aligned}
\hat{\chi}'_{ij}(\omega) &= \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\nu}{\nu^2-\omega^2}\, \varrho^A_{ij}(\nu) - \pi(1-e^{-\beta\hbar\omega})\, \varrho^B_{ij}(\omega) = +\hat{\chi}'_{ij}(-\omega) \\
\hat{\chi}''_{ij}(\omega) &= \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\omega}{\nu^2-\omega^2}\, \varrho^B_{ij}(\nu) + \pi(1-e^{-\beta\hbar\omega})\, \varrho^A_{ij}(\omega) = -\hat{\chi}''_{ij}(-\omega).
\end{aligned} \tag{10.50}$$

For the time ordered response functions, we find

$$\begin{aligned}
\hat{\chi}'^{\,\mathrm{T}}_{ij}(\omega) &= \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\nu}{\nu^2-\omega^2}\, \varrho^A_{ij}(\nu) - \pi(1+e^{-\beta\hbar\omega})\, \varrho^B_{ij}(\omega) \\
\hat{\chi}''^{\,\mathrm{T}}_{ij}(\omega) &= \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\omega}{\nu^2-\omega^2}\, \varrho^B_{ij}(\nu) + \pi(1+e^{-\beta\hbar\omega})\, \varrho^A_{ij}(\omega) \quad .
\end{aligned} \tag{10.51}$$

Hence, knowledge of either the retarded or the time-ordered response functions is sufficient to determine the full behavior of the other:

$$\hat{\chi}'_{ij}(\omega) = \frac{e^{\beta\hbar\omega}\,\hat{\chi}'^{\,\mathrm{T}}_{ij}(\omega)}{e^{\beta\hbar\omega}+1} + \frac{\hat{\chi}'^{\,\mathrm{T}}_{ji}(\omega)}{e^{\beta\hbar\omega}+1} \qquad , \qquad \hat{\chi}''_{ij}(\omega) = \frac{e^{\beta\hbar\omega}\,\hat{\chi}''^{\,\mathrm{T}}_{ij}(\omega)}{e^{\beta\hbar\omega}+1} - \frac{\hat{\chi}''^{\,\mathrm{T}}_{ji}(\omega)}{e^{\beta\hbar\omega}+1} \quad . \tag{10.52}$$

For the diagonal responses, with $i=j$, we then have

$$\hat{\chi}'_{jj}(\omega) = \hat{\chi}'^{\,\mathrm{T}}_{jj}(\omega) \qquad , \qquad \hat{\chi}''_{jj}(\omega) = \hat{\chi}''^{\,\mathrm{T}}_{jj}(\omega)\, \tanh(\tfrac{1}{2}\beta\hbar\omega) \quad . \tag{10.53}$$

10.2.3 Energy dissipation

The rate at which work is done by the external fields is the power dissipated, and is given by

$$\begin{aligned}
P(t) &= \frac{d}{dt}\,\langle\, \Psi(t)\,|\, \hat{H}_0 \,|\, \Psi(t)\,\rangle = -\frac{i}{\hbar}\,\langle\, \Psi(t)\,|\, [\hat{H}_0, \hat{H}_1(t)] \,|\, \Psi(t)\,\rangle \\
&= \frac{i}{\hbar}\sum_i \phi_i(t)\,\langle\, \Psi(t)\,|\, [\hat{H}_0, \hat{Q}_i] \,|\, \Psi(t)\,\rangle
\end{aligned} \tag{10.54}$$

Now recall $|\,\Psi(t)\,\rangle = \hat{U}(t,t_0)\,|\,\Psi(t_0)\,\rangle$, where we shall take $t_0 \to -\infty$. We will evaluate the power dissipated to quadratic order in the fields, and for this we need the expansion of the evolution operator $\hat{U}(t,t_0)$ to linear order in the fields, which is to say to linear order in the perturbation $\hat{H}_1$. From Eqn. 10.35 we have

$$\hat{U}(t,t_0) = \hat{U}_0(t,t_0) - \frac{i}{\hbar}\int\limits_{t_0}^{t} ds\, \hat{U}_0(t,s)\, \hat{H}_1(s)\, \hat{U}_0(s,t_0) + \ldots \tag{10.55}$$

where $\hat{U}_0(t_2,t_1)=e^{-i\hat{H}_0(t_2-t_1)/\hbar}$ and $\hat{H}_1(s)=-\sum_i \hat{Q}_i\,\phi_i(t)$. Thus, we have

$$\begin{aligned}
|\,\Psi(t)\,\rangle &= \hat{U}(t,t_0)\,|\,\Psi_0\,\rangle \\
&= e^{-i\hat{H}_0\,t/\hbar}\left\{1-\frac{i}{\hbar}\int\limits_{t_0}^{t}\!dt'\,e^{i\hat{H}_0\,t'/\hbar}\hat{H}_1(s)\,e^{-i\hat{H}_0\,t'/\hbar}+\ldots\right\}|\,\widetilde{\Psi}_0\,\rangle
\end{aligned} \tag{10.56}$$

Thus, to lowest nontrivial order in the fields,

$$\begin{aligned}
P(t) &= \frac{i}{\hbar}\sum_i \phi_i(t)\,\langle\,\Psi(t)\,|\,[\hat{H}_0,\hat{Q}_i]\,|\,\Psi(t)\,\rangle \\
&= -\frac{1}{\hbar^2}\sum_{i,j}\phi_i(t)\int\limits_{t_0}^{t}\!dt'\,\phi_j(t')\,\langle\,\widetilde{\Psi}_0\,|\,\big[[\hat{H}_0,\hat{Q}_i(t)],\hat{Q}_j(t')\big]\,|\,\widetilde{\Psi}_0\,\rangle \\
&= \frac{i}{\hbar}\sum_{i,j}\phi_i(t)\int\limits_{t_0}^{t}\!dt'\,\phi_j(t')\,\frac{d}{dt}\,\langle\,\widetilde{\Psi}_0\,|\,[\hat{Q}_i(t),\hat{Q}_j(t')]\,|\,\widetilde{\Psi}_0\,\rangle \\
&= \sum_{i,j}\phi_i(t)\int\limits_{-\infty}^{\infty}\!dt'\,\frac{d}{dt}\,\chi_{ij}(t-t')\,\phi_j(t') = \sum_i \phi_i(t)\,\frac{d\langle\hat{Q}_j(t)\rangle}{dt} \qquad .
\end{aligned} \tag{10.57}$$

The total energy dissipated is thus a functional of the external fields $\{\phi_i(t)\}$:

$$\begin{aligned}
W &= \int\limits_{-\infty}^{\infty}\!dt\,P(t) = -\int\limits_{-\infty}^{\infty}\!dt\int\limits_{-\infty}^{\infty}\!dt'\,\chi_{ij}(t-t')\,\dot{\phi}_i(t)\,\phi_j(t') \\
&= \int\limits_{-\infty}^{\infty}\!\frac{d\omega}{2\pi}\,(-i\omega)\,\hat{\phi}_i^*(\omega)\,\hat{\chi}_{ij}(\omega)\,\hat{\phi}_j(\omega) \quad ,
\end{aligned} \tag{10.58}$$

where we now adopt the convention that we sum on the repeated indices i and j. Since the $\{\hat{Q}_i\}$ are Hermitian observables, the $\{\phi_i(t)\}$ must be real fields, in which case their conjugates are given by $\hat{\phi}_i^*(\omega)=\hat{\phi}_j(-\omega)$, whence

$$\begin{aligned}
W &= \int\limits_{-\infty}^{\infty}\!\frac{d\omega}{4\pi}\,(-i\omega)\big[\hat{\chi}_{ij}(\omega)-\hat{\chi}_{ji}(-\omega)\big]\,\hat{\phi}_i^*(\omega)\,\hat{\phi}_j(\omega) \\
&= \int\limits_{-\infty}^{\infty}\!\frac{d\omega}{2\pi}\,\mathcal{M}_{ij}(\omega)\,\hat{\phi}_i^*(\omega)\,\hat{\phi}_j(\omega)
\end{aligned} \tag{10.59}$$

where

$$\begin{aligned}\mathcal{M}_{ij}(\omega) &\equiv \tfrac{1}{2}(-i\omega)\left\{\hat{\chi}_{ij}(\omega) - \hat{\chi}_{ji}(-\omega)\right\} \\ &= \pi\omega\left(1 - e^{-\beta\hbar\omega}\right)\left(\varrho^A_{ij}(\omega) + i\varrho^B_{ij}(\omega)\right) \quad .\end{aligned} \tag{10.60}$$

Note that as a matrix $\mathcal{M}(\omega) = \mathcal{M}^\dagger(\omega)$, so that $\mathcal{M}(\omega)$ has real eigenvalues.

10.2.4 Correlation functions

We define the *correlation function*

$$S_{ij}(t - t') \equiv \frac{1}{2\pi}\left\langle \hat{Q}_i(t)\,\hat{Q}_j(t')\right\rangle \quad , \tag{10.61}$$

which has the spectral representation

$$\begin{aligned}\hat{S}_{ij}(\omega) &= \hbar\varrho^A_{ij}(\omega) + i\hbar\varrho^B_{ij}(\omega) \\ &= \sum_{m,n} P_m\,\langle\, m\,|\,\hat{Q}_i\,|\,n\,\rangle\,\langle\, n\,|\,\hat{Q}_j\,|\,m\,\rangle\,\delta(\omega - \omega_n + \omega_m) \quad .\end{aligned} \tag{10.62}$$

Note that

$$\hat{S}_{ij}(-\omega) = e^{-\beta\hbar\omega}\,\hat{S}^*_{ij}(\omega) \qquad , \qquad \hat{S}_{ji}(\omega) = \hat{S}^*_{ij}(\omega) \quad . \tag{10.63}$$

and that

$$\mathcal{M}_{ij}(\omega) = \frac{\omega}{2i}\left\{\hat{\chi}_{ij}(\omega) - \hat{\chi}_{ji}(-\omega)\right\} = \frac{\pi\omega}{\hbar}\left(1 - e^{-\beta\hbar\omega}\right)\hat{S}_{ij}(\omega) \quad . \tag{10.64}$$

This result is known as the *fluctuation-dissipation theorem*, as it relates the equilibrium fluctuations $S_{ij}(\omega)$ to the dissipation kernel $\mathcal{M}_{ij}(\omega)$.

Time Reversal Symmetry

If the operators $\hat{Q}_i$ have a definite symmetry under time reversal, say

$$\hat{\mathcal{T}}\,\hat{Q}_i\hat{\mathcal{T}}^{-1} = \eta_i\,\hat{Q}_i \quad , \tag{10.65}$$

then the correlation function satisfies

$$\hat{S}_{ij}(\omega) = \eta_i\,\eta_j\,\hat{S}_{ji}(\omega) \quad . \tag{10.66}$$

10.2.5 Continuous systems

The indices i and j could contain spatial information as well. Typically we will separate out spatial degrees of freedom, and write

$$S_{ij}(\boldsymbol{x}-\boldsymbol{x}',t-t') = \frac{1}{2\pi}\,\big\langle \hat{Q}_i(\boldsymbol{x},t)\,\hat{Q}_j(\boldsymbol{x}',t')\big\rangle \quad , \tag{10.67}$$

where we have assumed space and time translation invariance. The Fourier transform is defined as

$$\begin{aligned}\hat{S}_{ij}(\boldsymbol{k},\omega) &= \int\limits_{-\infty}^{\infty}\!dt\int\! d^3\!x\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\, e^{i\omega t}\, S_{ij}(\boldsymbol{x},t)\\ &= \frac{1}{2\pi V}\int\limits_{-\infty}^{\infty}\!dt\; e^{+i\omega t}\,\big\langle \hat{Q}_i(\boldsymbol{k},t)\,\hat{Q}_j(-\boldsymbol{k},0)\big\rangle \quad .\end{aligned} \tag{10.68}$$

10.3 A Spin in a Magnetic Field

Consider a $S=\frac{1}{2}$ object in an external field, described by the Hamiltonian

$$\hat{H}_0 = \gamma B_0\, S^z \tag{10.69}$$

with $B_0>0$. (Without loss of generality, we can take the DC external field $\boldsymbol{B}_0$ to lie along $\hat{\boldsymbol{z}}$.) The eigenstates are $|\pm\rangle$, with $\omega_\pm = \pm\frac{1}{2}\gamma B_0$. We apply a perturbation,

$$\hat{H}_1(t) = \gamma \boldsymbol{S}\cdot\boldsymbol{B}_1(t) \quad . \tag{10.70}$$

At $T=0$, the susceptibility tensor is

$$\begin{aligned}\chi_{\alpha\beta}(\omega) &= \frac{\gamma^2}{\hbar}\sum_n \bigg\{ \frac{\langle -\,|\,S^\beta\,|\,n\,\rangle\langle\,n\,|\,S^\alpha\,|\,-\rangle}{\omega-\omega_- +\omega_n + i\epsilon} - \frac{\langle -\,|\,S^\alpha\,|\,n\,\rangle\langle\,n\,|\,S^\beta\,|\,-\rangle}{\omega+\omega_- -\omega_n + i\epsilon}\bigg\}\\ &= \frac{\gamma^2}{\hbar}\bigg\{ \frac{\langle -\,|\,S^\beta\,|\,+\rangle\langle +\,|\,S^\alpha\,|\,-\rangle}{\omega+\gamma B_0 + i\epsilon} - \frac{\langle -\,|\,S^\alpha\,|\,+\rangle\langle +\,|\,S^\beta\,|\,-\rangle}{\omega-\gamma B_0 + i\epsilon}\bigg\} \quad ,\end{aligned} \tag{10.71}$$

where we have dropped the hat on $\hat{\chi}_{\alpha\beta}(\omega)$ for notational convenience. The only nonzero matrix elements are

$$\chi_{+-}(\omega) = \frac{\hbar\gamma^2}{\omega+\gamma B_0+i\epsilon} \qquad , \qquad \chi_{-+}(\omega) = \frac{-\hbar\gamma^2}{\omega-\gamma B_0+i\epsilon} \quad , \tag{10.72}$$

or, equivalently,

$$\begin{aligned}\chi_{xx}(\omega) &= \tfrac{1}{4}\hbar\gamma^2 \left\{ \frac{1}{\omega + \gamma B_0 + i\epsilon} - \frac{1}{\omega - \gamma B_0 + i\epsilon} \right\} = +\chi_{yy}(\omega) \\ \chi_{xy}(\omega) &= \tfrac{i}{4}\hbar\gamma^2 \left\{ \frac{1}{\omega + \gamma B_0 + i\epsilon} + \frac{1}{\omega - \gamma B_0 + i\epsilon} \right\} = -\chi_{yx}(\omega) \quad .\end{aligned} \tag{10.73}$$

10.3.1 Bloch Equations

The torque exerted on a magnetic moment $\boldsymbol{\mu}$ by a magnetic field $\boldsymbol{H}$ is $\boldsymbol{N} = \boldsymbol{\mu} \times \boldsymbol{H}$, which is equal to the rate of change of the total angular momentum: $\dot{\boldsymbol{J}} = \boldsymbol{N}$. Since $\boldsymbol{\mu} = \gamma \boldsymbol{J}$, where γ is the gyromagnetic factor, we have $\dot{\boldsymbol{\mu}} = \gamma \boldsymbol{\mu} \times \boldsymbol{H}$. For noninteracting spins, the total magnetic moment, $\boldsymbol{M} = \sum_i \boldsymbol{\mu}_i$ then satisfies

$$\frac{d\boldsymbol{M}}{dt} = \gamma \boldsymbol{M} \times \boldsymbol{H} \quad . \tag{10.74}$$

Now suppose that $\boldsymbol{H} = H_0\,\hat{\boldsymbol{z}} + \boldsymbol{H}_\perp(t)$, where $\hat{\boldsymbol{z}} \cdot \boldsymbol{H}_\perp = 0$. In equilibrium, we have $\boldsymbol{M} = M_0\,\hat{\boldsymbol{z}}$, with $M_0 = \chi_0 H_0$, where χ_0 is the static susceptibility. Phenomenologically, we assume that the relaxation to this equilibrium state is described by a longitudinal and transverse relaxation time, respectively known as T_1 and T_2:

$$\begin{aligned}\dot{M}_x &= \gamma M_y H_z - \gamma M_z H_y - \frac{M_x}{T_2} \\ \dot{M}_y &= \gamma M_z H_x - \gamma M_x H_z - \frac{M_y}{T_2} \\ \dot{M}_z &= \gamma M_x H_y - \gamma M_y H_x - \frac{M_z - M_0}{T_1} \quad .\end{aligned} \tag{10.75}$$

These are known as the *Bloch equations*. Mathematically, they are a set of coupled linear, first order, time-dependent, inhomogeneous equations. These may be recast in the form

$$\dot{M}^\alpha + R_{\alpha\beta} M^\beta = \psi^\alpha \quad , \tag{10.76}$$

with $R_{\alpha\beta}(t) = T^{-1}_{\alpha\beta} - \gamma\,\epsilon_{\alpha\beta\delta} H^\delta(t)$, $\psi^\alpha = T^{-1}_{\alpha\beta}\, M^\beta_0$, and

$$T_{\alpha\beta} = \begin{pmatrix} T_2 & 0 & 0 \\ 0 & T_2 & 0 \\ 0 & 0 & T_1 \end{pmatrix} \quad . \tag{10.77}$$

The formal solution is written

$$\boldsymbol{M}(t) = \int_0^t dt'\, U(t-t')\, \boldsymbol{\psi}(t') + U(t)\, \boldsymbol{\psi}(0) \quad , \tag{10.78}$$

where the evolution matrix,

$$U(t) = \hat{\mathcal{T}} \exp\left\{ -\int_0^t dt'\, R(t') \right\} \quad , \tag{10.79}$$

is given in terms of the time-ordered exponential (earlier times to the right).

We can make analytical progress if we write write $\boldsymbol{M} = M_0\, \hat{\boldsymbol{z}} + \boldsymbol{m}$ and suppose $|\boldsymbol{H}_\perp| \ll H_0$ and $|\boldsymbol{m}| \ll M_0$, in which case we have

$$\begin{aligned} \dot{m}_x &= \gamma\, H_0\, m_y - \gamma\, H_y\, M_0 - \frac{m_x}{T_2} \\ \dot{m}_y &= \gamma\, H_x\, M_0 - \gamma\, H_0\, m_x - \frac{m_y}{T_2} \\ \dot{m}_z &= -\frac{m_z}{T_1} \quad , \end{aligned} \tag{10.80}$$

which are equivalent to the following:

$$\begin{aligned} \ddot{m}_x + 2T_2^{-1}\dot{m}_x + \big(\gamma^2 H_0^2 + T_2^{-2}\big) m_x &= \gamma\, M_0 \big(\gamma\, H_0 H_x - T_2^{-1} H_y - \dot{H}_y\big) \\ \ddot{m}_y + 2T_2^{-1}\dot{m}_y + \big(\gamma^2 H_0^2 + T_2^{-2}\big) m_y &= \gamma\, M_0 \big(\gamma\, H_0 H_y + T_2^{-1} H_x + \dot{H}_x\big) \end{aligned} \tag{10.81}$$

and $m_z(t) = m_z(0)\, \exp(-t/T_1)$. Solving the first two by Fourier transform,

$$\begin{aligned} \big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-2}\omega\big)\, \hat{m}_x(\omega) &= \gamma\, M_0 \big(\gamma\, H_0\, H_x(\omega) + (i\omega - T_2^{-1}) H_y(\omega)\big) \\ \big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-2}\omega\big)\, \hat{m}_y(\omega) &= \gamma\, M_0 \big(\gamma\, H_0\, H_y(\omega) - (i\omega - T_2^{-1}) H_x(\omega)\big) \quad , \end{aligned} \tag{10.82}$$

from which we read off

$$\begin{aligned} \chi_{xx}(\omega) &= \frac{\gamma^2 H_0\, M_0}{\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-1}\omega} = \chi_{yy}(\omega) \\ \chi_{xy}(\omega) &= \frac{(i\omega - T_2^{-1})\, \gamma\, M_0}{\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-1}\omega} = -\chi_{yx}(\omega) \quad . \end{aligned} \tag{10.83}$$

Note that Onsager reciprocity is satisfied:

$$\chi_{xy}(\omega, H_0) = \chi^{\mathsf{T}}_{yx}(\omega, H_0) = \chi_{yx}(\omega, -H_0) = -\chi_{yx}(\omega, H_0) \quad . \tag{10.84}$$

The lineshape is given by

$$\begin{aligned}\chi'_{xx}(\omega) &= \frac{(\gamma^2 H_0^2 + T_2^{-2} - \omega^2)\,\gamma^2\, H_0\, M_0}{\big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2\big)^2 + 4\,T_2^{-2}\omega^2} \\ \chi''_{xx}(\omega) &= \frac{2\,\gamma\, H_0\, M_0\, T_2^{-1}\omega}{\big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2\big)^2 + 4\,T_2^{-2}\omega^2} \quad ,\end{aligned} \tag{10.85}$$

so a measure of the linewidth is a measure of T_2^{-1}.

10.4 Density Response and Correlations

In many systems, external probes couple to the number density $\hat{n}(\boldsymbol{x}) = \sum_{i=1}^N \delta(\boldsymbol{x} - \boldsymbol{x}_i)$, and we may write the perturbing Hamiltonian as

$$\hat{H}_1(t) = -\int\! d^3\!x\; \hat{n}(\boldsymbol{x})\, \phi(\boldsymbol{x}, t) \quad . \tag{10.86}$$

The response $\delta n \equiv n - \langle n \rangle_0$ is given by

$$\begin{aligned}\langle \delta n(\boldsymbol{x}, t)\rangle &= \int\! dt' \!\int\! d^3\!x'\; \chi(\boldsymbol{x} - \boldsymbol{x}', t - t')\, \phi(\boldsymbol{x}', t') \\ \langle \delta\hat{n}(\boldsymbol{q}, \omega)\rangle &= \hat{\chi}(\boldsymbol{q}, \omega)\, \hat{\phi}(\boldsymbol{q}, \omega) \quad ,\end{aligned} \tag{10.87}$$

where

$$\begin{aligned}\hat{\chi}(\boldsymbol{q}, \omega) &= \frac{1}{\hbar V} \sum_{m,n} P_m \left\{ \frac{\big|\langle\, m \,|\, \hat{n}_{\boldsymbol{q}} \,|\, n \,\rangle\big|^2}{\omega - \omega_m + \omega_n + i\epsilon} - \frac{\big|\langle\, m \,|\, \hat{n}_{\boldsymbol{q}} \,|\, n \,\rangle\big|^2}{\omega + \omega_m - \omega_n + i\epsilon} \right\} \\ &= \frac{1}{\hbar} \int\limits_{-\infty}^{\infty}\! d\nu\; S(\boldsymbol{q}, \nu) \left\{ \frac{1}{\omega + \nu + i\epsilon} - \frac{1}{\omega - \nu + i\epsilon} \right\} \quad .\end{aligned} \tag{10.88}$$

The function

$$S(\boldsymbol{q}, \omega) = \frac{1}{V} \sum_{m,n} P_m\, \big|\langle\, m \,|\, \hat{n}_{\boldsymbol{q}} \,|\, n \,\rangle\big|^2\, \delta(\omega - \omega_n + \omega_m) \tag{10.89}$$

is known as the *dynamic structure factor* (dsf). Note that $\hat{n}_{\boldsymbol{q}} = \sum_{i=1}^N e^{-i\boldsymbol{q}\cdot\boldsymbol{x}_i}$ and that $\hat{n}^\dagger_{\boldsymbol{q}} = \hat{n}_{-\boldsymbol{q}}$. In a scattering experiment, where an incident probe (*e.g.* a neutron) interacts with the system via a potential $\phi(\boldsymbol{x}-\boldsymbol{R})$, where $\boldsymbol{R}$ is the probe particle position, Fermi's Golden Rule says that the rate at which the incident particle deposits momentum $\hbar\boldsymbol{q}$ and energy $\hbar\omega$ into the system is given by

$$\begin{aligned}\mathcal{I}(\boldsymbol{q},\omega) &= \frac{2\pi}{\hbar}\sum_{m,n} P_m \left|\left\langle\, m\,;\boldsymbol{p}\,\right|\hat{H}_1\left|\, n\,;\boldsymbol{p}-\hbar\boldsymbol{q}\,\right\rangle\right|^2 \delta(\omega-\omega_n+\omega_m)\\ &= \frac{2\pi}{\hbar}\,|\hat{\phi}(\boldsymbol{q})|^2\, S(\boldsymbol{q},\omega) \quad .\end{aligned} \tag{10.90}$$

The quantity $|\hat{\phi}(\boldsymbol{q})|^2$ is called the *form factor*. In neutron scattering, the "on-shell" condition requires that the incident energy ε and momentum $\boldsymbol{p}$ are related via the ballistic dispersion $\varepsilon=\boldsymbol{p}^2/2m_{\rm n}$. Similarly, the final energy and momentum are related, hence

$$\varepsilon-\hbar\omega=\frac{\boldsymbol{p}^2}{2m_{\rm n}}-\hbar\omega=\frac{(\boldsymbol{p}-\hbar\boldsymbol{q})^2}{2m_{\rm n}} \qquad \Longrightarrow \qquad \hbar\omega=\frac{\hbar\boldsymbol{q}\cdot\boldsymbol{p}}{m_{\rm n}}-\frac{\hbar^2\boldsymbol{q}^2}{2m_{\rm n}} \quad . \tag{10.91}$$

Hence, for fixed momentum transfer $\hbar\boldsymbol{q}$, the frequency ω can be varied by changing the incident momentum $\boldsymbol{p}$.

Another case of interest is the response of a system to a foreign object moving with trajectory $\boldsymbol{R}(t)=\boldsymbol{V}t$. In this case, $\phi(\boldsymbol{x},t)=\phi\big(\boldsymbol{x}-\boldsymbol{R}(t)\big)$, and

$$\hat{\phi}(\boldsymbol{q},\omega)=\int\! dt\!\int\! d^3\!x\, e^{-i\boldsymbol{q}\cdot\boldsymbol{x}}\, e^{i\omega t}\,\phi(\boldsymbol{x}-\boldsymbol{V}t)=2\pi\,\delta(\omega-\boldsymbol{q}\cdot\boldsymbol{V})\,\hat{\phi}(\boldsymbol{q}) \tag{10.92}$$

so that

$$\langle\delta n(\boldsymbol{q},\omega)\rangle=2\pi\,\delta(\omega-\boldsymbol{q}\cdot\boldsymbol{V})\,\hat{\chi}(\boldsymbol{q},\omega)\,\hat{\phi}(\boldsymbol{q}) \quad . \tag{10.93}$$

10.4.1 Sum rules

From eqn. (10.89) we find

$$\begin{aligned}\int\limits_{-\infty}^{\infty}\! d\omega\,\omega\, S(\boldsymbol{q},\omega) &= \frac{1}{V}\sum_{m,n} P_m\left|\langle\, m\,|\,\hat{n}_{\boldsymbol{q}}\,|\, n\,\rangle\right|^2(\omega_n-\omega_m)\\ &= \frac{1}{\hbar V}\sum_{m,n} P_m\,\langle\, m\,|\,\hat{n}_{\boldsymbol{q}}\,|\, n\,\rangle\,\langle\, n\,|\,[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\,|\, m\,\rangle\\ &= \frac{1}{\hbar V}\,\langle\hat{n}_{\boldsymbol{q}}\,[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\rangle=\frac{1}{2\hbar V}\left\langle\big[\hat{n}_{\boldsymbol{q}},[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\big]\right\rangle \quad ,\end{aligned} \tag{10.94}$$

where the last equality is guaranteed by $\boldsymbol{q}\to-\boldsymbol{q}$ symmetry. Now if the potential is velocity independent, *i.e.* if

$$\hat{H}=-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\boldsymbol{\nabla}_i^2+V(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N) \quad , \tag{10.95}$$

then with $\hat{n}^\dagger_{\boldsymbol{q}} = \sum_{i=1}^N e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i}$ we obtain

$$\begin{aligned}[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}] &= -\frac{\hbar^2}{2m}\sum_{i=1}^N \big[\boldsymbol{\nabla}_i^2\,,\,e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i}\big] = \frac{\hbar^2}{2im}\,\boldsymbol{q}\cdot\sum_{i=1}^N\Big(\boldsymbol{\nabla}_i\,e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i} + e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i}\,\boldsymbol{\nabla}_i\Big) \\ \big[\hat{n}_{\boldsymbol{q}},[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\big] &= \frac{\hbar^2}{2im}\,\boldsymbol{q}\cdot\sum_{i=1}^N\sum_{j=1}^N\Big[e^{-i\boldsymbol{q}\cdot\boldsymbol{x}_j},\,\boldsymbol{\nabla}_i\,e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i} + e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i}\,\boldsymbol{\nabla}_i\Big] = \frac{N\hbar^2\boldsymbol{q}^2}{m}\quad.\end{aligned} \tag{10.96}$$

We have derived the *f-sum rule*:

$$\int\limits_{-\infty}^{\infty} d\omega\,\omega\,S(\boldsymbol{q},\omega) = \frac{n\hbar\boldsymbol{q}^2}{2m}\quad, \tag{10.97}$$

where $n = N/V$ is the overall number density. Note that this integral, which is the first moment of the structure factor, is *independent of the potential!*. The n^{th} moment of the dsf distribution is given by

$$\int\limits_{-\infty}^{\infty} d\omega\,\omega^n\,S(\boldsymbol{q},\omega) = \frac{1}{\hbar V}\Big\langle \hat{n}_{\boldsymbol{q}}\Big[\overbrace{\hat{H},\big[\hat{H},\cdots[\hat{H},\hat{n}^\dagger_{\boldsymbol{q}}]\cdots\big]}^{n\text{ times}}\Big]\Big\rangle\quad. \tag{10.98}$$

Moments with $n \neq 1$ in general depend on the potential, unlike the $n = 1$ moment from the f-sum rule. The $n = 0$ moment gives

$$\begin{aligned}S(\boldsymbol{q}) \equiv \int\limits_{-\infty}^{\infty} d\omega\,S(\boldsymbol{q},\omega) &= \frac{1}{\hbar V}\,\langle \hat{n}^\dagger_{\boldsymbol{q}}\,\hat{n}_{\boldsymbol{q}}\rangle \\ &= \frac{1}{\hbar}\int d^3\!x\,\langle n(\boldsymbol{x})\,n(0)\rangle\,e^{-i\boldsymbol{q}\cdot\boldsymbol{x}}\quad,\end{aligned} \tag{10.99}$$

which is the Fourier transform of the density-density correlation function.

Compressibility sum rule

The isothermal compressibility is given by

$$\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial n}\bigg|_T = \frac{1}{n^2}\frac{\partial n}{\partial\mu}\bigg|_T\quad. \tag{10.100}$$

Since a constant potential $v(\boldsymbol{x},t)$ is equivalent to a chemical potential shift, we have

$$\langle\delta n\rangle = \hat{\chi}(\boldsymbol{q}=0,\omega=0)\,\delta\mu \quad\Longrightarrow\quad \kappa_T = \frac{2}{\hbar n^2}\lim_{\boldsymbol{q}\to 0}\int\limits_{-\infty}^{\infty} d\omega\,\frac{S(\boldsymbol{q},\omega)}{\omega}\quad. \tag{10.101}$$

This is known as the *compressibility sum rule*.

Single mode approximation at $T = 0$

For each wavevector $\boldsymbol{q}$, the dynamical structure factor $S(\boldsymbol{q},\omega)$ may be regarded as a distribution function of the frequency ω. The normalized average $n^{\rm th}$ moment $\langle \omega^n \rangle_{\boldsymbol{q}}$ is given by

$$\langle \omega^n \rangle_{\boldsymbol{q}} = \int\limits_{-\infty}^{\infty} \! d\omega \, \omega^n \, S(\boldsymbol{q},\omega) \bigg/ \int\limits_{-\infty}^{\infty} \! d\omega \, S(\boldsymbol{q},\omega) \quad . \tag{10.102}$$

Thus, we can define a set of quantities $\big\{ \Omega_{n,m}(\boldsymbol{q}) \big\}$, each of which has dimensions of frequency, according to

$$\big[\Omega_{n,m}(\boldsymbol{q}) \big]^{n-m} \equiv \frac{\langle \omega^n \rangle_{\boldsymbol{q}}}{\langle \omega^m \rangle_{\boldsymbol{q}}} = \int\limits_{-\infty}^{\infty} \! d\omega \, \omega^n \, S(\boldsymbol{q},\omega) \bigg/ \int\limits_{-\infty}^{\infty} \! d\omega \, \omega^m \, S(\boldsymbol{q},\omega) \quad . \tag{10.103}$$

If, for each wavevector $\boldsymbol{q}$, all the oscillator strength $|\langle\, \mathsf{G} \,|\, \hat{n}_{\boldsymbol{q}} \,|\, n \,\rangle|^2$ in the dsf is saturated by a single mode, then

$$S(\boldsymbol{q},\omega) \approx S_{\mathsf{SMA}}(\boldsymbol{q},\omega) \equiv S_{\mathsf{SMA}}(\boldsymbol{q}) \, \delta\big(\omega - \Omega_{\mathsf{SMA}}(\boldsymbol{q})\big) \quad . \tag{10.104}$$

If the SMA is exact, then $S_{\mathsf{SMA}}(\boldsymbol{q})$ is the static structure factor $S(\boldsymbol{q})$ from Eqn. 10.99. Within the SMA, the $n^{\rm th}$ moment of the dsf in Eqn. 10.98 is $\big[\Omega_{\mathsf{SMA}}(\boldsymbol{q})\big]^n \cdot S_{\mathsf{SMA}}(\boldsymbol{q})$, in which case each $\Omega_{n,m}(\boldsymbol{q})$ from Eqn. 10.103 is given by $\Omega_{\mathsf{SMA}}(\boldsymbol{q})$. Thus, the SMA frequency may be approximated by $\Omega_{n,m}(\boldsymbol{q})$ for any n and m. For example, if we take $n = +1$ and $m = -1$, we have

$$\Omega^2_{1,-1}(\boldsymbol{q}) = \frac{n\boldsymbol{q}^2}{m\hat{\chi}(\boldsymbol{q})} \quad , \tag{10.105}$$

where

$$\hat{\chi}(\boldsymbol{q}) = \frac{2}{\hbar} \int\limits_0^{\infty} \! d\omega \, \frac{S(\boldsymbol{q},\omega)}{\omega} \tag{10.106}$$

is the static susceptibility. If instead we were to choose $n = 1$ and $m = 0$, we arrive at

$$\Omega_{1,0}(\boldsymbol{q}) = \frac{n\hbar\boldsymbol{q}^2}{2S(\boldsymbol{q})} \quad . \tag{10.107}$$

Note that within the SMA, we have $\hat{\chi}(\boldsymbol{q}) \approx \hat{\chi}_{\mathsf{SMA}}(\boldsymbol{q}) = 2S_{\mathsf{SMA}}(\boldsymbol{q})/\hbar\Omega_{\mathsf{SMA}}(\boldsymbol{q})\,$.

10.4.2 Dynamic Structure Factor for the Electron Gas

The dynamic structure factor $S(\boldsymbol{q},\omega)$ tells us about the spectrum of density fluctuations. The density operator $\hat{n}^\dagger_{\boldsymbol{q}} = \sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i}$ increases the wavevector by $\boldsymbol{q}$. At $T = 0$, in order for $\langle\, n \,|\, \hat{n}^\dagger_{\boldsymbol{q}} \,|\, \mathsf{G} \,\rangle$

to be nonzero (where $|\mathsf{G}\rangle$ is the ground state, *i.e.* the filled Fermi sphere), the state n must correspond to a *particle-hole excitation*. For a given $\boldsymbol{q}$, the maximum excitation frequency is obtained by taking an electron just inside the Fermi sphere, with wavevector $\boldsymbol{k} = k_{\rm F}\,\hat{\boldsymbol{q}}$ and transferring it to a state outside the Fermi sphere with wavevector $\boldsymbol{k}+\boldsymbol{q}$. For $|\boldsymbol{q}| < 2k_{\rm F}$, the minimum excitation frequency is zero – one can always form particle-hole excitations with states adjacent to the Fermi sphere. For $|\boldsymbol{q}| > 2k_{\rm F}$, the minimum excitation frequency is obtained by taking an electron just inside the Fermi sphere with wavevector $\boldsymbol{k} = -k_{\rm F}\,\hat{\boldsymbol{q}}$ to an unfilled state outside the Fermi sphere with wavevector $\boldsymbol{k}+\boldsymbol{q}$. These cases are depicted in fig. 10.4.

We therefore have

$$\omega_{\mathsf{max}}(q) = \frac{\hbar q^2}{2m} + \frac{\hbar k_{\rm F} q}{m} \tag{10.108}$$

and

$$\omega_{\rm min}(q) = \begin{cases} 0 & \text{if } q \leqslant 2k_{\rm F} \\ \frac{\hbar q^2}{2m} - \frac{\hbar k_{\rm F} q}{m} & \text{if } q > 2k_{\rm F} \end{cases} \quad . \tag{10.109}$$

This is depicted in fig. 10.2. Outside of the region bounded by $\omega_{\rm min}(q)$ and $\omega_{\mathsf{max}}(q)$, there are no single pair excitations. It is of course easy to create *multiple pair* excitations with arbitrary energy and momentum, as depicted in fig. 10.3. However, these multipair states do not couple to the ground state $|\,\mathsf{G}\,\rangle$ through a single application of the density operator $\hat{n}^\dagger_{\boldsymbol{q}}$, hence they have zero oscillator strength: $\langle\, n\,|\,\hat{n}^\dagger_{\boldsymbol{q}}\,|\,\mathsf{G}\,\rangle = 0$ for any multipair state $|\,n\,\rangle$.

Explicit $T=0$ calculation

We start with

$$\begin{aligned} 2\pi\, S(\boldsymbol{x},t) &= \langle n(\boldsymbol{x},t)\, n(0,0)\rangle \\ &= \int\!\frac{d^3\!k}{(2\pi)^3}\int\!\frac{d^3\!k'}{(2\pi)^3}\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \sum_{i,j} \big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i(t)}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{x}_j}\big\rangle \quad . \end{aligned} \tag{10.110}$$

The time evolution of the operator $\boldsymbol{x}_i(t)$ is given by $\boldsymbol{x}_i(t) = \boldsymbol{x}_i + \boldsymbol{p}_i t/m$, where $\boldsymbol{p}_i = -i\hbar\boldsymbol{\nabla}_i$. Using the result

$$e^{A+B} = e^A\, e^B\, e^{-\frac{1}{2}[A,B]} \quad , \tag{10.111}$$

which is valid when $[A,[A,B]] = [B,[A,B]] = 0$, we have

$$e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i(t)} = e^{i\hbar\boldsymbol{k}^2 t/2m}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{p}_i\, t/m} \quad , \tag{10.112}$$

hence

$$2\pi\, S(\boldsymbol{x},t) = \int\!\frac{d^3\!k}{(2\pi)^3}\int\!\frac{d^3\!k'}{(2\pi)^3}\, e^{i\hbar\boldsymbol{k}^2 t/2m}\, e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \sum_{i,j} \big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{x}_j}\big\rangle \quad . \tag{10.113}$$

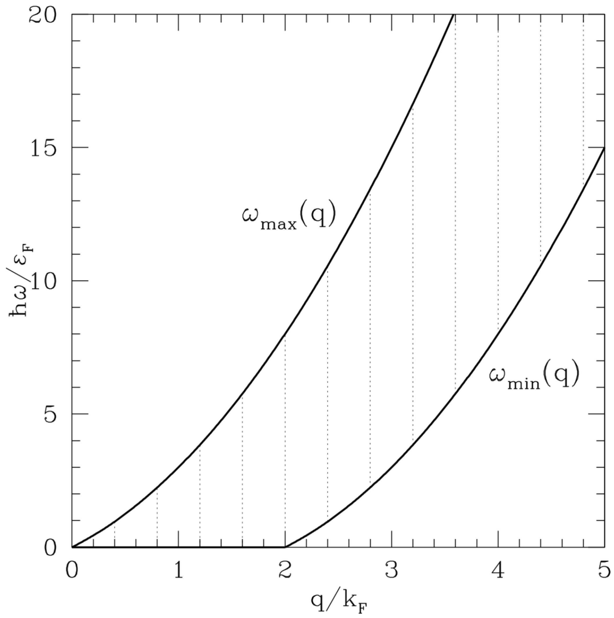

Figure 10.2: Spread of particle-hole excitation frequencies ω in units of $\varepsilon_F/\hbar$ *versus* wavevector q in units of k_F. Outside the hatched areas, there are no *single pair* excitations.

We now break the sum up into diagonal ($i = j$) and off-diagonal ($i \neq j$) terms.

For the diagonal terms, with $i = j$, we have

$$\begin{aligned}\left\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{x}_i}\right\rangle &= e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{k}' t/m}\left\langle e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{x}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\right\rangle \\ &= e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{k}' t/m}\,\frac{(2\pi)^3}{NV}\,\delta(\boldsymbol{k}-\boldsymbol{k}')\sum_{\boldsymbol{q}}\Theta(k_F - q)\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m} \quad ,\end{aligned} \tag{10.114}$$

since the ground state $|\,\mathsf{G}\,\rangle$ is a Slater determinant formed of single particle wavefunctions $\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \exp(i\boldsymbol{q}\cdot\boldsymbol{x})/\sqrt{V}$ with $q < k_F$.

For $i \neq j$, we must include exchange effects. We then have

$$\begin{aligned}\left\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i}\, e^{-i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{x}_j}\right\rangle &= \frac{1}{N(N-1)}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'}\Theta(k_F - q)\,\Theta(k_F - q') \\ &\qquad \times\int\frac{d^3x_i}{V}\int\frac{d^3x_j}{V}\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\left\{e^{-i\boldsymbol{k}\cdot\boldsymbol{x}_i}\, e^{i\boldsymbol{k}'\boldsymbol{x}_j} - e^{i(\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{k})\cdot\boldsymbol{x}_i}\, e^{i(\boldsymbol{q}'-\boldsymbol{q}+\boldsymbol{k}')\cdot\boldsymbol{x}_j}\right\} \\ &= \frac{(2\pi)^6}{N(N-1)V^2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'}\Theta(k_F - q)\,\Theta(k_F - q') \\ &\qquad \times e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\left\{\delta(\boldsymbol{k})\,\delta(\boldsymbol{k}') - \delta(\boldsymbol{k}-\boldsymbol{k}')\,\delta(\boldsymbol{k}+\boldsymbol{q}'-\boldsymbol{q})\right\} \quad .\end{aligned} \tag{10.115}$$

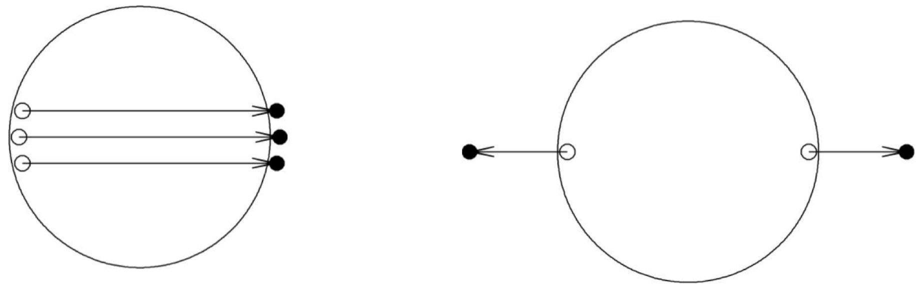

Figure 10.3: With multiple pair excitations, every part of $(\boldsymbol{q},\omega)$ space is accessible. However, these states to not couple to the ground state $|\mathsf{G}\rangle$ through a *single* application of the density operator $\hat{n}^\dagger_{\boldsymbol{q}}$.

Summing over the $i=j$ terms gives

$$2\pi\, S_{\rm diag}(\boldsymbol{x},t) = \int\!\frac{d^3\!k}{(2\pi)^3}\; e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\, e^{-i\hbar\boldsymbol{k}^2 t/2m}\!\int\!\frac{d^3\!q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\quad , \tag{10.116}$$

while the off-diagonal terms yield

$$\begin{aligned} 2\pi\, S_{\rm off-diag}(\boldsymbol{x},t) &= \int\!\frac{d^3\!k}{(2\pi)^3}\; e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\!\int\!\frac{d^3\!q}{(2\pi)^3}\int\!\frac{d^3\!q'}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-q') \\ &\qquad\qquad \times (2\pi)^3\Big\{\delta(\boldsymbol{k}) - e^{+i\hbar\boldsymbol{k}^2 t/2m}\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\,\delta(\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{k})\Big\} \\ &= n^2 - \int\!\frac{d^3\!k}{(2\pi)^3}\; e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\, e^{+i\hbar\boldsymbol{k}^2 t/2m}\!\int\!\frac{d^3\!q}{(2\pi)^3}\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-|\boldsymbol{k}-\boldsymbol{q}|)\,e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\quad , \end{aligned} \tag{10.117}$$

and hence

$$\begin{aligned} 2\pi\, S(\boldsymbol{k},\omega) &= n^2\,(2\pi)^4\delta(\boldsymbol{k})\,\delta(\omega) + \int\!\frac{d^3\!q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\bigg\{2\pi\,\delta\Big(\omega - \frac{\hbar\boldsymbol{k}^2}{2m} - \frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big) \\ &\qquad\qquad - \Theta(k_{\rm F}-|\boldsymbol{k}-\boldsymbol{q}|)\,2\pi\delta\Big(\omega + \frac{\hbar\boldsymbol{k}^2}{2m} - \frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big)\bigg\} \\ &= (2\pi)^4 n^2\delta(\boldsymbol{k})\delta(\omega) + \int\!\frac{d^3\!q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,\Theta(|\boldsymbol{k}+\boldsymbol{q}|-k_{\rm F})\cdot 2\pi\delta\Big(\omega - \frac{\hbar\boldsymbol{k}^2}{2m} - \frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big). \end{aligned} \tag{10.118}$$

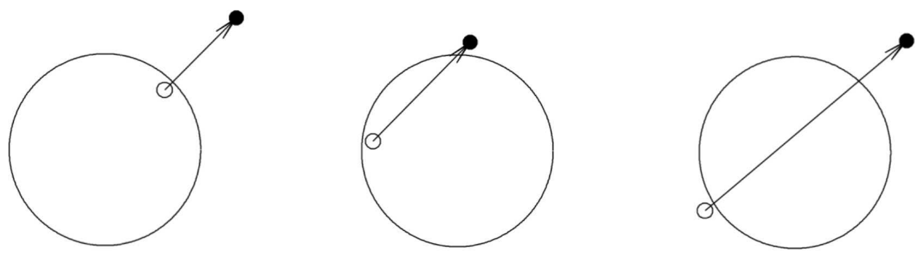

Figure 10.4: Minimum and maximum frequency particle-hole excitations in the free electron gas at $T = 0$. (a) To construct a maximum frequency excitation for a given $\boldsymbol{q}$, create a hole just inside the Fermi sphere at $\boldsymbol{k} = k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ and an electron at $\boldsymbol{k}' = \boldsymbol{k}+\boldsymbol{q}$. (b) For $|\boldsymbol{q}| < 2k_{\mathrm{F}}$ the minumum excitation frequency is zero. (c) For $|\boldsymbol{q}| > 2k_{\mathrm{F}}$, the minimum excitation frequency is obtained by placing a hole at $\boldsymbol{k} = -k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ and an electron at $\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{q}$.

For $\boldsymbol{k}, \omega \neq 0$, then,

$$
\begin{aligned}
2\pi\, S(\boldsymbol{k},\omega) &= \frac{1}{2\pi}\int\limits_0^{k_{\mathrm{F}}}\! dq\, q^2 \int\limits_{-1}^{1}\! dx\, \Theta\big(\sqrt{k^2+q^2+2kqx} - k_{\mathrm{F}}\big)\, \delta\Big(\omega - \frac{\hbar k^2}{2m} - \frac{\hbar k q}{m}\, x\Big) \\
&= \frac{m}{2\pi\hbar k}\int\limits_0^{k_{\mathrm{F}}}\! dq\, q\, \Theta\Big(\sqrt{q^2 + \frac{2m\omega}{\hbar}} - k_{\mathrm{F}}\Big) \int\limits_{-1}^{1}\! dx\, \delta\Big(x + \frac{k}{2q} - \frac{m\omega}{\hbar k q}\Big) \\
&= \frac{m}{4\pi\hbar k}\int\limits_0^{k_{\mathrm{F}}^2}\! du\, \Theta\Big(u + \frac{2m\omega}{\hbar} - k_{\mathrm{F}}^2\Big)\, \Theta\bigg(u - \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2\bigg) \quad .
\end{aligned}
\tag{10.119}
$$

The constraints on u are

$$
k_{\mathrm{F}}^2 \geqslant u \geqslant \mathsf{max}\bigg(k_{\mathrm{F}}^2 - \frac{2m\omega}{\hbar}\,,\, \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2\bigg) \quad . \tag{10.120}
$$

Clearly $\omega > 0$ is required. There are two cases to consider.

The first case is

$$
k_{\mathrm{F}}^2 - \frac{2m\omega}{\hbar} \geqslant \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2 \quad\Longrightarrow\quad 0 \leqslant \omega \leqslant \frac{\hbar k_{\mathrm{F}} k}{m} - \frac{\hbar k^2}{2m} \quad , \tag{10.121}
$$

which in turn requires $k \leqslant 2k_{\mathrm{F}}$. In this case, we have

$$
2\pi\, S(\boldsymbol{k},\omega) = \frac{m}{4\pi\hbar k}\bigg\{k_{\mathrm{F}}^2 - \Big(k_{\mathrm{F}}^2 - \frac{2m\omega}{\hbar}\Big)\bigg\} = \frac{m^2\omega}{2\pi\hbar^2 k} \quad . \tag{10.122}
$$

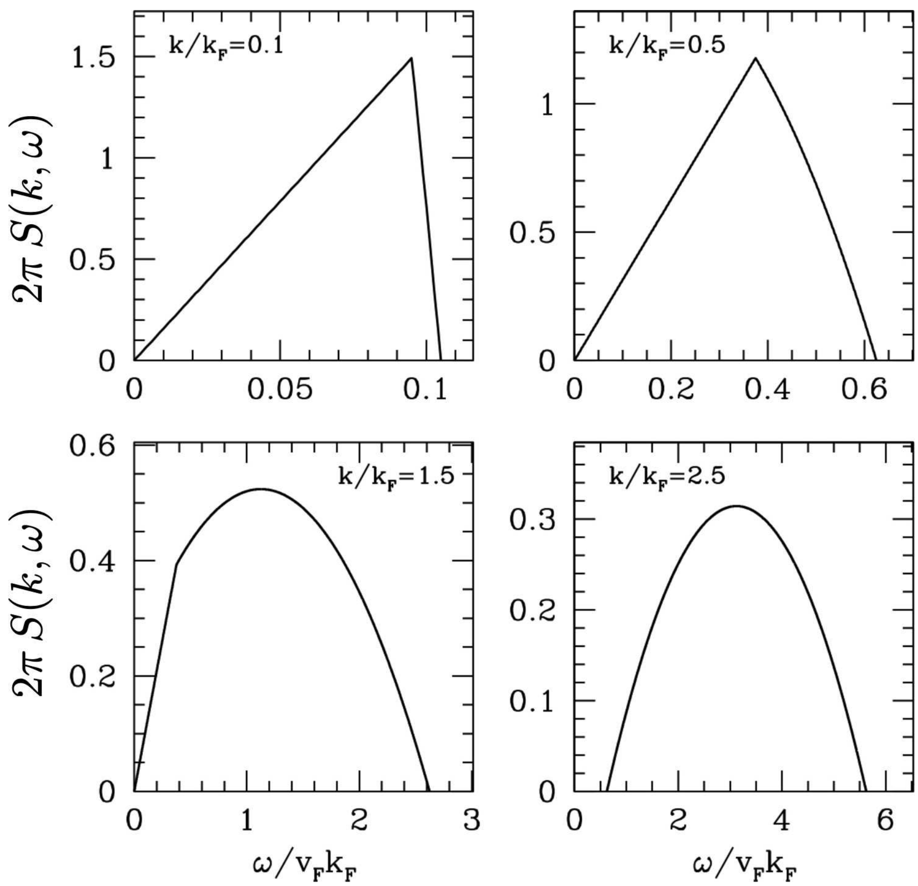

Figure 10.5: The dynamic structure factor $S(k,\omega)$ for the electron gas at various values of $k/k_{\rm F}$.

The second case

$$k_{\rm F}^2 - \frac{2m\omega}{\hbar} \leqslant \left| \frac{k}{2} - \frac{m\omega}{\hbar k} \right|^2 \quad \Longrightarrow \quad \omega \geqslant \frac{\hbar k_{\rm F} k}{m} - \frac{\hbar k^2}{2m} \quad . \tag{10.123}$$

However, we also have that

$$\left| \frac{k}{2} - \frac{m\omega}{\hbar k} \right|^2 \leqslant k_{\rm F}^2 \quad , \tag{10.124}$$

hence ω is restricted to the range

$$\frac{\hbar k}{2m}\,|k - 2k_{\rm F}| \leqslant \omega \leqslant \frac{\hbar k}{2m}\,|k + 2k_{\rm F}| \quad . \tag{10.125}$$

The integral in (10.119) then gives

$$2\pi\, S(\boldsymbol{k},\omega) = \frac{m}{4\pi\hbar k} \left\{ k_{\rm F}^2 - \left| \frac{k}{2} - \frac{m\omega}{\hbar k} \right|^2 \right\} \quad . \tag{10.126}$$

Putting it all together,

$$2\pi\, S(\boldsymbol{k},\omega) = \begin{cases} \frac{mk_{\rm F}}{\pi^2\hbar^2}\cdot\frac{\pi\omega}{2v_{\rm F}k} & \text{if } 0<\omega\leqslant v_{\rm F}k-\frac{\hbar k^2}{2m} \\ \frac{mk_{\rm F}}{\pi^2\hbar^2}\cdot\frac{\pi k_{\rm F}}{4k}\left[1-\left(\frac{\omega}{v_{\rm F}k}-\frac{k}{2k_{\rm F}}\right)^2\right] & \text{if } \left|v_{\rm F}k-\frac{\hbar k^2}{2m}\right|\leqslant\omega\leqslant v_{\rm F}k+\frac{\hbar k^2}{2m} \\ 0 & \text{if } \omega\geqslant v_{\rm F}k+\frac{\hbar k^2}{2m} \quad . \end{cases} \tag{10.127}$$

Integrating over all frequency gives the static structure factor,

$$S(\boldsymbol{k}) = \frac{1}{V}\,\langle n^\dagger_{\boldsymbol{k}}\, n_{\boldsymbol{k}}\rangle = \int\limits_{-\infty}^{\infty} d\omega\, S(\boldsymbol{k},\omega) \quad . \tag{10.128}$$

The result is

$$S(\boldsymbol{k}) = \begin{cases} \left(\frac{3k}{4k_{\rm F}}-\frac{k^3}{16k_{\rm F}^3}\right)n & \text{if } 0<k\leqslant 2k_{\rm F} \\ n & \text{if } k\geqslant 2k_{\rm F} \\ Vn^2 & \text{if } k=0 \quad , \end{cases} \tag{10.129}$$

where $n = k_{\rm F}^3/6\pi^2$ is the density (per spin polarization).

10.5 Charged Systems: Screening and Dielectric Response

10.5.1 Definition of the charge response functions

Consider a many-electron system in the presence of a time-varying external charge density $\rho_{\rm ext}(\boldsymbol{x},t)$. The perturbing Hamiltonian is then

$$\begin{aligned} \hat H_1 &= -e\int d^3\!x\int d^3\!x'\,\frac{n(\boldsymbol{x})\,\rho_{\rm ext}(\boldsymbol{x}',t)}{\left|\boldsymbol{x}-\boldsymbol{x}'\right|} \\ &= -e\int\frac{d^3\!k}{(2\pi)^3}\,\frac{4\pi}{\boldsymbol{k}^2}\,\hat n(\boldsymbol{k})\,\hat\rho_{\rm ext}(-\boldsymbol{k},t) \quad . \end{aligned} \tag{10.130}$$

The induced charge is $-e\,\delta n$, where δn is the induced number density:

$$\delta\hat n(\boldsymbol{q},\omega) = \frac{4\pi e}{\boldsymbol{q}^2}\,\hat\chi(\boldsymbol{q},\omega)\,\hat\rho_{\rm ext}(\boldsymbol{q},\omega) \quad . \tag{10.131}$$

We can use this to determine the dielectric function $\epsilon(\boldsymbol{q},\omega)$:

$$\begin{aligned} \boldsymbol{\nabla}\cdot\boldsymbol{D} &= 4\pi\rho_{\rm ext} \\ \boldsymbol{\nabla}\cdot\boldsymbol{E} &= 4\pi\big(\rho_{\rm ext}-e\,\langle\delta n\rangle\big) \quad . \end{aligned} \tag{10.132}$$

In Fourier space,

$$\begin{aligned} i\boldsymbol{q}\cdot\boldsymbol{D}(\boldsymbol{q},\omega) &= 4\pi\hat{\rho}_{\text{ext}}(\boldsymbol{q},\omega) \\ i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega) &= 4\pi\hat{\rho}_{\text{ext}}(\boldsymbol{q},\omega) - 4\pi e\,\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle \quad , \end{aligned} \tag{10.133}$$

so that from $\boldsymbol{D}(\boldsymbol{q},\omega)=\epsilon(\boldsymbol{q},\omega)\,\boldsymbol{E}(\boldsymbol{q},\omega)$ follows

$$\begin{aligned} \frac{1}{\epsilon(\boldsymbol{q},\omega)} = \frac{i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega)}{i\boldsymbol{q}\cdot\boldsymbol{D}(\boldsymbol{q},\omega)} &= 1 - \frac{\delta\hat{n}(\boldsymbol{q},\omega)}{Z\hat{n}_{\text{ext}}(\boldsymbol{q},\omega)} \\ &= 1 - \frac{4\pi e^2}{\boldsymbol{q}^2}\,\hat{\chi}(\boldsymbol{q},\omega) \quad . \end{aligned} \tag{10.134}$$

A system is said to exhibit *perfect screening* if

$$\epsilon(\boldsymbol{q}\to 0,\omega=0)=\infty \qquad \Longrightarrow \qquad \lim_{\boldsymbol{q}\to 0}\frac{4\pi e^2}{\boldsymbol{q}^2}\,\hat{\chi}(\boldsymbol{q},0)=1 \quad . \tag{10.135}$$

Here, $\hat{\chi}(\boldsymbol{q},\omega)$ is the usual density-density response function,

$$\hat{\chi}(\boldsymbol{q},\omega)=\frac{1}{\hbar V}\sum_j \frac{2\omega_j}{\omega_j^2-(\omega+i\epsilon)^2}\,\big|\langle\, j\,|\,\hat{n}_{\boldsymbol{q}}\,|\,0\,\rangle\big|^2 \quad , \tag{10.136}$$

where we content ourselves to work at $T=0$, and where $\omega_j\equiv(E_j-E_0)/\hbar$ is the excitation frequency for the state $|\,n\,\rangle$.

From $\boldsymbol{j}_{\text{charge}}=\sigma\boldsymbol{E}$ and the continuity equation

$$i\boldsymbol{q}\cdot\langle\hat{\boldsymbol{j}}_{\text{charge}}(\boldsymbol{q},\omega)\rangle = -ie\omega\langle\hat{n}(\boldsymbol{q},\omega)\rangle = i\sigma(\boldsymbol{q},\omega)\,\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega) \quad , \tag{10.137}$$

we find

$$\overbrace{\Big(4\pi\hat{\rho}_{\text{ext}}(\boldsymbol{q},\omega)-4\pi e\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle\Big)}^{i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega)}\,\sigma(\boldsymbol{q},\omega) = -i\omega e\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle \quad , \tag{10.138}$$

or

$$\frac{4\pi i}{\omega}\,\sigma(\boldsymbol{q},\omega)=\frac{\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle}{e^{-1}\hat{\rho}_{\text{ext}}(\boldsymbol{q},\omega)-\big\langle\delta\hat{n}(\boldsymbol{q},\omega)\big\rangle}=\frac{1-\epsilon^{-1}(\boldsymbol{q},\omega)}{\epsilon^{-1}(\boldsymbol{q}\omega)}=\epsilon(\boldsymbol{q},\omega)-1 \quad . \tag{10.139}$$

Thus, we arrive at

$$\frac{1}{\epsilon(\boldsymbol{q},\omega)}=1-\frac{4\pi e^2}{\boldsymbol{q}^2}\,\hat{\chi}(\boldsymbol{q},\omega) \qquad , \qquad \epsilon(\boldsymbol{q},\omega)=1+\frac{4\pi i}{\omega}\,\sigma(\boldsymbol{q},\omega) \quad . \tag{10.140}$$

Taken together, these two equations allow us to relate the conductivity and the charge response function,

$$\sigma(\boldsymbol{q},\omega)=-\frac{i\omega}{\boldsymbol{q}^2}\,\frac{e^2\hat{\chi}(\boldsymbol{q},\omega)}{1-\frac{4\pi e^2}{\boldsymbol{q}^2}\hat{\chi}(\boldsymbol{q},\omega)} \quad . \tag{10.141}$$

10.5.2 Static screening: Thomas-Fermi approximation

Imagine a time-independent, slowly varying electrical potential $\phi(\boldsymbol{x})$. We may define the 'local chemical potential' $\widetilde{\mu}(\boldsymbol{x})$ as

$$\mu \equiv \widetilde{\mu}(\boldsymbol{x}) - e\phi(\boldsymbol{x}) \quad , \tag{10.142}$$

where μ is the bulk chemical potential. The local chemical potential is related to the local density by local thermodynamics. At $T = 0$,

$$\begin{aligned} \widetilde{\mu}(\boldsymbol{x}) &\equiv \frac{\hbar^2}{2m}\, k_{\rm F}^2(\boldsymbol{x}) = \frac{\hbar^2}{2m}\Big(3\pi^2 n + 3\pi^2 \delta n(\boldsymbol{x})\Big)^{2/3} \\ &= \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}\left\{1 + \frac{2}{3}\,\frac{\delta n(\boldsymbol{x})}{n} + \ldots\right\} \quad , \end{aligned} \tag{10.143}$$

hence, to lowest order,

$$\delta n(\boldsymbol{x}) = \frac{3en}{2\mu}\,\phi(\boldsymbol{x}) \quad . \tag{10.144}$$

This makes sense – a positive potential induces an increase in the local electron number density. In Fourier space,

$$\langle \delta\hat{n}(\boldsymbol{q},\omega=0)\rangle = \frac{3en}{2\mu}\,\hat{\phi}(\boldsymbol{q},\omega=0) \quad . \tag{10.145}$$

Poisson's equation is $-\nabla^2\phi = 4\pi\rho_{\rm tot}$, *i.e.*

$$\begin{aligned} i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},0) = \boldsymbol{q}^2\,\hat{\phi}(\boldsymbol{q},0) &= 4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},0) - 4\pi e\,\langle\delta\hat{n}(\boldsymbol{q},0)\rangle \\ &= 4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},0) - \frac{6\pi n e^2}{\mu}\,\hat{\phi}(\boldsymbol{q},0) \quad , \end{aligned} \tag{10.146}$$

and defining the Thomas-Fermi wavevector $q_{\rm TF}$ by

$$q_{\rm TF}^2 \equiv \frac{6\pi n e^2}{\mu} \quad , \tag{10.147}$$

we have

$$\hat{\phi}(\boldsymbol{q},0) = \frac{4\pi\hat{\rho}_{\rm ext}(\boldsymbol{q},0)}{\boldsymbol{q}^2 + q_{\rm TF}^2} \quad , \tag{10.148}$$

hence

$$e\,\langle\delta\hat{n}(\boldsymbol{q},0)\rangle = \frac{q_{\rm TF}^2}{\boldsymbol{q}^2 + q_{\rm TF}^2}\cdot\hat{\rho}_{\rm ext}(\boldsymbol{q},0) \qquad \Longrightarrow \qquad \epsilon(\boldsymbol{q},0) = 1 + \frac{q_{\rm TF}^2}{\boldsymbol{q}^2} \quad . \tag{10.149}$$

Note that $\epsilon(\boldsymbol{q}\to 0,\omega=0) = \infty$, so there is perfect screening.

The Thomas-Fermi wavelength is $\lambda_{\rm TF} = q_{\rm TF}^{-1}$, and may be written as

$$\lambda_{\rm TF} = \left(\frac{\pi}{12}\right)^{1/6}\sqrt{r_s}\,a_{\rm B} \simeq 0.800\,\sqrt{r_s}\,a_{\rm B} \quad , \tag{10.150}$$

where r_s is the dimensionless free electron sphere radius, given in units of the Bohr radius $a_{\rm B} = \hbar^2/me^2 = 0.529$Å, defined by $\frac{4}{3}\pi(r_s a_{\rm B})^3 n = 1$, hence $r_s \propto n^{-1/3}$. Small r_s corresponds to high density. Since Thomas-Fermi theory is a statistical theory, it can only be valid if there are many particles within a sphere of radius $\lambda_{\rm TF}$, *i.e.* $\frac{4}{3}\pi\lambda_{\rm TF}^3\, n > 1$, or $r_s \lesssim (\pi/12)^{1/3} \simeq 0.640$. TF theory is applicable only in the high density limit.

In the presence of a δ-function external charge density $\rho_{\rm ext}(\boldsymbol{x}) = Ze\,\delta(\boldsymbol{x})$, we have its Fourier transform $\hat{\rho}_{\rm ext}(\boldsymbol{q},0) = Ze$, and

$$\langle \delta\hat{n}(\boldsymbol{q},0)\rangle = \frac{Z q_{\rm TF}^2}{\boldsymbol{q}^2 + q_{\rm TF}^2} \qquad \Longrightarrow \qquad \langle \delta n(\boldsymbol{x})\rangle = \frac{Z\, e^{-r/\lambda_{\rm TF}}}{4\pi r} \tag{10.151}$$

Note the decay on the scale of $\lambda_{\rm TF}$. Note also the perfect screening:

$$e\,\langle \delta\hat{n}(\boldsymbol{q}\to 0, \omega = 0)\rangle = \hat{\rho}_{\rm ext}(\boldsymbol{q}\to 0, \omega=0) = Ze \quad . \tag{10.152}$$

10.5.3 High frequency behavior of $\epsilon(\boldsymbol{q},\omega)$

We have

$$\epsilon^{-1}(\boldsymbol{q},\omega) = 1 - \frac{4\pi e^2}{\boldsymbol{q}^2}\,\hat{\chi}(\boldsymbol{q},\omega) \tag{10.153}$$

and, at $T=0$,

$$\hat{\chi}(\boldsymbol{q},\omega) = \frac{1}{\hbar V}\sum_j \big|\langle\, j\,|\, \hat{n}^\dagger_{\boldsymbol{q}}\,|\, 0\,\rangle\big|^2 \left\{ \frac{1}{\omega + \omega_j + i\epsilon} - \frac{1}{\omega - \omega_j + i\epsilon}\right\} \quad , \tag{10.154}$$

where the number density operator is

$$\hat{n}^\dagger_{\boldsymbol{q}} = \begin{cases} \sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{x}_i} & (1^{\rm st}\ \text{quantized}) \\ \sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}+\boldsymbol{q}}\,\psi_{\boldsymbol{k}} & (2^{\rm nd}\ \text{quantized: } \{\psi_{\boldsymbol{k}},\psi^\dagger_{\boldsymbol{k}'}\} = \delta_{\boldsymbol{k}\boldsymbol{k}'}) \quad . \end{cases} \tag{10.155}$$

Taking the limit $\omega\to\infty$, we find

$$\hat{\chi}(\boldsymbol{q},\omega\to\infty) = -\frac{2}{\hbar V\omega^2}\sum_j \big|\langle\, j\,|\,\hat{n}^\dagger_{\boldsymbol{q}}\,|\,0\,\rangle\big|^2\,\omega_j = -\frac{2}{\hbar\omega^2}\int\limits_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\,\omega'\,S(\boldsymbol{q},\omega') \quad . \tag{10.156}$$

Invoking the f-sum rule, the above integral is $n\hbar\boldsymbol{q}^2/2m$, hence

$$\hat{\chi}(\boldsymbol{q},\omega\to\infty) = -\frac{n\boldsymbol{q}^2}{m\omega^2} \quad , \tag{10.157}$$

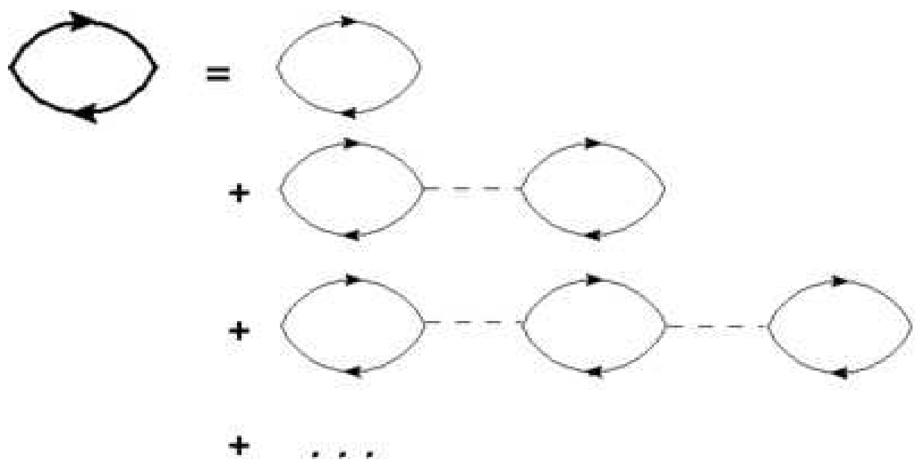

Figure 10.6: Perturbation expansion for RPA susceptibility bubble. Each bare bubble contributes a factor $\chi^0(\boldsymbol{q},\omega)$ and each wavy interaction line $\hat{v}(\boldsymbol{q})$. The infinite series can be summed, yielding eqn. 10.162.

and

$$\epsilon^{-1}(\boldsymbol{q},\omega\to\infty) = 1 + \frac{\omega_{\rm p}^2}{\omega^2} \quad , \tag{10.158}$$

where

$$\omega_{\rm p} \equiv \sqrt{\frac{4\pi n e^2}{m}} \tag{10.159}$$

is the *plasma frequency*.

10.5.4 Random phase approximation (RPA)

The electron charge appears nowhere in the free electron gas response function $\chi^0(\boldsymbol{q},\omega)$. An interacting electron gas certainly does know about electron charge, since the Coulomb repulsion between electrons is part of the Hamiltonian. The idea behind the RPA is to obtain an approximation to the interacting $\hat{\chi}(\boldsymbol{q},\omega)$ from the noninteracting $\chi^0(\boldsymbol{q},\omega)$ by self-consistently adjusting the charge so that the perturbing charge density is not $\rho_{\rm ext}(\boldsymbol{x})$, but rather $\rho_{\rm ext}(\boldsymbol{x},t) - e\,\langle\delta n(\boldsymbol{x},t)\rangle$. Thus, we write

$$\begin{aligned} e\,\langle\delta\hat{n}(\boldsymbol{q},\omega)\rangle &= \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^{\rm RPA}(\boldsymbol{q},\omega)\,\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega) \\ &= \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^0(\boldsymbol{q},\omega)\,\Big\{\hat{\rho}_{\rm ext}(\boldsymbol{q},\omega) - e\,\langle\delta\hat{n}(\boldsymbol{q},\omega)\rangle\Big\} \quad , \end{aligned} \tag{10.160}$$

which gives

$$\chi^{\rm RPA}(\boldsymbol{q},\omega) = \frac{\chi^0(\boldsymbol{q},\omega)}{1 + \frac{4\pi e^2}{\boldsymbol{q}^2}\chi^0(\boldsymbol{q},\omega)} \quad . \tag{10.161}$$

Several comments are in order.

1. If the electron-electron interaction were instead given by a general $\hat{v}(\boldsymbol{q})$ rather than the specific Coulomb form $\hat{v}(\boldsymbol{q}) = 4\pi e^2/\boldsymbol{q}^2$, we would obtain

$$\chi^{\text{RPA}}(\boldsymbol{q},\omega) = \frac{\chi^0(\boldsymbol{q},\omega)}{1 + \hat{v}(\boldsymbol{q})\,\chi^0(\boldsymbol{q},\omega)} \quad . \tag{10.162}$$

2. Within the RPA, there is perfect screening:

$$\lim_{\boldsymbol{q}\to 0} \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^{\text{RPA}}(\boldsymbol{q},\omega) = 1 \quad . \tag{10.163}$$

3. The RPA expression may be expanded in an infinite series,

$$\chi^{\text{RPA}} = \chi^0 - \chi^0\,\hat{v}\,\chi^0 + \chi^0\,\hat{v}\,\chi^0\,\hat{v}\,\chi^0 - \ldots \quad , \tag{10.164}$$

which has a diagrammatic interpretation, depicted in fig. 10.6. The perturbative expansion in the interaction $\hat{v}$ may be resummed to yield the RPA result.

4. The RPA dielectric function takes the simple form

$$\epsilon^{\text{RPA}}(\boldsymbol{q},\omega) = 1 + \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^0(\boldsymbol{q},\omega) \quad . \tag{10.165}$$

5. Explicitly,

$$\begin{aligned}\mathsf{Re}\ \epsilon^{\text{RPA}}(\boldsymbol{q},\omega) = 1 + \frac{q_{\text{TF}}^2}{q^2}\Bigg\{\frac{1}{2} + \frac{k_{\text{F}}}{4q}\Bigg[&\bigg(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\text{F}}q)^2}\bigg)\ln\bigg|\frac{\omega - v_{\text{F}}q - \hbar q^2/2m}{\omega + v_{\text{F}}q - \hbar q^2/2m}\bigg| \\ &+ \bigg(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\text{F}}q)^2}\bigg)\ln\bigg|\frac{\omega - v_{\text{F}}q + \hbar q^2/2m}{\omega + v_{\text{F}}q + \hbar q^2/2m}\bigg|\Bigg]\Bigg\}\end{aligned} \tag{10.166}$$

and

$$\mathsf{Im}\ \epsilon^{\text{RPA}}(\boldsymbol{q},\omega) = \begin{cases} \frac{\pi\omega}{2v_{\text{F}}q}\cdot\frac{q_{\text{TF}}^2}{q^2} & \text{if } 0 \leqslant \omega \leqslant v_{\text{F}}q - \hbar q^2/2m \\ \frac{\pi k_{\text{F}}}{4q}\Big(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\text{F}}q)^2}\Big)\,\frac{q_{\text{TF}}^2}{q^2} & \text{if } v_{\text{F}}q - \hbar q^2/2m \leqslant \omega \leqslant v_{\text{F}}q + \hbar q^2/2m \\ 0 & \text{if } \omega > v_{\text{F}}q + \hbar q^2/2m \end{cases} \tag{10.167}$$

6. Note that
$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q},\omega\to\infty)=1-\frac{\omega_{\mathrm{p}}^2}{\omega^2}\quad, \tag{10.168}$$
in agreement with the f-sum rule, and
$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q}\to 0,\omega=0)=1+\frac{q_{\mathrm{TF}}^2}{q^2}\quad, \tag{10.169}$$
in agreement with Thomas-Fermi theory.

7. When $\omega=0$ we have
$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q},0)=1+\frac{q_{\mathrm{TF}}^2}{q^2}\left\{\frac{1}{2}+\frac{k_{\mathrm{F}}}{2q}\left(1-\frac{q^2}{4k_{\mathrm{F}}^2}\right)\ln\left|\frac{q+2k_{\mathrm{F}}}{q-2k_{\mathrm{F}}}\right|\right\}\quad, \tag{10.170}$$
which is real and which has a singularity at $q=2k_{\mathrm{F}}$. This means that the long-distance behavior of $\langle\delta n(\boldsymbol{x})\rangle$ must oscillate. For a local charge perturbation, $\rho_{\mathrm{ext}}(\boldsymbol{x})=Ze\,\delta(\boldsymbol{x})$, we have
$$\langle\delta n(\boldsymbol{x})\rangle=\frac{Z}{2\pi^2 r}\int\limits_0^\infty dq\,q\sin(qr)\left\{1-\frac{1}{\epsilon(\boldsymbol{q},0)}\right\}\quad, \tag{10.171}$$
and within the RPA one finds for long distances
$$\langle\delta n(\boldsymbol{x})\rangle\sim\frac{Z\cos(2k_{\mathrm{F}}r)}{r^3}\quad, \tag{10.172}$$
rather than the Yukawa form familiar from Thomas-Fermi theory.

10.5.5 Plasmons

The RPA response function diverges when $\hat{v}(\boldsymbol{q})\,\chi^0(\boldsymbol{q},\omega)=-1$. For a given value of $\boldsymbol{q}$, this occurs for a specific value (or for a discrete set of values) of ω, *i.e.* it defines a dispersion relation $\omega=\Omega(\boldsymbol{q})$. The poles of χ^{RPA} and are identified with elementary excitations of the electron gas known as *plasmons*.

To find the plasmon dispersion, we first derive a result for $\chi^0(\boldsymbol{q},\omega)$, starting with
$$\begin{aligned}\chi^0(\boldsymbol{q},t)&=\frac{i}{\hbar V}\left\langle\big[\hat{n}(\boldsymbol{q},t),\hat{n}(-\boldsymbol{q},0)\big]\right\rangle\Theta(t)\\&=\frac{i}{\hbar V}\left\langle\Big[\sum_{\boldsymbol{k}\sigma}\psi^\dagger_{\boldsymbol{k},\sigma}\,\psi_{\boldsymbol{k}+\boldsymbol{q},\sigma},\sum_{\boldsymbol{k}',\sigma'}\psi^\dagger_{\boldsymbol{k}',\sigma'}\,\psi_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}\Big]\right\rangle e^{i(\varepsilon(\boldsymbol{k})-\varepsilon(\boldsymbol{k}+\boldsymbol{q}))t/\hbar}\,\Theta(t)\quad,\end{aligned} \tag{10.173}$$

where $\varepsilon(\boldsymbol{k})$ is the noninteracting electron dispersion. For a free electron gas, $\varepsilon(\boldsymbol{k}) = \hbar^2\boldsymbol{k}^2/2m$. Next, using

$$\big[AB, CD\big] = A\big\{B, C\big\}D - \big\{A, C\big\}BD + CA\big\{B, D\big\} - C\big\{A, D\big\}B \tag{10.174}$$

we obtain

$$\chi^0(\boldsymbol{q}, t) = \frac{i}{\hbar V}\sum_{\boldsymbol{k}\sigma}(f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}})\, e^{i(\varepsilon(\boldsymbol{k})-\varepsilon(\boldsymbol{k}+\boldsymbol{q}))t/\hbar}\,\Theta(t) \quad , \tag{10.175}$$

and therefore

$$\chi^0(\boldsymbol{q}, \omega) = 2\int\!\frac{d^3k}{(2\pi)^3}\;\frac{f_{\boldsymbol{k}+\boldsymbol{q}} - f_{\boldsymbol{k}}}{\hbar\omega - \varepsilon(\boldsymbol{k}+\boldsymbol{q}) + \varepsilon(\boldsymbol{k}) + i\epsilon} \quad . \tag{10.176}$$

Here,

$$f_{\boldsymbol{k}} = \frac{1}{e^{(\varepsilon(\boldsymbol{k})-\mu)/k_\mathrm{B}T} + 1} \tag{10.177}$$

is the Fermi distribution. At $T = 0$, $f_{\boldsymbol{k}} = \Theta(k_\mathrm{F} - k)$, and for $\omega \gg v_\mathrm{F}q$ we can expand $\chi^0(\boldsymbol{q}, \omega)$ in powers of ω^{-2}, yielding

$$\chi^0(\boldsymbol{q}, \omega) = -\frac{k_\mathrm{F}^3}{3\pi^2}\cdot\frac{q^2}{m\omega^2}\left\{1 + \frac{3}{5}\left(\frac{\hbar k_\mathrm{F} q}{m\omega}\right)^2 + \ldots\right\} \quad , \tag{10.178}$$

so the resonance condition becomes

$$\begin{aligned} 0 &= 1 + \frac{4\pi e^2}{q^2}\,\chi^0(\boldsymbol{q}, \omega) \\ &= 1 - \frac{\omega_\mathrm{p}^2}{\omega^2}\left\{1 + \frac{3}{5}\left(\frac{v_\mathrm{F} q}{\omega}\right)^2 + \ldots\right\} \quad . \end{aligned} \tag{10.179}$$

This gives the dispersion

$$\omega = \omega_\mathrm{p}\left\{1 + \frac{3}{10}\left(\frac{v_\mathrm{F} q}{\omega_\mathrm{p}}\right)^2 + \ldots\right\} \quad . \tag{10.180}$$

Recall that the particle-hole continuum frequencies are bounded by $\omega_{\mathrm{min}}(q)$ and $\omega_{\mathsf{max}}(q)$, which are given in eqs. 10.109 and 10.108. Eventually the plasmon penetrates the particle-hole continuum, at which point it becomes heavily damped since it can decay into particle-hole excitations.

10.5.6 Jellium

Finally, consider an electron gas in the presence of a neutralizing ionic background. We assume one species of ion with mass M_i and charge $+Z_\mathrm{i}e$, and we smear the ionic charge into a continuum as an approximation. This nonexistent material is known in the business of many-body physics as *jellium*. Let the ion number density be n_{i}, and the electron number density be n_{e}. Then Laplace's equation says

$$\nabla^2\phi = -4\pi\rho_{\mathrm{charge}} = -4\pi e\big(n_{\mathrm{i}} - n_{\mathrm{e}} + n_{\mathrm{ext}}\big) \quad , \tag{10.181}$$

where $n_{\mathrm{ext}} = \rho_{\mathrm{ext}}/e$, where ρ_{ext} is the test charge density, regarded as a perturbation to the jellium. The ions move according to

$$M_{\mathrm{i}}\,\frac{d\boldsymbol{v}}{dt} = Z_{\mathrm{i}}\,e\boldsymbol{E} = -Z_{\mathrm{i}}\,e\,\boldsymbol{\nabla}\phi \quad . \tag{10.182}$$

They also satisfy continuity, which to lowest order in small quantities is governed by the equation

$$n_{\mathrm{i}}^0\,\boldsymbol{\nabla}\!\cdot\!\boldsymbol{v} + \frac{\partial n_{\mathrm{i}}}{\partial t} = 0 \quad , \tag{10.183}$$

where n_i^0 is the average ionic number density. Taking the time derivative of the above equation, and invoking Newton's law for the ion's as well as Laplace, we find

$$-\frac{\partial^2 n_{\mathrm{i}}(\boldsymbol{x},t)}{\partial t^2} = \frac{4\pi n_{\mathrm{i}}^0 Z_{\mathrm{i}} e^2}{M_{\mathrm{i}}}\,\Big(n_{\mathrm{i}}(\boldsymbol{x},t) + n_{\mathrm{ext}}(\boldsymbol{x},t) - n_{\mathrm{e}}(\boldsymbol{x},t)\Big) \quad . \tag{10.184}$$

In Fourier space,

$$\omega^2\,\hat{n}_{\mathrm{i}}(\boldsymbol{q},\omega) = \mathit{\Omega}_{\mathrm{p,i}}^2\Big(\hat{n}_{\mathrm{i}}(\boldsymbol{q},\omega) + \hat{n}_{\mathrm{ext}}(\boldsymbol{q},\omega) - \hat{n}_{\mathrm{e}}(\boldsymbol{q},\omega)\Big) \quad , \tag{10.185}$$

where

$$\mathit{\Omega}_{\mathrm{p,i}} = \sqrt{\frac{4\pi n_{\mathrm{i}}^0 Z_{\mathrm{i}} e^2}{M_{\mathrm{i}}}} \tag{10.186}$$

is the ionic plasma frequency. Typically $\mathit{\Omega}_{\mathrm{p,i}} \approx 10^{13}\,\mathrm{s}^{-1}$.

Since the ionic mass M_{i} is much greater than the electron mass, the ionic plasma frequency is much greater than the electron plasma frequency. We assume that the ions may be regarded as 'slow' and that the electrons respond according to Eqn. 10.131, *viz.*

$$\hat{n}_{\mathrm{e}}(\boldsymbol{q},\omega) = \frac{4\pi e}{\boldsymbol{q}^2}\,\chi_{\mathrm{e}}(\boldsymbol{q},\omega)\,\Big(\hat{n}_{\mathrm{i}}(\boldsymbol{q},\omega) + \hat{n}_{\mathrm{ext}}(\boldsymbol{q},\omega)\Big) \quad . \tag{10.187}$$

We then have

$$\frac{\omega^2}{\mathit{\Omega}_{\mathrm{p,i}}^2}\,\hat{n}_{\mathrm{i}}(\boldsymbol{q},\omega) = \frac{\hat{n}_{\mathrm{i}}(\boldsymbol{q},\omega) + \hat{n}_{\mathrm{ext}}(\boldsymbol{q},\omega)}{\epsilon_{\mathrm{e}}(\boldsymbol{q},\omega)} \quad . \tag{10.188}$$

From this equation, we obtain $\hat{n}_{\mathrm{i}}(\boldsymbol{q},\omega)$ and then $n_{\mathrm{tot}} \equiv n_{\mathrm{i}} - n_{\mathrm{e}} + n_{\mathrm{ext}}$. We thereby obtain

$$\hat{n}_{\mathrm{tot}}(\boldsymbol{q},\omega) = \frac{\hat{n}_{\mathrm{ext}}(\boldsymbol{q},\omega)}{\epsilon_{\mathrm{e}}(\boldsymbol{q},\omega) - \omega^{-2}\,\mathit{\Omega}_{\mathrm{p,i}}^2} \quad . \tag{10.189}$$

Finally, the dielectric function of the jellium system is given by

$$\begin{aligned}\epsilon(\boldsymbol{q},\omega) &= \frac{\hat{n}_{\text{ext}}(\boldsymbol{q},\omega)}{\hat{n}_{\text{tot}}(\boldsymbol{q},\omega)} \\ &= \epsilon_{\text{e}}(\boldsymbol{q},\omega) - \frac{\omega^2}{\Omega^2_{\text{p,i}}} \quad .\end{aligned} \tag{10.190}$$

At frequencies low compared to the electron plasma frequency, we approximate $\epsilon_{\text{e}}(\boldsymbol{q},\omega)$ by the Thomas-Fermi form, $\epsilon_{\text{e}}(\boldsymbol{q},\omega) \approx \big(q^2 + q^2_{\text{TF}}\big)/q^2$. Then

$$\epsilon(\boldsymbol{q},\omega) \approx 1 + \frac{q^2_{\text{TF}}}{q^2} - \frac{\Omega^2_{\text{p,i}}}{\omega^2} \quad . \tag{10.191}$$

The zeros of this function, given by $\epsilon(\boldsymbol{q},\omega_{\boldsymbol{q}}) = 0$, occur for

$$\omega_{\boldsymbol{q}} = \frac{\Omega_{\text{p,i}}\, q}{\sqrt{q^2 + q^2_{\text{TF}}}} \quad . \tag{10.192}$$

This allows us to write

$$\frac{4\pi e^2}{\boldsymbol{q}^2}\,\frac{1}{\epsilon(\boldsymbol{q},\omega)} = \frac{4\pi e^2}{\boldsymbol{q}^2 + q^2_{\text{TF}}} \cdot \frac{\omega^2}{\omega^2 - \omega^2_{\boldsymbol{q}}} \quad . \tag{10.193}$$

This is interpreted as the effective interaction between charges in the jellium model, arising from both electronic and ionic screening. Note that the interaction is negative, *i.e.* attractive, for $\omega^2 < \omega^2_{\boldsymbol{q}}$. At frequencies high compared to $\omega_{\boldsymbol{q}}$, but low compared to the electronic plasma frequency, the effective potential is of the Yukawa form. Only the electrons then participate in screening, because the phonons are too slow.

10.6 Electromagnetic Response

Consider an interacting system consisting of electrons of charge $-e$ in the presence of a time-varying electromagnetic field. The electromagnetic field is given in terms of the 4-potential $A^\mu = (A^0, \boldsymbol{A})$:

$$\boldsymbol{E} = -\boldsymbol{\nabla} A^0 - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} \qquad , \qquad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} \quad . \tag{10.194}$$

The Hamiltonian for an N-particle system is

$$\begin{aligned}\hat{H}(A^\mu) &= \sum_{i=1}^N \left\{ \frac{1}{2m}\Big(\boldsymbol{p}_i + \frac{e}{c}\boldsymbol{A}(\boldsymbol{x}_i,t)\Big)^2 - eA^0(\boldsymbol{x}_i,t) + v_{\text{ext}}(\boldsymbol{x}_i)\right\} + \sum_{i<j} u(\boldsymbol{x}_i - \boldsymbol{x}_j) \\ &= \hat{H}(0) - \frac{1}{c}\int\! d^3\!x\; j^{\text{p}}_\mu(\boldsymbol{x})\, A^\mu(\boldsymbol{x},t) + \frac{e^2}{2mc^2}\int\! d^3\!x\; n(\boldsymbol{x})\, \boldsymbol{A}^2(\boldsymbol{x},t) \quad ,\end{aligned} \tag{10.195}$$

where we have defined

$$\begin{aligned} n(\boldsymbol{x}) &\equiv \sum_{i=1}^{N} \delta(\boldsymbol{x}-\boldsymbol{x}_i) \\ j^{\rm p}_0(\boldsymbol{x}) &\equiv c\,e\,n(\boldsymbol{x}) \\ \boldsymbol{j}^{\rm p}(\boldsymbol{x}) &\equiv -\frac{e}{2m}\sum_{i=1}^{N} \Big\{\boldsymbol{p}_i\,\delta(\boldsymbol{x}-\boldsymbol{x}_i)+\delta(\boldsymbol{x}-\boldsymbol{x}_i)\,\boldsymbol{p}_i\Big\} \quad . \end{aligned} \tag{10.196}$$

Throughout this discussion we invoke covariant/contravariant notation, using the metric

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad , \tag{10.197}$$

so that

$$\begin{aligned} j^\mu &= (j^0, j^1, j^2, j^3) \equiv (j^0, \boldsymbol{j}) \\ j_\mu &= g_{\mu\nu} j^\nu = (-j^0, j^1, j^2, j^3) \\ j_\mu A^\mu &= j^\mu g_{\mu\nu}\, A^\nu = -j^0 A^0 + \boldsymbol{j}\cdot\boldsymbol{A} \equiv j\cdot A \end{aligned} \tag{10.198}$$

The quantity $j^{\rm p}_\mu(\boldsymbol{x})$ is known as the *paramagnetic current density*. The physical current density $j_\mu(\boldsymbol{x})$ also contains a *diamagnetic* contribution:

$$\begin{aligned} j_\mu(\boldsymbol{x}) &= -c\,\frac{\delta\hat{H}}{\delta A^\mu(\boldsymbol{x})} = j^{\rm p}_\mu(\boldsymbol{x}) + j^{\rm d}_\mu(\boldsymbol{x}) \\ j^{\rm d}_0(\boldsymbol{x}) &= 0 \\ \boldsymbol{j}^{\rm d}(\boldsymbol{x}) &= -\frac{e^2}{mc}\, n(\boldsymbol{x})\boldsymbol{A}(\boldsymbol{x}) = -\frac{e}{mc^2}\, j^{\rm p}_0(\boldsymbol{x})\,\boldsymbol{A}(\boldsymbol{x}) \quad . \end{aligned} \tag{10.199}$$

The electromagnetic response tensor $K_{\mu\nu}$ is defined via

$$\big\langle j_\mu(\boldsymbol{x},t)\big\rangle = -\frac{c}{4\pi}\int\! dt' \!\int\! d^3\!x'\; K_{\mu\nu}(\boldsymbol{x}t;\boldsymbol{x}'t')\, A^\nu(\boldsymbol{x}',t') \quad , \tag{10.200}$$

valid to first order in the external 4-potential A^μ. From

$$\begin{aligned} \big\langle j^{\rm p}_\mu(\boldsymbol{x},t)\big\rangle &= \frac{i}{\hbar c}\int\! dt' \!\int\! d^3\!x'\; \big\langle \big[j^{\rm p}_\mu(\boldsymbol{x},t), j^{\rm p}_\nu(\boldsymbol{x}',t')\big]\big\rangle\; \Theta(t-t')\, A^\nu(\boldsymbol{x}',t') \\ \big\langle j^{\rm d}_\mu(\boldsymbol{x},t)\big\rangle &= -\frac{e}{mc^2}\,\big\langle j^{\rm p}_0(\boldsymbol{x},t)\big\rangle\, A^\mu(\boldsymbol{x},t)\,(1-\delta_{\mu 0}) \quad , \end{aligned} \tag{10.201}$$

we conclude

$$\begin{aligned} K_{\mu\nu}(\boldsymbol{x}t;\boldsymbol{x}'t') &= \frac{4\pi}{i\hbar c^2} \left\langle \left[j^{\text{p}}_\mu(\boldsymbol{x},t), j^{\text{p}}_\nu(\boldsymbol{x}',t') \right] \right\rangle \Theta(t-t') \\ &\qquad + \frac{4\pi e}{mc^2} \left\langle j^{\text{p}}_0(\boldsymbol{x},t) \right\rangle \delta(\boldsymbol{x}-\boldsymbol{x}')\, \delta(t-t')\, \delta_{\mu\nu}\, (1-\delta_{\mu 0}) \quad . \end{aligned} \tag{10.202}$$

The first term is sometimes known as the *paramagnetic response kernel*,

$$K^{\text{p}}_{\mu\nu}(x;x') = \frac{4\pi}{i\hbar c^2} \left\langle \left[j^{\text{p}}_\mu(x), j^{\text{p}}_\nu(x') \right] \right\rangle \Theta(t-t') \quad , \tag{10.203}$$

is not directly calculable by perturbation theory. Rather, one obtains the time-ordered response function $K^{\text{p;T}}_{\mu\nu}(x;x') = (4\pi/i\hbar c^2) \left\langle \hat{\mathcal{T}} j^{\text{p}}_\mu(x)\, j^{\text{p}}_\nu(x') \right\rangle$, where $x^\mu \equiv (ct, \boldsymbol{x})$.

Second quantized notation

In the presence of an electromagnetic field described by the 4-potential $A^\mu = (c\phi, \boldsymbol{A})$, the Hamiltonian of an interacting electron system takes the form

$$\begin{aligned} \hat{H} = \sum_\sigma \int \! d^3\!x\, \psi^\dagger_\sigma(\boldsymbol{x}) \left\{ \frac{1}{2m} \Big(\frac{\hbar}{i} \boldsymbol{\nabla} + \frac{e}{c} \boldsymbol{A} \Big)^2 - eA^0(\boldsymbol{x}) + v_{\mathsf{ext}}(\boldsymbol{x}) \right\} \psi_\sigma(\boldsymbol{x}) \\ + \frac{1}{2} \sum_{\sigma,\sigma'} \int \! d^3\!x \int \! d^3\!x'\, \psi^\dagger_\sigma(\boldsymbol{x})\, \psi^\dagger_{\sigma'}(\boldsymbol{x}')\, u(\boldsymbol{x}-\boldsymbol{x}')\, \psi_{\sigma'}(\boldsymbol{x}')\, \psi_\sigma(\boldsymbol{x}) \quad , \end{aligned} \tag{10.204}$$

where $v(\boldsymbol{x}-\boldsymbol{x}')$ is a two-body interaction, *e.g.* $e^2/|\boldsymbol{x}-\boldsymbol{x}'|$, and $U(\boldsymbol{x})$ is the external scalar potential. Expanding in powers of A^μ,

$$\hat{H}(A^\mu) = \hat{H}(0) - \frac{1}{c} \int \! d^3\!x\, j^{\text{p}}_\mu(\boldsymbol{x})\, A^\mu(\boldsymbol{x}) + \frac{e^2}{2mc^2} \sum_\sigma \int \! d^3\!x\, \psi^\dagger_\sigma(\boldsymbol{x})\, \psi_\sigma(\boldsymbol{x})\, \boldsymbol{A}^2(\boldsymbol{x}) \quad , \tag{10.205}$$

where the paramagnetic current density $j^{\text{p}}_\mu(\boldsymbol{x})$ is defined by

$$\begin{aligned} j^{\text{p}}_0(\boldsymbol{x}) &= c\, e \sum_\sigma \psi^\dagger_\sigma(\boldsymbol{x})\, \psi_\sigma(\boldsymbol{x}) \\ \boldsymbol{j}^{\text{p}}(\boldsymbol{x}) &= \frac{ie\hbar}{2m} \sum_\sigma \left\{ \psi^\dagger_\sigma(\boldsymbol{x})\, \boldsymbol{\nabla}\, \psi_\sigma(\boldsymbol{x}) - \Big(\boldsymbol{\nabla} \psi^\dagger_\sigma(\boldsymbol{x}) \Big)\, \psi_\sigma(\boldsymbol{x}) \right\} \quad . \end{aligned} \tag{10.206}$$

10.6.1 Gauge invariance and charge conservation

In Fourier space, with $q^\mu = (\omega/c, \boldsymbol{q})$, we have, for homogeneous systems,

$$\left\langle j_\mu(q) \right\rangle = -\frac{c}{4\pi}\, K_{\mu\nu}(q)\, A^\nu(q) \quad . \tag{10.207}$$

Note our convention on Fourier transforms:

$$\begin{aligned} H(x) &= \int \frac{d^4k}{(2\pi)^4}\, \hat{H}(k)\, e^{+ik\cdot x} \\ \hat{H}(k) &= \int d^4\!x\, H(x)\, e^{-ik\cdot x} \quad , \end{aligned} \tag{10.208}$$

where $k\cdot x \equiv k_\mu x^\mu = \boldsymbol{k}\cdot\boldsymbol{x} - \omega t$. Under a gauge transformation, $A^\mu \to A^\mu + \partial^\mu \Lambda$, *i.e.*

$$A^\mu(q) \to A^\mu(q) + i\Lambda(q)\, q^\mu \quad , \tag{10.209}$$

where Λ is an arbitrary scalar function. Since the physical current must be unchanged by a gauge transformation, we conclude that $K_{\mu\nu}(q)\, q^\nu = 0$. We also have the continuity equation, $\partial^\mu j_\mu = 0$, the Fourier space version of which says $q^\mu\, j_\mu(q) = 0$, which in turn requires $q^\mu\, K_{\mu\nu}(q) = 0$. Therefore,

$$\sum_\mu q^\mu\, K_{\mu\nu}(q) = \sum_\nu K_{\mu\nu}(q)\, q^\nu = 0 \quad . \tag{10.210}$$

In fact, the above conditions are identical owing to the reciprocity relations,

$$\begin{aligned} \mathsf{Re}\ K_{\mu\nu}(q) &= +\mathsf{Re}\ K_{\nu\mu}(-q) \\ \mathsf{Im}\ K_{\mu\nu}(q) &= -\mathsf{Im}\ K_{\nu\mu}(-q) \quad , \end{aligned} \tag{10.211}$$

which follow from the spectral representation of $K_{\mu\nu}(q)$. Thus,

$$\text{gauge invariance} \Longleftrightarrow \text{charge conservation} \quad . \tag{10.212}$$

10.6.2 A sum rule

If we work in a gauge where $A^0 = 0$, then $\boldsymbol{E} = -c^{-1}\dot{\boldsymbol{A}}$, hence $\boldsymbol{E}(q) = iq^0 \boldsymbol{A}(q)$, and

$$\begin{aligned} \big\langle j_i(q) \big\rangle &= -\frac{c}{4\pi}\, K_{ij}(q)\, A^j(q) \\ &= -\frac{c}{4\pi}\, K_{ij}(q)\, \frac{c}{i\omega}\, E^j(q) \equiv \sigma_{ij}(q)\, E^j(q) \quad . \end{aligned}$$

Thus, the conductivity tensor is given by

$$\sigma_{ij}(\boldsymbol{q},\omega) = \frac{ic^2}{4\pi\omega}\, K_{ij}(\boldsymbol{q},\omega) \quad . \tag{10.213}$$

If, in the $\omega \to 0$ limit, the conductivity is to remain finite, then we must have

$$\int\limits_0^\infty \! dt \int \! d^3\!x\, \Big\langle \big[j_i^{\rm p}(\boldsymbol{x},t), j_j^{\rm p}(0,0) \big] \Big\rangle\, e^{+i\omega t} = \frac{ie^2 n}{m}\, \delta_{ij} \quad , \tag{10.214}$$

where n is the electron number density. This relation is spontaneously violated in a superconductor, where $\sigma(\omega) \propto \omega^{-1}$ as $\omega \to 0$.

10.6.3 Longitudinal and transverse response

In an isotropic system, the spatial components of $K_{\mu\nu}$ may be resolved into longitudinal and transverse components, since the only preferred spatial vector is $\boldsymbol{q}$ itself. Thus, we may write

$$K_{ij}(\boldsymbol{q},\omega) = K_{\parallel}(\boldsymbol{q},\omega)\,\hat{q}_i\,\hat{q}_j + K_{\perp}(\boldsymbol{q},\omega)\,\big(\delta_{ij} - \hat{q}_i\,\hat{q}_j\big) \quad , \tag{10.215}$$

where $\hat{q}_i \equiv q_i/|\boldsymbol{q}|$. We now invoke current conservation, which says $q^\mu\,K_{\mu\nu}(q) = 0$. When $\nu = j$ is a spatial index,

$$q^0\,K_{0j} + q^i\,K_{ij} = \frac{\omega}{c}\,K_{0j} + K_{\parallel}\,q_j \quad , \tag{10.216}$$

which yields

$$K_{0j}(\boldsymbol{q},\omega) = -\frac{c}{\omega}\,q^j\,K_{\parallel}(\boldsymbol{q},\omega) = K_{j0}(\boldsymbol{q},\omega) \quad . \tag{10.217}$$

In other words, the three components of $K_{0j}(q)$ are in fact completely determined by $K_{\parallel}(q)$ and q itself. When $\nu = 0$,

$$0 = q^0\,K_{00} + q^i\,K_{i0} = \frac{\omega}{c}\,K_{00} - \frac{c}{\omega}\,\boldsymbol{q}^2\,K_{\parallel} \quad , \tag{10.218}$$

which says

$$K_{00}(\boldsymbol{q},\omega) = \frac{c^2}{\omega^2}\,\boldsymbol{q}^2\,K_{\parallel}(\boldsymbol{q},\omega) \quad . \tag{10.219}$$

Thus, of the 10 freedoms of the symmetric 4×4 tensor $K_{\mu\nu}(q)$, there are only two independent ones – the functions $K_{\parallel}(q)$ and $K_{\perp}(q)$.

10.6.4 Neutral systems

In neutral systems, we define the number density and number current density as

$$\begin{aligned} n(\boldsymbol{x}) &= \sum_{i=1}^N \delta(\boldsymbol{x} - \boldsymbol{x}_i) \\ \boldsymbol{j}(\boldsymbol{x}) &= \frac{1}{2m}\sum_{i=1}^N \Big\{ \boldsymbol{p}_i\,\delta(\boldsymbol{x} - \boldsymbol{x}_i) + \delta(\boldsymbol{x} - \boldsymbol{x}_i)\,\boldsymbol{p}_i \Big\} \quad . \end{aligned} \tag{10.220}$$

The charge and current susceptibilities are then given by

$$\begin{aligned} \chi(\boldsymbol{x},t) &= \frac{i}{\hbar}\,\big\langle \big[n(\boldsymbol{x},t), n(0,0)\big]\big\rangle\,\Theta(t) \\ \chi_{ij}(\boldsymbol{x},t) &= \frac{i}{\hbar}\,\big\langle \big[j_i(\boldsymbol{x},t), j_j(0,0)\big]\big\rangle\,\Theta(t) \quad . \end{aligned} \tag{10.221}$$

We define the longitudinal and transverse susceptibilities for homogeneous systems according to

$$\chi_{ij}(\boldsymbol{q},\omega) = \chi_{\parallel}(\boldsymbol{q},\omega)\,\hat{q}_i\,\hat{q}_j + \chi_{\perp}(\boldsymbol{q},\omega)\,(\delta_{ij} - \hat{q}_i\,\hat{q}_j) \quad . \tag{10.222}$$

From the continuity equation,

$$\nabla \cdot \boldsymbol{j} + \frac{\partial n}{\partial t} = 0 \tag{10.223}$$

follows the relation

$$\chi_{\|}(\boldsymbol{q},\omega) = \frac{n}{m} + \frac{\omega^2}{\boldsymbol{q}^2}\,\hat{\chi}(\boldsymbol{q},\omega) \quad . \tag{10.224}$$

EXERCISE: Derive eqn. (10.224).

The relation between $K_{\mu\nu}(q)$ and the neutral susceptibilities defined above is then

$$\begin{aligned} K_{00}(\boldsymbol{x},t) &= -4\pi e^2\,\chi(\boldsymbol{x},t) \\ K_{ij}(\boldsymbol{x},t) &= \frac{4\pi e^2}{c^2}\left\{\frac{n}{m}\,\delta(\boldsymbol{x})\,\delta(t) - \chi_{ij}(\boldsymbol{x},t)\right\} \quad , \end{aligned} \tag{10.225}$$

and therefore

$$\begin{aligned} K_{\|}(\boldsymbol{q},\omega) &= \frac{4\pi e^2}{c^2}\left\{\frac{n}{m} - \chi_{\|}(\boldsymbol{q},\omega)\right\} \\ K_{\perp}(\boldsymbol{q},\omega) &= \frac{4\pi e^2}{c^2}\left\{\frac{n}{m} - \chi_{\perp}(\boldsymbol{q},\omega)\right\} \quad . \end{aligned} \tag{10.226}$$

10.6.5 The Meissner effect and superfluid density

Suppose we apply an electromagnetic field $\boldsymbol{E}$. We adopt a gauge in which $A^0 = 0$, $\boldsymbol{E} = -c^{-1}\dot{\boldsymbol{A}}$, and $\boldsymbol{B} = \nabla \times \boldsymbol{A}$. To satisfy Maxwell's equations[5], we have $\boldsymbol{q}\cdot\boldsymbol{A}(\boldsymbol{q},\omega) = 0$, *i.e.* $\boldsymbol{A}(\boldsymbol{q},\omega)$ is purely transverse. But then

$$\big\langle \boldsymbol{j}(\boldsymbol{q},\omega)\big\rangle = -\frac{c}{4\pi}\,K_{\perp}(\boldsymbol{q},\omega)\,\boldsymbol{A}(\boldsymbol{q},\omega) \quad . \tag{10.227}$$

This leads directly to the Meissner effect whenever $\lim_{\boldsymbol{q}\to 0} K_{\perp}(\boldsymbol{q},0)$ is finite. To see this, we write

$$\begin{aligned} \nabla \times \boldsymbol{B} &= \nabla\,(\nabla\cdot\boldsymbol{A}) - \nabla^2\boldsymbol{A} \\ &= \frac{4\pi}{c}\,\boldsymbol{j} + \frac{1}{c}\frac{\partial \boldsymbol{E}}{\partial t} \\ &= \frac{4\pi}{c}\left(-\frac{c}{4\pi}\right) K_{\perp}(-i\nabla, i\,\partial_t)\,\boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2\boldsymbol{A}}{\partial t^2} \quad , \end{aligned} \tag{10.228}$$

which yields

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\boldsymbol{A} = K_{\perp}(-i\nabla, i\,\partial_t)\boldsymbol{A} \quad . \tag{10.229}$$

[5] *I.e.* if $\nabla\cdot\boldsymbol{E} = 0$, which pertains when there is local charge neutrality.

In the static limit, $\boldsymbol{\nabla}^2 \boldsymbol{A} = K_\perp(-i\boldsymbol{\nabla}, 0)\boldsymbol{A}$, and we define

$$\frac{1}{\lambda_{\rm L}^2} \equiv \lim_{\boldsymbol{q}\to 0} K_\perp(\boldsymbol{q}, 0) \quad . \tag{10.230}$$

$\lambda_{\rm L}$ is the *London penetration depth*, which is related to the *superfluid density* $n_{\rm s}$ by

$$n_{\rm s} \equiv \frac{mc^2}{4\pi e^2 \lambda_{\rm L}^2} = n - m \lim_{\boldsymbol{q}\to 0} \chi_\perp(\boldsymbol{q}, 0) \quad . \tag{10.231}$$

Since the function $K_\perp(\boldsymbol{q}, 0)$ has dimensions of L^{-2}, assuming spatial isotropy, we may define another length scale, λ, by

$$\lambda = \frac{2}{\pi} \int\limits_0^\infty \frac{dq}{q^2 + K_\perp(q, 0)} \quad . \tag{10.232}$$

Note that if $K_\perp(q, 0)$ is q-independent then $\lambda = \lambda_{\rm L}$.

Ideal Bose gas

We start from

$$\begin{aligned} \chi_{ij}(\boldsymbol{q}, t) &= \frac{i}{\hbar V} \big\langle \big[j_i(\boldsymbol{q}, t), j_j(-\boldsymbol{q}, 0) \big] \big\rangle \, \Theta(t) \\ j_i(\boldsymbol{q}) &= \frac{\hbar}{2m} \sum_{\boldsymbol{k}} (2k_i + q_i) \, \psi^\dagger_{\boldsymbol{k}} \, \psi_{\boldsymbol{k}+\boldsymbol{q}} \quad . \end{aligned} \tag{10.233}$$

For the free Bose gas, with dispersion $\omega_{\boldsymbol{k}} = \hbar \boldsymbol{k}^2/2m$,

$$\begin{aligned} j_i(\boldsymbol{q}, t) &= \frac{\hbar}{2m} \sum_{\boldsymbol{k}} (2k_i + q_i) \, e^{i(\omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}})t} \, \psi^\dagger_{\boldsymbol{k}} \, \psi_{\boldsymbol{k}+\boldsymbol{q}} \\ \big[j_i(\boldsymbol{q}, t), j_j(-\boldsymbol{q}, 0) \big] &= \frac{\hbar^2}{4m^2} \sum_{\boldsymbol{k},\boldsymbol{k}'} (2k_i + q_i)(2k'_j - q_j) \, e^{i(\omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}})t} \big[\psi^\dagger_{\boldsymbol{k}} \, \psi_{\boldsymbol{k}+\boldsymbol{q}}, \psi^\dagger_{\boldsymbol{k}'} \, \psi_{\boldsymbol{k}'-\boldsymbol{q}} \big] \end{aligned} \tag{10.234}$$

Using

$$[AB, CD] = A \, [B, C] \, D + AC \, [B, D] + C \, [A, D] \, B + [A, C] \, DB \quad , \tag{10.235}$$

we obtain

$$\big[j_i(\boldsymbol{q}, t), j_j(-\boldsymbol{q}, 0) \big] = \frac{\hbar^2}{4m^2} \sum_{\boldsymbol{k}} (2k_i + q_i)(2k_j + q_j) \, e^{i(\omega_{\boldsymbol{k}} - \omega_{\boldsymbol{k}+\boldsymbol{q}})t} \, \big\{ n^0(\omega_{\boldsymbol{k}}) - n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}}) \big\} \quad , \tag{10.236}$$

where $n^0(\omega)$ is the equilibrium Bose distribution[6],

$$n^0(\omega) = \frac{1}{e^{\beta\hbar\omega} \, e^{-\beta\mu} - 1} \quad . \tag{10.237}$$

[6]Recall that $\mu = 0$ in the condensed phase.

Thus,

$$\begin{aligned}\chi_{ij}(\boldsymbol{q},\omega) &= \frac{\hbar}{4m^2V}\sum_{\boldsymbol{k}}(2k_i+q_i)(2k_j+q_j)\,\frac{n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}})-n^0(\omega_{\boldsymbol{k}})}{\omega+\omega_{\boldsymbol{k}}-\omega_{\boldsymbol{k}+\boldsymbol{q}}+i\epsilon} \\ &= \frac{\hbar n_0}{4m^2}\left\{\frac{1}{\omega+\omega_{\boldsymbol{q}}+i\epsilon}-\frac{1}{\omega-\omega_{\boldsymbol{q}}+i\epsilon}\right\}q_i\,q_j+\frac{\hbar}{m^2}\int\!\frac{d^3k}{(2\pi)^3}\,\frac{n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}/2})-n^0(\omega_{\boldsymbol{k}-\boldsymbol{q}/2})}{\omega+\omega_{\boldsymbol{k}-\boldsymbol{q}/2}-\omega_{\boldsymbol{k}+\boldsymbol{q}/2}+i\epsilon}\,k_i\,k_j \quad ,\end{aligned} \tag{10.238}$$

where $n_0 = N_0/V$ is the condensate number density. Taking the $\omega = 0$, $\boldsymbol{q} \to 0$ limit yields

$$\chi_{ij}(\boldsymbol{q}\to 0,0) = \frac{n_0}{m}\,\hat{q}_i\,\hat{q}_j + \frac{n'}{m}\,\delta_{ij} \quad , \tag{10.239}$$

where n' is the density of uncondensed bosons. From this we read off

$$\chi_{\|}(\boldsymbol{q}\to 0,0) = \frac{n}{m} \qquad , \qquad \chi_{\perp}(\boldsymbol{q}\to 0,0) = \frac{n'}{m} \quad , \tag{10.240}$$

where $n = n_0 + n'$ is the total boson number density. The superfluid density, according to (10.231), is $n_{\mathrm{s}} = n_0(T)$.

In fact, the ideal Bose gas is *not* a superfluid. Its excitation spectrum is too 'soft' - any superflow is unstable toward decay into single particle excitations.