Chapter 3

Linear Response Theory

3.1 Response and Resonance

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

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = f(t) \ , \tag{3.1}$$

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 $H(t)$:

$$H(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \hat{H}(\omega) \, e^{-i\omega t} \tag{3.2}$$

$$\hat{H}(\omega) = \int\limits_{-\infty}^{\infty} dt \, H(t) \, e^{+i\omega t} \ . \tag{3.3}$$

Note that if $H(t)$ is a real function, then $\hat{H}(-\omega) = \hat{H}^*(\omega)$. In Fourier space, then, eqn. (3.1) becomes

$$(\omega_0^2 - 2i\gamma\omega - \omega^2) \, \hat{\boldsymbol{x}}(\omega) = \hat{f}(\omega) \ , \tag{3.4}$$

with the solution

$$\hat{\boldsymbol{x}}(\omega) = \frac{\hat{f}(\omega)}{\omega_0^2 - 2i\gamma\omega - \omega^2} \equiv \hat{\chi}(\omega) \, \hat{f}(\omega) \tag{3.5}$$

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

$$\hat{\chi}(\omega) = \frac{1}{\omega_0^2 - 2i\gamma\omega - \omega^2} = \frac{-1}{(\omega - \omega_+)(\omega - \omega_-)} \ , \tag{3.6}$$

with

$$\omega_\pm = -i\gamma \pm \sqrt{\omega_0^2 - \gamma^2} \ . \tag{3.7}$$

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

The complete solution to (3.1) is then

$$x(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, \frac{\hat{f}(\omega)\, e^{-i\omega t}}{\omega_0^2 - 2i\gamma\omega - \omega^2} + x_{\rm h}(t) \tag{3.8}$$

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

$$x_{\rm h}(t) = A_+ e^{-i\omega_+ t} + A_- e^{-i\omega_- t} \ . \tag{3.9}$$

Since $\text{Im}(\omega_\pm) < 0$, $x_{\rm h}(t)$ 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

$$x(t) = \int_{-\infty}^{\infty} dt' \ \chi(t-t') \, f(t') \tag{3.10}$$

$$\chi(s) \equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \ \hat{\chi}(\omega)\, e^{-i\omega s} \ , \tag{3.11}$$

which brings us to a very important and sensible result:

<u>Claim</u>: 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.

<u>Proof</u>: Consider eqn. (3.11). 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 (3.6), we close in the LHP for $s > 0$ and obtain

$$\begin{aligned} \chi(s>0) &= (-2\pi i) \sum_{\omega \in \text{LHP}} \text{Res} \left\{ \frac{1}{2\pi} \, \hat{\chi}(\omega)\, e^{-i\omega s} \right\} \\ &= \frac{i e^{-i\omega_+ s}}{\omega_+ - \omega_-} + \frac{i e^{-i\omega_- s}}{\omega_- - \omega_+} \ , \end{aligned} \tag{3.12}$$

i.e.

$$\chi(s) = \begin{cases} \frac{e^{-\gamma s}}{\sqrt{\omega_0^2 - \gamma^2}} \, \sin\!\left(\sqrt{\omega_0^2 - \gamma^2}\right) \Theta(s) & \text{if } \omega_0^2 > \gamma^2 \\ \\ \frac{e^{-\gamma s}}{\sqrt{\gamma^2 - \omega_0^2}} \, \sinh\!\left(\sqrt{\gamma^2 - \omega_0^2}\right) \Theta(s) & \text{if } \omega_0^2 < \gamma^2 \ , \end{cases} \tag{3.13}$$

where $\Theta(s)$ is the step function: $\Theta(s \geq 0) = 1$, $\Theta(s < 0) = 0$. 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 $t = 0$.

3.1.1 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

$$P(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,(-i\omega)\,\hat{\chi}(\omega)\,\hat{f}(\omega)\,e^{-i\omega t} \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi}\,\hat{f}^*(\nu)\,e^{+i\nu t} \tag{3.14}$$

$$\Delta E = \int\limits_{-\infty}^{\infty} dt\,P(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,(-i\omega)\,\hat{\chi}(\omega)\,\big|\hat{f}(\omega)\big|^2 \ . \tag{3.15}$$

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

$$\hat{\chi}(\omega) = \hat{\chi}'(\omega) + i\hat{\chi}''(\omega) \ , \tag{3.16}$$

we find for our example

$$\hat{\chi}'(\omega) = \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + 4\gamma^2\omega^2} = +\hat{\chi}'(-\omega) \tag{3.17}$$

$$\hat{\chi}''(\omega) = \frac{2\gamma\omega}{(\omega_0^2 - \omega^2)^2 + 4\gamma^2\omega^2} = -\hat{\chi}''(-\omega). \tag{3.18}$$

The energy dissipated may now be written

$$\Delta E = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\omega\,\hat{\chi}''(\omega)\,\big|\hat{f}(\omega)\big|^2 \ . \tag{3.19}$$

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.

3.2 Kramers-Kronig Relations

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

$$\oint\limits_{\mathcal{C}} \frac{dz}{2\pi i}\,\frac{\chi(z)}{z-\zeta} = 0 \ , \tag{3.20}$$

whenever $\mathrm{Im}(\zeta) \le 0$, where $\mathcal{C}$ is the contour depicted in fig. 3.1.

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

$$\chi(\omega) \equiv \lim_{\epsilon\to 0^+} \chi(\omega + i\epsilon) \ . \tag{3.21}$$

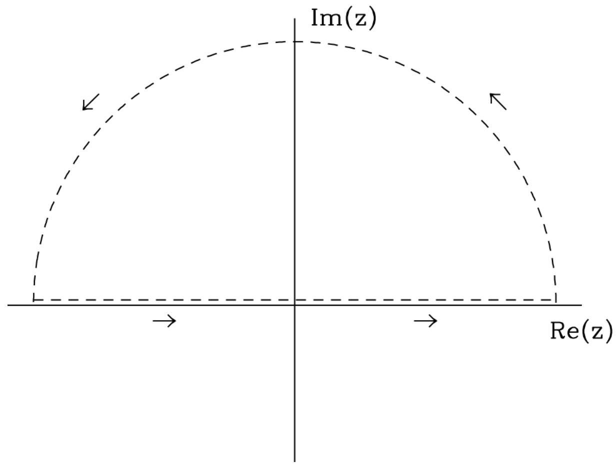

Figure 3.1: The complex integration contour $\mathcal{C}$.

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

$$\begin{aligned} 0 &= \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \, \frac{\chi(\nu)}{\nu - \omega + i\epsilon} \\ &= \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \, \big[\chi'(\nu) + i\chi''(\nu)\big] \left[\frac{\mathcal{P}}{\nu - \omega} - i\pi\delta(\nu - \omega)\right] \end{aligned} \tag{3.22}$$

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

$$\chi'(\omega) = \mathcal{P}\int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi} \, \frac{\chi''(\nu)}{\nu - \omega} \tag{3.23}$$

$$\chi''(\omega) = -\mathcal{P}\int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi} \, \frac{\chi'(\nu)}{\nu - \omega} \ . \tag{3.24}$$

The Kramers-Kronig relations are valid for any function $\chi(z)$ which is analytic in the upper half plane.

If $\chi(z)$ is analytic everywhere off the $\mathrm{Im}(z) = 0$ axis, we may write

$$\chi(z) = \int\limits_{-\infty}^{\infty} \frac{d\nu}{\pi} \, \frac{\chi''(\nu)}{\nu - z} \ . \tag{3.25}$$

This immediately yields the result

$$\lim_{\epsilon \to 0^+} \big[\chi(\omega + i\epsilon) - \chi(\omega - i\epsilon)\big] = 2i\,\chi''(\omega) \ . \tag{3.26}$$

As an example, consider the function

$$\chi''(\omega) = \frac{\omega}{\omega^2 + \gamma^2} \ . \tag{3.27}$$

Then, choosing $\gamma > 0$,

$$\chi(z) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \, \frac{1}{\omega - z} \cdot \frac{\omega}{\omega^2 + \gamma^2} = \begin{cases} i/(z + i\gamma) & \text{if } \text{Im}(z) > 0 \\ \\ -i/(z - i\gamma) & \text{if } \text{Im}(z) < 0 \ . \end{cases} \tag{3.28}$$

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

EXERCISE: Show that eqn. (3.26) is satisfied for $\chi(\omega) = \omega/(\omega^2 + \gamma^2)$.

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

$$\tilde{\chi}(z) = \frac{i}{z + i\gamma} \ . \tag{3.29}$$

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

3.3 Quantum Mechanical Response Functions

Now consider a general quantum mechanical system with a Hamiltonian $\mathcal{H}_0$ subjected to a time-dependent perturbation, $\mathcal{H}_1(t)$, where

$$\mathcal{H}_1(t) = -\sum_i Q_i \, \phi_i(t) \ . \tag{3.30}$$

Here, the $\{Q_i\}$ are a set of Hermitian operators, and the $\{\phi_i(t)\}$ are fields or potentials. Some examples:

$$\mathcal{H}_1(t) = \begin{cases} -\boldsymbol{M} \cdot \boldsymbol{B}(t) & \text{magnetic moment -- magnetic field} \\ \\ \int d^3\!r \, \varrho(\boldsymbol{r}) \, \phi(\boldsymbol{r}, t) & \text{density -- scalar potential} \\ \\ -\frac{1}{c} \int d^3\!r \, \boldsymbol{j}(\boldsymbol{r}) \cdot \boldsymbol{A}(\boldsymbol{r}, t) & \text{electromagnetic current -- vector potential} \end{cases}$$

We now ask, what is $\langle Q_i(t) \rangle$? We assume that the lowest order response is linear, *i.e.*

$$\langle Q_i(t) \rangle = \int_{-\infty}^{\infty} dt' \, \chi_{ij}(t - t') \, \phi_j(t') + \mathcal{O}(\phi_k \, \phi_l) \ . \tag{3.31}$$

Note that we assume that the $\mathcal{O}(\phi^0)$ term vanishes, which can be assured with a judicious choice of the $\{Q_i\}$[2]. We also assume that the responses are all causal, *i.e.* $\chi_{ij}(t - t') = 0$ for

[2] If not, define $\delta Q_i \equiv Q_i - \langle Q_i \rangle_0$ and consider $\langle \delta Q_i(t) \rangle$.

$t < t'$. To compute $\chi_{ij}(t-t')$, we will use first order perturbation theory to obtain $\langle Q_i(t)\rangle$ and then functionally differentiate with respect to $\phi_j(t')$:

$$\chi_{ij}(t-t') = \frac{\delta\big\langle Q_i(t)\big\rangle}{\delta\phi_j(t')} \ . \tag{3.32}$$

The first step is to establish the result,

$$\big|\,\Psi(t)\,\big\rangle = \mathcal{T}\,\exp\bigg\{-\frac{i}{\hbar}\int\limits_{t_0}^{t}\!dt'\,\big[\mathcal{H}_0 + \mathcal{H}_1(t')\big]\bigg\}\big|\,\Psi(t_0)\,\big\rangle \ , \tag{3.33}$$

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

$$i\hbar\frac{d}{dt}\big|\,\Psi(t)\,\big\rangle = \mathcal{H}(t)\big|\,\Psi(t)\,\big\rangle \ , \tag{3.34}$$

where $\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t)$. Integrating this equation from t to $t+dt$ gives

$$\big|\,\Psi(t+dt)\,\big\rangle = \Big(1 - \frac{i}{\hbar}\mathcal{H}(t)\,dt\Big)\,\big|\,\Psi(t)\,\big\rangle \tag{3.35}$$

$$\big|\,\Psi(t_0+N\,dt)\,\big\rangle = \Big(1 - \frac{i}{\hbar}\mathcal{H}(t_0+(N-1)dt)\Big)\cdots\Big(1 - \frac{i}{\hbar}\mathcal{H}(t_0)\Big)\,\big|\,\Psi(t_0)\,\big\rangle \ , \tag{3.36}$$

hence

$$\big|\,\Psi(t_2)\,\big\rangle = U(t_2,t_1)\,\big|\,\Psi(t_1)\,\big\rangle \tag{3.37}$$

$$U(t_2,t_1) = \mathcal{T}\exp\bigg\{-\frac{i}{\hbar}\int\limits_{t_1}^{t_2}\!dt\,\mathcal{H}(t)\bigg\} \ . \tag{3.38}$$

$U(t_2,t_1)$ is a unitary operator (*i.e.* $U^\dagger = U^{-1}$), known as the *time evolution operator* between times t_1 and t_2.

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

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

$$\frac{\delta U(t_2,t_1)}{\delta\phi_j(t)} = \frac{i}{\hbar}\,U(t_2,t)\,Q_j\,U(t,t_1) \ , \tag{3.39}$$

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

$$\begin{aligned}\frac{\delta\big|\,\Psi(t)\,\big\rangle}{\delta\phi_j(t')}\bigg|_{\{\phi_i=0\}} &= \frac{i}{\hbar}\,e^{-i\mathcal{H}_0(t-t')/\hbar}\,Q_j\,e^{-i\mathcal{H}_0(t'-t_0)/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\Theta(t-t')\\ &= \frac{i}{\hbar}\,e^{-i\mathcal{H}_0 t/\hbar}\,Q_j(t')\,e^{+i\mathcal{H}_0\,t_0/\hbar}\,\big|\,\Psi(t_0)\,\big\rangle\Theta(t-t') \ ,\end{aligned} \tag{3.40}$$

where

$$Q_j(t) \equiv e^{i\mathcal{H}_0 t/\hbar}\, Q_j \, e^{-i\mathcal{H}_0 t/\hbar} \tag{3.41}$$

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

$$\begin{aligned}
\chi_{ij}(t-t') &= \frac{\delta}{\delta\phi_j(t')} \big\langle\, \Psi(t) \,\big|\, Q_i \,\big|\, \Psi(t) \,\big\rangle \\
&= \frac{\delta\big\langle\, \Psi(t) \,\big|}{\delta\phi_j(t')}\, Q_i \big|\, \Psi(t) \,\big\rangle + \big\langle\, \Psi(t) \,\big| Q_i \, \frac{\delta\big|\, \Psi(t) \,\big\rangle}{\delta\phi_j(t')} \\
&= \bigg\{ -\frac{i}{\hbar} \big\langle\, \Psi(t_0) \,\big|\, e^{-i\mathcal{H}_0\, t_0/\hbar}\, Q_j(t')\, e^{+i\mathcal{H}_0 t/\hbar}\, Q_i \,\big|\, \Psi(t) \,\big\rangle \\
&\qquad + \frac{i}{\hbar} \big\langle\, \Psi(t) \,\big|\, Q_i\, e^{-i\mathcal{H}_0 t/\hbar}\, Q_j(t')\, e^{+i\mathcal{H}_0 t_0/\hbar} \,\big|\, \Psi(t_0) \,\big\rangle \bigg\}\, \Theta(t-t') \\
&= \frac{i}{\hbar} \big\langle \big[Q_i(t), Q_j(t') \big] \big\rangle\, \Theta(t-t') \ ,
\end{aligned} \tag{3.42}$$

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

$$\boxed{\chi_{ij}(t-t') = \frac{i}{\hbar} \big\langle \big[Q_i(t), Q_j(t') \big] \big\rangle\, \Theta(t-t')} \tag{3.43}$$

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

3.3.1 Spectral Representation

We now derive an expression for the response functions in terms of the spectral properties of the Hamiltonian $\mathcal{H}_0$. We stress that $\mathcal{H}_0$ may describe a fully interacting system. Write $\mathcal{H}_0 \big|\, n \,\big\rangle = \hbar\omega_n \big|\, n \,\big\rangle$, in which case

$$\begin{aligned}
\hat\chi_{ij}(\omega) &= \frac{i}{\hbar} \int\limits_0^\infty \! dt \; e^{i\omega t}\, \big\langle \big[Q_i(t), Q_j(0) \big] \big\rangle \\
&= \frac{i}{\hbar} \int\limits_0^\infty \! dt \; e^{i\omega t}\, \frac{1}{Z} \sum_{m,n} e^{-\beta\hbar\omega_m} \Big\{ \big\langle\, m \,\big|\, Q_i \,\big|\, n \,\big\rangle \big\langle\, n \,\big|\, Q_j \,\big|\, m \,\big\rangle\, e^{+i(\omega_m - \omega_n)t} \\
&\qquad\qquad - \big\langle\, m \,\big|\, Q_j \,\big|\, n \,\big\rangle \big\langle\, n \,\big|\, Q_i \,\big|\, m \,\big\rangle\, e^{+i(\omega_n - \omega_m)t} \Big\} \ ,
\end{aligned} \tag{3.44}$$

where $\beta = 1/k_{\rm B}T$ and Z is the partition function. Regularizing the integrals at $t \to \infty$ with $\exp(-\epsilon t)$ with $\epsilon = 0^+$, we use

$$\int\limits_0^\infty \! dt \; e^{i(\omega - \Omega + i\epsilon)t} = \frac{i}{\omega - \Omega + i\epsilon} \tag{3.45}$$

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

$$\boxed{\hat\chi_{ij}(\omega+i\epsilon)=\frac{1}{\hbar Z}\sum_{m,n}e^{-\beta\hbar\omega_m}\left\{\frac{\langle\, m\,|\,Q_j\,|\,n\,\rangle\,\langle\, n\,|\,Q_i\,|\,m\,\rangle}{\omega-\omega_m+\omega_n+i\epsilon}-\frac{\langle\, m\,|\,Q_i\,|\,n\,\rangle\,\langle\, n\,|\,Q_j\,|\,m\,\rangle}{\omega+\omega_m-\omega_n+i\epsilon}\right\}} \tag{3.46}$$

We will refer to this as $\hat\chi_{ij}(\omega)$; formally $\hat\chi_{ij}(\omega)$ has poles or a branch cut (for continuous spectra) along the $\mathrm{Re}(\omega)$ axis. Diagrammatic perturbation theory does not give us $\hat\chi_{ij}(\omega)$, but rather the *time-ordered* response function,

$$\begin{aligned}\chi^{\mathrm{T}}_{ij}(t-t')&\equiv\frac{i}{\hbar}\big\langle \mathcal{T}\,Q_i(t)\,Q_j(t')\big\rangle\\&=\frac{i}{\hbar}\big\langle Q_i(t)\,Q_j(t')\big\rangle\,\Theta(t-t')+\frac{i}{\hbar}\big\langle Q_j(t')\,Q_i(t)\big\rangle\,\Theta(t'-t)\ .\end{aligned} \tag{3.47}$$

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

$$\boxed{\hat\chi^{\mathrm{T}}_{ij}(\omega+i\epsilon)=\frac{1}{\hbar Z}\sum_{m,n}e^{-\beta\hbar\omega_m}\left\{\frac{\langle\, m\,|\,Q_j\,|\,n\,\rangle\langle\, n\,|\,Q_i\,|\,m\,\rangle}{\omega-\omega_m+\omega_n-i\epsilon}-\frac{\langle\, m\,|\,Q_i\,|\,n\,\rangle\langle\, n\,|\,Q_j\,|\,m\,\rangle}{\omega+\omega_m-\omega_n+i\epsilon}\right\}} \tag{3.48}$$

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:

$$\langle\, m\,|\,Q_i\,|\,n\,\rangle\langle\, n\,|\,Q_j\,|\,m\,\rangle\equiv A_{mn}(ij)+iB_{mn}(ij)\ . \tag{3.49}$$

That is[4],

$$A_{mn}(ij)=\frac{1}{2}\,\langle\, m\,|\,Q_i\,|\,n\,\rangle\,\langle\, n\,|\,Q_j\,|\,m\,\rangle+\frac{1}{2}\,\langle\, m\,|\,Q_j\,|\,n\,\rangle\,\langle\, n\,|\,Q_i\,|\,m\,\rangle \tag{3.50}$$

$$B_{mn}(ij)=\frac{1}{2i}\langle\, m\,|\,Q_i\,|\,n\,\rangle\,\langle\, n\,|\,Q_j\,|\,m\,\rangle-\frac{1}{2i}\langle\, m\,|\,Q_j\,|\,n\,\rangle\,\langle\, n\,|\,Q_i\,|\,m\,\rangle. \tag{3.51}$$

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:

$$A_{mn}(ij)=+A_{nm}(ij)=A_{nm}(ji)=+A_{mn}(ji) \tag{3.52}$$

$$B_{mn}(ij)=-B_{nm}(ij)=B_{nm}(ji)=-B_{mn}(ji)\ . \tag{3.53}$$

We define the *spectral densities*

$$\left\{\begin{matrix}\varrho^A_{ij}(\omega)\\ \varrho^B_{ij}(\omega)\end{matrix}\right\}\equiv\frac{1}{\hbar Z}\sum_{m,n}e^{-\beta\hbar\omega_m}\left\{\begin{matrix}A_{mn}(ij)\\ B_{mn}(ij)\end{matrix}\right\}\delta(\omega-\omega_n+\omega_m)\ , \tag{3.54}$$

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

[4]We assume all the Q_i are Hermitian, *i.e.* $Q_i=Q_i^\dagger$.

which satisfy

$$\varrho^A_{ij}(\omega) = +\varrho^A_{ji}(\omega) \quad , \quad \varrho^A_{ij}(-\omega) = +e^{-\beta\hbar\omega}\, \varrho^A_{ij}(\omega) \tag{3.55}$$

$$\varrho^B_{ij}(\omega) = -\varrho^B_{ji}(\omega) \quad , \quad \varrho^B_{ij}(-\omega) = -e^{-\beta\hbar\omega}\, \varrho^B_{ij}(\omega)\ . \tag{3.56}$$

In terms of these spectral densities,

$$\hat\chi'_{ij}(\omega) = \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\nu}{\nu^2-\omega^2}\, \varrho^A_{ij}(\nu) - \pi(1-e^{-\beta\hbar\omega})\, \varrho^B_{ij}(\omega) = +\hat\chi'_{ij}(-\omega) \tag{3.57}$$

$$\hat\chi''_{ij}(\omega) = \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\omega}{\nu^2-\omega^2}\, \varrho^B_{ij}(\nu) + \pi(1-e^{-\beta\hbar\omega})\, \varrho^A_{ij}(\omega) = -\hat\chi''_{ij}(-\omega). \tag{3.58}$$

For the time ordered response functions, we find

$$\hat\chi'^{\,\mathrm{T}}_{ij}(\omega) = \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\nu}{\nu^2-\omega^2}\, \varrho^A_{ij}(\nu) - \pi(1+e^{-\beta\hbar\omega})\, \varrho^B_{ij}(\omega) \tag{3.59}$$

$$\hat\chi''^{\,\mathrm{T}}_{ij}(\omega) = \mathcal{P}\int\limits_{-\infty}^{\infty} d\nu\, \frac{2\omega}{\nu^2-\omega^2}\, \varrho^B_{ij}(\nu) + \pi(1+e^{-\beta\hbar\omega})\, \varrho^A_{ij}(\omega)\ . \tag{3.60}$$

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

$$\big[\hat\chi'_{ij}(\omega) + \hat\chi'_{ji}(\omega)\big] = \big[\hat\chi'^{\,\mathrm{T}}_{ij}(\omega) + \hat\chi'^{\,\mathrm{T}}_{ji}(\omega)\big] \tag{3.61}$$

$$\big[\hat\chi'_{ij}(\omega) - \hat\chi'_{ji}(\omega)\big] = \big[\hat\chi'^{\,\mathrm{T}}_{ij}(\omega) - \hat\chi'^{\,\mathrm{T}}_{ji}(\omega)\big] \times \tanh(\tfrac{1}{2}\beta\hbar\omega) \tag{3.62}$$

$$\big[\hat\chi''_{ij}(\omega) + \hat\chi''_{ji}(\omega)\big] = \big[\hat\chi''^{\,\mathrm{T}}_{ij}(\omega) + \hat\chi''^{\,\mathrm{T}}_{ji}(\omega)\big] \times \tanh(\tfrac{1}{2}\beta\hbar\omega) \tag{3.63}$$

$$\big[\hat\chi''_{ij}(\omega) - \hat\chi''_{ji}(\omega)\big] = \big[\hat\chi''^{\,\mathrm{T}}_{ij}(\omega) - \hat\chi''^{\,\mathrm{T}}_{ji}(\omega)\big]\ . \tag{3.64}$$

3.3.2 Energy Dissipation

The work done on the system must be positive! he rate at which work is done by the external fields is the power dissipated,

$$\begin{aligned} P &= \frac{d}{dt}\,\big\langle\, \Psi(t) \,\big|\, \mathcal{H}(t) \,\big|\, \Psi(t) \,\big\rangle \\ &= \Big\langle \Psi(t) \Big| \frac{\partial \mathcal{H}_1(t)}{\partial t} \Big| \Psi(t) \Big\rangle = -\sum_i \big\langle Q_i(t) \big\rangle\, \dot\phi_i(t)\ , \end{aligned} \tag{3.65}$$

where we have invoked the Feynman-Hellman theorem. The total energy dissipated is thus a functional of the external fields $\{\phi_i(t)\}$:

$$W = \int_{-\infty}^{\infty} dt\, P(t) = -\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt'\, \chi_{ij}(t-t')\, \dot\phi_i(t)\, \phi_j(t')$$
$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, (-i\omega)\, \hat\phi^*_i(\omega)\, \hat\chi_{ij}(\omega)\, \hat\phi_j(\omega)\ . \tag{3.66}$$

Since the $\{Q_i\}$ are Hermitian observables, the $\{\phi_i(t)\}$ must be real fields, in which case $\hat\phi^*_i(\omega) = \hat\phi_j(-\omega)$, whence

$$W = \int_{-\infty}^{\infty} \frac{d\omega}{4\pi}\, (-i\omega) \big[\hat\chi_{ij}(\omega) - \hat\chi_{ji}(-\omega)\big]\, \hat\phi^*_i(\omega)\, \hat\phi_j(\omega)$$
$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \mathcal{M}_{ij}(\omega)\, \hat\phi^*_i(\omega)\, \hat\phi_j(\omega) \tag{3.67}$$

where

$$\mathcal{M}_{ij}(\omega) \equiv \tfrac{1}{2}(-i\omega)\big[\hat\chi_{ij}(\omega) - \hat\chi_{ji}(-\omega)\big]$$
$$= \pi\omega\left(1 - e^{-\beta\hbar\omega}\right)\Big(\varrho^A_{ij}(\omega) + i\varrho^B_{ij}(\omega)\Big)\ . \tag{3.68}$$

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

3.3.3 Correlation Functions

We define the *correlation function*

$$S_{ij}(t) \equiv \big\langle Q_i(t)\, Q_j(t')\big\rangle\ , \tag{3.69}$$

which has the spectral representation

$$\hat S_{ij}(\omega) = 2\pi\hbar\Big[\varrho^A_{ij}(\omega) + i\varrho^B_{ij}(\omega)\Big]$$
$$= \frac{2\pi}{Z}\sum_{m,n} e^{-\beta\hbar\omega_m}\, \langle\, m \,|\, Q_i \,|\, n\,\rangle \langle\, n \,|\, Q_j \,|\, n\,\rangle\, \delta(\omega - \omega_n + \omega_m)\ . \tag{3.70}$$

Note that

$$\hat S_{ij}(-\omega) = e^{-\beta\hbar\omega}\, \hat S^*_{ij}(\omega) \qquad , \qquad \hat S_{ji}(\omega) = \hat S^*_{ij}(\omega)\ . \tag{3.71}$$

and that

$$\boxed{\hat\chi_{ij}(\omega) - \hat\chi_{ji}(-\omega) = \frac{i}{\hbar}\left(1 - e^{-\beta\hbar\omega}\right)\hat S_{ij}(\omega)} \tag{3.72}$$

This result is known as the *fluctuation-dissipation theorem*, as it relates the equilibrium fluctuations $S_{ij}(\omega)$ to the dissipative quantity $\hat\chi_{ij}(\omega) - \hat\chi_{ji}(-\omega)$.

Time Reversal Symmetry

If the operators Q_i have a definite symmetry under time reversal, say

$$\mathcal{T}\, Q_i \mathcal{T}^{-1} = \eta_i \, Q_i \ , \tag{3.73}$$

then the correlation function satisfies

$$\hat{S}_{ij}(\omega) = \eta_i \, \eta_j \, \hat{S}_{ji}(\omega) \ . \tag{3.74}$$

3.3.4 Continuous Systems

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

$$S_{ij}(\boldsymbol{r}-\boldsymbol{r}', t-t') = \big\langle Q_i(\boldsymbol{r},t)\, Q_j(\boldsymbol{r}',t')\big\rangle \ , \tag{3.75}$$

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

$$\hat{S}(\boldsymbol{k},\omega) = \int\! d^3\!r \int\limits_{-\infty}^{\infty}\! dt \ e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\, S(\boldsymbol{r},t) \tag{3.76}$$

$$= \frac{1}{V}\int\limits_{-\infty}^{\infty}\! dt \ e^{+i\omega t}\, \big\langle \hat{Q}(\boldsymbol{k},t)\, \hat{Q}(-\boldsymbol{k},0)\big\rangle \ . \tag{3.77}$$

3.4 Example: $S = \frac{1}{2}$ Object in a Magnetic Field

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

$$\mathcal{H}_0 = \gamma B_0 \, S^z \tag{3.78}$$

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 $\big|\pm\big\rangle$, with $\omega_\pm = \pm\frac{1}{2}\gamma B_0$. We apply a perturbation,

$$\mathcal{H}_1(t) = \gamma \boldsymbol{S}\cdot\boldsymbol{B}_1(t) \ . \tag{3.79}$$

At $T = 0$, the susceptibility tensor is

$$\begin{aligned}\chi_{\alpha\beta}(\omega) &= \frac{\gamma^2}{\hbar}\sum_n \left\{ \frac{\big\langle - \,\big|\, S^\beta \,\big|\, n\big\rangle\big\langle n \,\big|\, S^\alpha \,\big|\, -\big\rangle}{\omega - \omega_- + \omega_n + i\epsilon} - \frac{\big\langle - \,\big|\, S^\alpha \,\big|\, n\big\rangle\big\langle n \,\big|\, S^\beta \,\big|\, -\big\rangle}{\omega + \omega_- - \omega_n + i\epsilon}\right\} \\ &= \frac{\gamma^2}{\hbar}\left\{ \frac{\big\langle - \,\big|\, S^\beta \,\big|\, +\big\rangle\big\langle + \,\big|\, S^\alpha \,\big|\, -\big\rangle}{\omega + \gamma B_0 + i\epsilon} - \frac{\big\langle - \,\big|\, S^\alpha \,\big|\, +\big\rangle\big\langle + \,\big|\, S^\beta \,\big|\, -\big\rangle}{\omega - \gamma B_0 + i\epsilon}\right\} \ , \end{aligned} \tag{3.80}$$

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

$$\chi_{+-}(\omega) = \frac{\hbar\gamma^2}{\omega + \gamma B_0 + i\epsilon} \tag{3.81}$$

$$\chi_{-+}(\omega) = \frac{-\hbar\gamma^2}{\omega - \gamma B_0 + i\epsilon} \ , \tag{3.82}$$

or, equivalently,

$$\chi_{xx}(\omega) = \tfrac{1}{4}\hbar\gamma^2 \left\{ \frac{1}{\omega + \gamma B_0 + i\epsilon} - \frac{1}{\omega - \gamma B_0 + i\epsilon} \right\} = +\chi_{yy}(\omega) \tag{3.83}$$

$$\chi_{xy}(\omega) = \tfrac{i}{4}\hbar\gamma^2 \left\{ \frac{1}{\omega + \gamma B_0 + i\epsilon} + \frac{1}{\omega - \gamma B_0 + i\epsilon} \right\} = -\chi_{yx}(\omega) \ . \tag{3.84}$$

3.4.1 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

$$\frac{d\boldsymbol{M}}{dt} = \gamma \boldsymbol{M} \times \boldsymbol{H} \ . \tag{3.85}$$

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:

$$\dot{M}_x = \gamma M_y H_z - \gamma M_z H_y - \frac{M_x}{T_2} \tag{3.86}$$

$$\dot{M}_y = \gamma M_z H_x - \gamma M_x H_z - \frac{M_y}{T_2} \tag{3.87}$$

$$\dot{M}_z = \gamma M_x H_y - \gamma M_y H_x - \frac{M_z - M_0}{T_1} \ . \tag{3.88}$$

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

$$\dot{M}^\alpha + R_{\alpha\beta} M^\beta = \psi^\alpha \ , \tag{3.89}$$

with $R_{\alpha\beta}(t) = T^{-1}_{\alpha\beta} - \gamma\, \epsilon_{\alpha\beta\delta} H^\delta(t)$, $\psi^\alpha = T^{-1}_{\alpha\beta}\, M_0^\beta$, and

$$T_{\alpha\beta} = \begin{pmatrix} T_2 & 0 & 0 \\ 0 & T_2 & 0 \\ 0 & 0 & T_1 \end{pmatrix} \ . \tag{3.90}$$

The formal solution is written

$$\boldsymbol{M}(t) = \int_0^t dt'\, U(t-t')\, \boldsymbol{\psi}(t') + U(t)\, \boldsymbol{\psi}(0) \ , \tag{3.91}$$

where the evolution matrix,

$$U(t) = \mathcal{T} \ \exp\left\{ - \int_0^t dt'\, R(t') \right\} \ , \tag{3.92}$$

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

$$\dot{m}_x = \gamma\, H_0\, m_y - \gamma\, H_y\, M_0 - \frac{m_x}{T_2} \tag{3.93}$$

$$\dot{m}_y = \gamma\, H_x\, M_0 - \gamma\, H_0\, m_x - \frac{m_y}{T_2} \tag{3.94}$$

$$\dot{m}_z = -\frac{m_z}{T_1} \ , \tag{3.95}$$

which are equivalent to the following:

$$\ddot{m}_x + 2T_2^{-1} \dot{m}_x + \big(\gamma^2 H_0^2 + T_2^{-2}\big) m_x = \gamma\, M_0 \big(\gamma\, H_0 H_x - T_2^{-1} H_y - \dot{H}_y\big) \tag{3.96}$$

$$\ddot{m}_y + 2T_2^{-1} \dot{m}_y + \big(\gamma^2 H_0^2 + T_2^{-2}\big) m_y = \gamma\, M_0 \big(\gamma\, H_0 H_y + T_2^{-1} H_x + \dot{H}_x\big) \tag{3.97}$$

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

$$\big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-2}\omega\big)\, \hat{m}_x(\omega) = \gamma\, M_0 \big(\gamma\, H_0\, H_x(\omega) + (i\omega - T_2^{-1}) H_y(\omega)\big) \tag{3.98}$$

$$\big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-2}\omega\big)\, \hat{m}_y(\omega) = \gamma\, M_0 \big(\gamma\, H_0\, H_y(\omega) - (i\omega - T_2^{-1}) H_x(\omega)\big) \ , \tag{3.99}$$

from which we read off

$$\chi_{xx}(\omega) = \frac{\gamma^2 H_0\, M_0}{\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-1}\omega} = \chi_{yy}(\omega) \tag{3.100}$$

$$\chi_{xy}(\omega) = \frac{(i\omega - T_2^{-1})\, \gamma\, M_0}{\gamma^2 H_0^2 + T_2^{-2} - \omega^2 - 2iT_2^{-1}\omega} = -\chi_{yx}(\omega) \ . \tag{3.101}$$

Note that Onsager reciprocity is satisfied:

$$\chi_{xy}(\omega, H_0) = \chi^{\mathrm{t}}_{yx}(\omega, H_0) = \chi_{yx}(\omega, -H_0) = -\chi_{yx}(\omega, H_0) \ . \tag{3.102}$$

The lineshape is given by

$$\chi'_{xx}(\omega) = \frac{(\gamma^2 H_0^2 + T_2^{-2} - \omega^2)\, \gamma^2\, H_0\, M_0}{\big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2\big)^2 + 4\, T_2^{-2} \omega^2} \tag{3.103}$$

$$\chi''_{xx}(\omega) = \frac{2\, \gamma\, H_0\, M_0\, T_2^{-1} \omega}{\big(\gamma^2 H_0^2 + T_2^{-2} - \omega^2\big)^2 + 4\, T_2^{-2} \omega^2} \ , \tag{3.104}$$

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

3.5 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 $A^\mu = (A^0, \boldsymbol{A})$:

$$\boldsymbol{E} = -\boldsymbol{\nabla} A^0 - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} \tag{3.105}$$

$$\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} \ . \tag{3.106}$$

The Hamiltonian for an N-particle system is

$$\begin{aligned}\mathcal{H}(A^\mu) &= \sum_{i=1}^{N} \left\{ \frac{1}{2m}\Big(\boldsymbol{p}_i + \frac{e}{c}\boldsymbol{A}(\boldsymbol{x}_i,t)\Big)^2 - eA^0(\boldsymbol{x}_i,t) + U(\boldsymbol{x}_i)\right\} + \sum_{i<j} v(\boldsymbol{x}_i - \boldsymbol{x}_j) \\ &= \mathcal{H}(0) - \frac{1}{c}\int\! d^3x \, j^{\rm p}_\mu(\boldsymbol{x})\, A^\mu(\boldsymbol{x},t) + \frac{e^2}{2mc^2}\int\! d^3x\, n(\boldsymbol{x})\, \boldsymbol{A}^2(\boldsymbol{x},t) \ ,\end{aligned} \tag{3.107}$$

where we have defined

$$n(\boldsymbol{x}) \equiv \sum_{i=1}^{N} \delta(\boldsymbol{x} - \boldsymbol{x}_i) \tag{3.108}$$

$$\boldsymbol{j}^{\rm p}(\boldsymbol{x}) \equiv -\frac{e}{2m}\sum_{i=1}^{N} \Big\{ \boldsymbol{p}_i\, \delta(\boldsymbol{x} - \boldsymbol{x}_i) + \delta(\boldsymbol{x} - \boldsymbol{x}_i)\, \boldsymbol{p}_i \Big\} \tag{3.109}$$

$$j^{\rm p}_0(\boldsymbol{x}) \equiv c\, e\, n(\boldsymbol{x}) \ . \tag{3.110}$$

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

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \ , \tag{3.111}$$

so that

$$j^\mu = (j^0, j^1, j^2, j^3) \equiv (j^0, \boldsymbol{j}) \tag{3.112}$$

$$j_\mu = g_{\mu\nu} j^\nu = (-j^0, j^1, j^2, j^3) \tag{3.113}$$

$$j_\mu A^\mu = j^\mu g_{\mu\nu}\, A^\nu = -j^0 A^0 + \boldsymbol{j}\cdot\boldsymbol{A} \equiv j \cdot A \tag{3.114}$$

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:

$$j_\mu(\boldsymbol{x}) = -c\,\frac{\delta\mathcal{H}}{\delta A^\mu(\boldsymbol{x})} = j^{\rm p}_\mu(\boldsymbol{x}) + j^{\rm d}_\mu(\boldsymbol{x}) \tag{3.115}$$

$$\boldsymbol{j}^{\rm d}(\boldsymbol{x}) = -\frac{e^2}{mc}\, n(\boldsymbol{x})\boldsymbol{A}(\boldsymbol{x}) = -\frac{e}{mc^2}\, j^{\rm p}_0(\boldsymbol{x})\, \boldsymbol{A}(\boldsymbol{x}) \tag{3.116}$$

$$j^{\rm d}_0(\boldsymbol{x}) = 0 \ . \tag{3.117}$$

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

$$\big\langle j_\mu(\boldsymbol{x},t)\big\rangle = -\frac{c}{4\pi}\int\!d^3x'\!\int\!dt\;K_{\mu\nu}(\boldsymbol{x}t;\boldsymbol{x}'t')\,A^\nu(\boldsymbol{x}',t')\ , \tag{3.118}$$

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

$$\big\langle j^{\rm p}_\mu(\boldsymbol{x},t)\big\rangle = \frac{i}{\hbar c}\int\!d^3x'\!\int\!dt'\;\big\langle\big[j^{\rm p}_\mu(\boldsymbol{x},t),j^{\rm p}_\nu(\boldsymbol{x}',t')\big]\big\rangle\,\Theta(t-t')\,A^\nu(\boldsymbol{x}',t') \tag{3.119}$$

$$\big\langle j^{\rm d}_\mu(\boldsymbol{x},t)\big\rangle = -\frac{e}{mc^2}\,\big\langle j^{\rm p}_0(\boldsymbol{x},t)\big\rangle\,A^\mu(\boldsymbol{x},t)\,(1-\delta_{\mu 0})\ , \tag{3.120}$$

we conclude

$$\begin{aligned}K_{\mu\nu}(\boldsymbol{x}t;\boldsymbol{x}'t') &= \frac{4\pi}{i\hbar c^2}\,\Big\langle\big[j^{\rm p}_\mu(\boldsymbol{x},t),j^{\rm p}_\nu(\boldsymbol{x}',t')\big]\Big\rangle\,\Theta(t-t')\\ &\qquad + \frac{4\pi e}{mc^2}\,\big\langle j^{\rm p}_0(\boldsymbol{x},t)\big\rangle\,\delta(\boldsymbol{x}-\boldsymbol{x}')\,\delta(t-t')\,\delta_{\mu\nu}\,(1-\delta_{\mu 0})\ .\end{aligned} \tag{3.121}$$

The first term is sometimes known as the *paramagnetic response kernel*, $K^{\rm p}_{\mu\nu}(x;x') = (4\pi i/i\hbar c^2)\big\langle\big[j^{\rm p}_\mu(x),j^{\rm p}_\nu(x')\big]\big\rangle\,\Theta(t-t')$ is not directly calculable by perturbation theory. Rather, one obtains the time-ordered response function $K^{\rm p,T}_{\mu\nu}(x;x') = (4\pi/i\hbar c^2)\big\langle\mathcal{T}\,j^{\rm p}_\mu(x)\,j^{\rm p}_\nu(x')\big\rangle$, 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

$$\begin{aligned}\mathcal{H} &= \sum_\sigma\int\!d^3x\;\psi^\dagger_\sigma(\boldsymbol{x})\bigg\{\frac{1}{2m}\Big(\frac{\hbar}{i}\boldsymbol{\nabla}+\frac{e}{c}\boldsymbol{A}\Big)^2 - eA^0(\boldsymbol{x}) + U(\boldsymbol{x})\bigg\}\,\psi_\sigma(\boldsymbol{x})\\ &\quad + \frac{1}{2}\sum_{\sigma,\sigma'}\int\!d^3x\!\int\!d^3x'\;\psi^\dagger_\sigma(\boldsymbol{x})\,\psi^\dagger_{\sigma'}(\boldsymbol{x}')\,v(\boldsymbol{x}-\boldsymbol{x}')\,\psi_{\sigma'}(\boldsymbol{x}')\,\psi_\sigma(\boldsymbol{x})\ ,\end{aligned} \tag{3.122}$$

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,

$$\mathcal{H}(A^\mu) = \mathcal{H}(0) - \frac{1}{c}\int\!d^3x\;j^{\rm p}_\mu(\boldsymbol{x})\,A^\mu(\boldsymbol{x}) + \frac{e^2}{2mc^2}\sum_\sigma\int\!d^3x\;\psi^\dagger_\sigma(\boldsymbol{x})\,\psi_\sigma(\boldsymbol{x})\,\boldsymbol{A}^2(\boldsymbol{x})\ , \tag{3.123}$$

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

$$j^{\rm p}_0(\boldsymbol{x}) = c\,e\sum_\sigma \psi^\dagger_\sigma(\boldsymbol{x})\,\psi_\sigma(\boldsymbol{x}) \tag{3.124}$$

$$\boldsymbol{j}^{\rm p}(\boldsymbol{x}) = \frac{ie\hbar}{2m}\sum_\sigma\Big\{\psi^\dagger_\sigma(\boldsymbol{x})\,\boldsymbol{\nabla}\,\psi_\sigma(\boldsymbol{x}) - \Big(\boldsymbol{\nabla}\psi^\dagger_\sigma(\boldsymbol{x})\Big)\,\psi_\sigma(\boldsymbol{x})\Big\}\ . \tag{3.125}$$

3.5.1 Gauge Invariance and Charge Conservation

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

$$\big\langle j_\mu(q)\big\rangle = -\frac{c}{4\pi}\, K_{\mu\nu}(q)\, A^\nu(q) \ . \tag{3.126}$$

Note our convention on Fourier transforms:

$$H(x) = \int\!\frac{d^4\!k}{(2\pi)^4}\ \hat H(k)\, e^{+ik\cdot x} \tag{3.127}$$

$$\hat H(k) = \int\! d^4\!x\, H(x)\, e^{-ik\cdot x} \ , \tag{3.128}$$

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.*

$$A^\mu(q) \to A^\mu(q) + i\Lambda(q)\, q^\mu \ , \tag{3.129}$$

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,

$$\boxed{\sum_\mu q^\mu\, K_{\mu\nu}(q) = \sum_\nu K_{\mu\nu}(q)\, q^\nu = 0} \tag{3.130}$$

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

$$\mathrm{Re}\, K_{\mu\nu}(q) = +\mathrm{Re}\, K_{\nu\mu}(-q) \tag{3.131}$$

$$\mathrm{Im}\, K_{\mu\nu}(q) = -\mathrm{Im}\, K_{\nu\mu}(-q) \ , \tag{3.132}$$

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

$$\boxed{\text{gauge invariance} \Longleftrightarrow \text{charge conservation}} \tag{3.133}$$

3.5.2 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

$$\begin{aligned}\big\langle j_i(q)\big\rangle &= -\frac{c}{4\pi}\, K_{ij}(q)\, A^j(q)\\ &= -\frac{c}{4\pi}\, K_{ij}(q)\, \frac{c}{i\omega}\, E^j(q)\\ &\equiv \sigma_{ij}(q)\, E^j(q) \ .\end{aligned} \tag{3.134}$$

Thus, the conductivity tensor is given by

$$\sigma_{ij}(\boldsymbol{q},\omega) = \frac{ic^2}{4\pi\omega}\, K_{ij}(\boldsymbol{q},\omega) \ . \tag{3.135}$$

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

$$\int\! d^3\!x \int_0^\infty\! dt \, \Big\langle \big[j^{\rm p}_i(\boldsymbol{x},t), j^{\rm p}_j(0,0) \big] \Big\rangle \, e^{+i\omega t} = \frac{ie^2 n}{m} \, \delta_{ij} \ , \tag{3.136}$$

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

3.5.3 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

$$K_{ij}(\boldsymbol{q},\omega) = K_{\parallel}(\boldsymbol{q},\omega)\, \hat q_i \, \hat q_j + K_{\perp}(\boldsymbol{q},\omega) \, \big(\delta_{ij} - \hat q_i \, \hat q_j \big) \ , \tag{3.137}$$

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,

$$q^0 \, K_{0j} + q^i \, K_{ij} = \frac{\omega}{c} \, K_{0j} + K_{\parallel} \, q_j \ , \tag{3.138}$$

which yields

$$\boxed{K_{0j}(\boldsymbol{q},\omega) = -\frac{c}{\omega} \, q^j \, K_{\parallel}(\boldsymbol{q},\omega) = K_{j0}(\boldsymbol{q},\omega)} \tag{3.139}$$

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

$$0 = q^0 \, K_{00} + q^i \, K_{i0} = \frac{\omega}{c} \, K_{00} - \frac{c}{\omega} \, \boldsymbol{q}^2 \, K_{\parallel} \ , \tag{3.140}$$

which says

$$\boxed{K_{00}(\boldsymbol{q},\omega) = \frac{c^2}{\omega^2} \, \boldsymbol{q}^2 \, K_{\parallel}(\boldsymbol{q},\omega)} \tag{3.141}$$

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 $K_{\perp}(q)$.

3.5.4 Neutral Systems

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

$$n(\boldsymbol{x}) = \sum_{i=1}^N \delta(\boldsymbol{x} - \boldsymbol{x}_i) \tag{3.142}$$

$$\boldsymbol{j}(\boldsymbol{x}) = \frac{1}{2m} \sum_{i=1}^N \Big\{ \boldsymbol{p}_i \, \delta(\boldsymbol{x} - \boldsymbol{x}_i) + \delta(\boldsymbol{x} - \boldsymbol{x}_i) \, \boldsymbol{p}_i \Big\} \ . \tag{3.143}$$

The charge and current susceptibilities are then given by

$$\chi(\boldsymbol{x},t) = \frac{i}{\hbar}\big\langle\big[n(\boldsymbol{x},t),n(0,0)\big]\big\rangle \tag{3.144}$$

$$\chi_{ij}(\boldsymbol{x},t) = \frac{i}{\hbar}\big\langle\big[j_i(\boldsymbol{x},t),j_j(0,0)\big]\big\rangle \ . \tag{3.145}$$

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

$$\chi_{ij}(\boldsymbol{q},\omega) = \chi_{\parallel}(\boldsymbol{q},\omega)\,\hat{q}_i\,\hat{q}_j + \chi_{\perp}(\boldsymbol{q},\omega)\,(\delta_{ij} - \hat{q}_i\,\hat{q}_j) \ . \tag{3.146}$$

From the continuity equation,

$$\boldsymbol{\nabla}\cdot\boldsymbol{j} + \frac{\partial n}{\partial t} = 0 \tag{3.147}$$

follows the relation

$$\chi_{\parallel}(\boldsymbol{q},\omega) = \frac{n}{m} + \frac{\omega^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega) \ . \tag{3.148}$$

EXERCISE: Derive eqn. (3.148).

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

$$K_{00}(\boldsymbol{x},t) = -4\pi e^2\,\chi(\boldsymbol{x},t) \tag{3.149}$$

$$K_{ij}(\boldsymbol{x},t) = \frac{4\pi e^2}{c^2}\bigg\{\frac{n}{m}\,\delta(\boldsymbol{x})\,\delta(t) - \chi_{ij}(\boldsymbol{x},t)\bigg\} \ , \tag{3.150}$$

and therefore

$$K_{\parallel}(\boldsymbol{q},\omega) = \frac{4\pi e^2}{c^2}\bigg\{\frac{n}{m} - \chi_{\parallel}(\boldsymbol{q},\omega)\bigg\} \tag{3.151}$$

$$K_{\perp}(\boldsymbol{q},\omega) = \frac{4\pi e^2}{c^2}\bigg\{\frac{n}{m} - \chi_{\perp}(\boldsymbol{q},\omega)\bigg\} \ . \tag{3.152}$$

3.5.5 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 $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$. To satisfy Maxwell's equations, we have $\boldsymbol{q}\cdot\boldsymbol{A}(\boldsymbol{q},\omega) = 0$, *i.e.* $\boldsymbol{A}(\boldsymbol{q},\omega)$ is purely transverse. But then

$$\big\langle\boldsymbol{j}(\boldsymbol{q},\omega)\big\rangle = -\frac{c}{4\pi}\,K_{\perp}(\boldsymbol{q},\omega)\,\boldsymbol{A}(\boldsymbol{q},\omega) \ . \tag{3.153}$$

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

$$\begin{aligned}\boldsymbol{\nabla}\times\boldsymbol{B} &= \boldsymbol{\nabla}\,(\boldsymbol{\nabla}\cdot\boldsymbol{A}) - \boldsymbol{\nabla}^{\,2}\boldsymbol{A} \\ &= \frac{4\pi}{c}\,\boldsymbol{j} + \frac{1}{c}\frac{\partial\boldsymbol{E}}{\partial t} \\ &= \frac{4\pi}{c}\Big(-\frac{c}{4\pi}\Big)\,K_{\perp}(-i\boldsymbol{\nabla},i\,\partial_t)\,\boldsymbol{A} - \frac{1}{c^2}\frac{\partial^2\boldsymbol{A}}{\partial t^2} \ ,\end{aligned} \tag{3.154}$$

which yields

$$\Big(\boldsymbol{\nabla}^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Big)\boldsymbol{A} = K_\perp(-i\boldsymbol{\nabla}, i\,\partial_t)\boldsymbol{A} \ . \tag{3.155}$$

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

$$\frac{1}{\lambda_{\rm L}^2} \equiv \lim_{\boldsymbol{q}\to 0} K_\perp(\boldsymbol{q},0) \ . \tag{3.156}$$

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

$$n_{\rm s} \equiv \frac{mc^2}{4\pi e^2\lambda_{\rm L}^2} \tag{3.157}$$

$$= n - m \lim_{\boldsymbol{q}\to 0} \chi_\perp(\boldsymbol{q},0) \ . \tag{3.158}$$

Ideal Bose Gas

We start from

$$\chi_{ij}(\boldsymbol{q},t) = \frac{i}{\hbar V}\big\langle\big[j_i(\boldsymbol{q},t), j_j(-\boldsymbol{q},0)\big]\big\rangle \tag{3.159}$$

$$j_i(\boldsymbol{q}) = \frac{\hbar}{2m}\sum_{\boldsymbol{k}}(2k_i+q_i)\,\psi^\dagger_{\boldsymbol{k}}\,\psi_{\boldsymbol{k}+\boldsymbol{q}} \ . \tag{3.160}$$

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

$$j_i(\boldsymbol{q},t) = (2k_i+q_i)\,e^{i(\omega_{\boldsymbol{k}}-\omega_{\boldsymbol{k}+\boldsymbol{q}})t}\,\psi^\dagger_{\boldsymbol{k}}\,\psi_{\boldsymbol{k}+\boldsymbol{q}} \tag{3.161}$$

$$\big[j_i(\boldsymbol{q},t), j_j(-\boldsymbol{q},0)\big] = \frac{\hbar^2}{4m^2}\sum_{\boldsymbol{k},\boldsymbol{k}'}(2k_i+q_i)(2k'_j-q_j)\,e^{i(\omega_{\boldsymbol{k}}-\omega_{\boldsymbol{k}+\boldsymbol{q}})t} \times \big[\psi^\dagger_{\boldsymbol{k}}\,\psi_{\boldsymbol{k}+\boldsymbol{q}}, \psi^\dagger_{\boldsymbol{k}'}\,\psi_{\boldsymbol{k}'-\boldsymbol{q}}\big] \tag{3.162}$$

Using

$$[AB,CD] = A\,[B,C]\,D + AC\,[B,D] + C\,[A,D]\,B + [A,C]\,DB \ , \tag{3.163}$$

we obtain

$$\big[j_i(\boldsymbol{q},t), j_j(-\boldsymbol{q},0)\big] = \frac{\hbar^2}{4m^2}\sum_{\boldsymbol{k}}(2k_i+q_i)(2k_j+q_j)\,e^{i(\omega_{\boldsymbol{k}}-\omega_{\boldsymbol{k}+\boldsymbol{q}})t}\,\big\{n^0(\omega_{\boldsymbol{k}})-n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}})\big\} \ , \tag{3.164}$$

where $n^0(\omega)$ is the equilibrium Bose distribution[5],

$$n^0(\omega) = \frac{1}{e^{\beta\hbar\omega}\,e^{-\beta\mu}-1} \ . \tag{3.165}$$

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

Thus,

$$\chi_{ij}(\boldsymbol{q},\omega) = \frac{\hbar}{4m^2V}\sum_{\boldsymbol{k}}(2k_i+q_i)(2k_j+q_j)\,\frac{n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}})-n^0(\omega_{\boldsymbol{k}})}{\omega+\omega_{\boldsymbol{k}}-\omega_{\boldsymbol{k}+\boldsymbol{q}}+i\epsilon} \tag{3.166}$$

$$= \frac{\hbar n_0}{4m^2}\left\{\frac{1}{\omega+\omega_{\boldsymbol{q}}+i\epsilon}-\frac{1}{\omega-\omega_{\boldsymbol{q}}+i\epsilon}\right\} q_i\,q_j + \frac{\hbar}{m^2}\int\!\frac{d^3\!k}{(2\pi)^3}\,\frac{n^0(\omega_{\boldsymbol{k}+\boldsymbol{q}/2})-n^0(\omega_{\boldsymbol{k}-\boldsymbol{q}/2})}{\omega+\omega_{\boldsymbol{k}-\boldsymbol{q}/2}-\omega_{\boldsymbol{k}+\boldsymbol{q}/2}+i\epsilon}\,k_i\,k_j\ , \tag{3.167}$$

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

$$\chi_{ij}(\boldsymbol{q}\to 0,0) = \frac{n_0}{m}\,\hat{q}_i\,\hat{q}_j + \frac{n'}{m}\,\delta_{ij}\ , \tag{3.168}$$

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

$$\chi_{\parallel}(\boldsymbol{q}\to 0,0) = \frac{n}{m}\qquad , \qquad \chi_{\perp}(\boldsymbol{q}\to 0,0) = \frac{n'}{m}\ , \tag{3.169}$$

where $n = n_0 + n'$ is the total boson number density. The superfluid density, according to (3.158), is $n_{\rm s} = n_0(T)$.

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.

3.6 Density-Density Correlations

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

$$\mathcal{H}_1(t) = -\int\! d^3\!r\; n(\boldsymbol{r})\,U(\boldsymbol{r},t)\ . \tag{3.170}$$

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

$$\langle\delta n(\boldsymbol{r},t)\rangle = \int\! d^3\!r'\!\int\! dt'\;\chi(\boldsymbol{r}-\boldsymbol{r}',t-t')\,U(\boldsymbol{r}',t') \tag{3.171}$$

$$\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q},\omega)\rangle = \chi(\boldsymbol{q},\omega)\,\hat{U}(\boldsymbol{q},\omega)\ , \tag{3.172}$$

where

$$\begin{aligned}\chi(\boldsymbol{q},\omega) &= \frac{1}{\hbar V Z}\sum_{m,n} e^{-\beta\hbar\omega_m}\left\{\frac{\big|\langle\, m\,|\,\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,|\,n\,\rangle\big|^2}{\omega-\omega_m+\omega_n+i\epsilon} - \frac{\big|\langle\, m\,|\,\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,|\,n\,\rangle\big|^2}{\omega+\omega_m-\omega_n+i\epsilon}\right\} \\ &= \frac{1}{\hbar}\int\limits_{-\infty}^{\infty} d\nu\, S(\boldsymbol{q},\nu)\left\{\frac{1}{\omega+\nu+i\epsilon} - \frac{1}{\omega-\nu+i\epsilon}\right\} \end{aligned} \tag{3.173}$$

$$S(\boldsymbol{q},\omega) = \frac{2\pi}{VZ}\sum_{m,n} e^{-\beta\hbar\omega_m}\,\big|\langle\, m\,|\,\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,|\,n\,\rangle\big|^2\,\delta(\omega-\omega_n+\omega_m)\ . \tag{3.174}$$

Note that

$$\hat{\boldsymbol{n}}_{\boldsymbol{q}} = \sum_{i=1}^{N} e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i}\ , \tag{3.175}$$

and that $\hat{\boldsymbol{n}}_{\boldsymbol{q}}^\dagger = \hat{\boldsymbol{n}}_{-\boldsymbol{q}}$. $S(\boldsymbol{q},\omega)$ is known as the *dynamic structure factor*. In a scattering experiment, where an incident probe (*e.g.* a neutron) interacts with the system via a potential $U(\boldsymbol{r}-\boldsymbol{R})$, 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

$$\begin{aligned}\mathcal{I}(\boldsymbol{q},\omega) &= \frac{2\pi}{\hbar Z}\sum_{m,n} e^{-\beta\hbar\omega_m}\,\big|\langle\, m;\boldsymbol{p}\,|\,\mathcal{H}_1\,|\,n;\boldsymbol{p}-\hbar\boldsymbol{q}\,\rangle\big|^2\,\delta(\omega-\omega_n+\omega_m) \\ &= \frac{1}{\hbar}\,\big|\hat{U}(\boldsymbol{q})\big|^2\,S(\boldsymbol{q},\omega)\ . \end{aligned} \tag{3.176}$$

The quantity $\big|\hat{U}(\boldsymbol{q})\big|^2$ 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

$$\varepsilon - \hbar\omega = \frac{\boldsymbol{p}^2}{2m_{\rm n}} - \hbar\omega = \frac{(\boldsymbol{p}-\hbar\boldsymbol{q})^2}{2m_{\rm n}} \qquad \Longrightarrow \qquad \hbar\omega = \frac{\hbar\boldsymbol{q}\cdot\boldsymbol{p}}{m_{\rm n}} - \frac{\hbar^2\boldsymbol{q}^2}{2m_{\rm n}}\ . \tag{3.177}$$

Hence, for fixed momentum transfer $\hbar\boldsymbol{q}$, 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, $U(\boldsymbol{r},t) = U\big(\boldsymbol{r}-\boldsymbol{R}(t)\big)$, and

$$\begin{aligned}\hat{U}(\boldsymbol{q},\omega) &= \int\! d^3\!r \!\int\! dt\, e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\, e^{i\omega t}\, U(\boldsymbol{r}-\boldsymbol{V}t) \\ &= 2\pi\,\delta(\omega-\boldsymbol{q}\cdot\boldsymbol{V})\,\hat{U}(\boldsymbol{q}) \end{aligned} \tag{3.178}$$

so that

$$\langle\delta n(\boldsymbol{q},\omega)\rangle = 2\pi\,\delta(\omega-\boldsymbol{q}\cdot\boldsymbol{V})\,\chi(\boldsymbol{q},\omega)\ . \tag{3.179}$$

3.6.1 Sum Rules

From eqn. (3.174) we find

$$\begin{aligned}\int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\,S(\boldsymbol{q},\omega) &= \frac{1}{VZ}\sum_{m,n} e^{-\beta\hbar\omega_m}\,\Big|\big\langle\, m\,\big|\,\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,\big|\,n\,\big\rangle\Big|^2\,(\omega_n-\omega_m)\\ &= \frac{1}{\hbar VZ}\sum_{m,n} e^{-\beta\hbar\omega_m}\,\big\langle\, m\,\big|\,\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,\big|\,n\,\big\rangle\,\big\langle\, n\,\big|\,[\mathcal{H},\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}]\,\big|\,m\,\big\rangle\\ &= \frac{1}{\hbar V}\big\langle\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,[\mathcal{H},\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}]\big\rangle = \frac{1}{2\hbar V}\big\langle\big[\hat{\boldsymbol{n}}_{\boldsymbol{q}},[\mathcal{H},\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}]\big]\big\rangle\ , \qquad (3.180)\end{aligned}$$

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

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^N \boldsymbol{\nabla}_i^{\,2} + V(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)\ , \qquad (3.181)$$

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

$$\begin{aligned}[\mathcal{H},\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}] &= -\frac{\hbar^2}{2m}\sum_{i=1}^N\big[\boldsymbol{\nabla}_i^{\,2},e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}\big] \qquad (3.182)\\ &= \frac{\hbar^2}{2im}\,\boldsymbol{q}\cdot\sum_{i=1}^N\Big(\boldsymbol{\nabla}_i\,e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}+e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}\,\boldsymbol{\nabla}_i\Big)\\ \big[\hat{\boldsymbol{n}}_{\boldsymbol{q}},[\mathcal{H},\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}]\big] &= \frac{\hbar^2}{2im}\,\boldsymbol{q}\cdot\sum_{i=1}^N\sum_{j=1}^N\Big[e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_j},\boldsymbol{\nabla}_i\,e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}+e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}\,\boldsymbol{\nabla}_i\Big]\\ &= N\hbar^2\boldsymbol{q}^2/m\ . \qquad (3.183)\end{aligned}$$

We have derived the *f-sum rule*:

$$\int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\,S(\boldsymbol{q},\omega) = \frac{N\hbar\boldsymbol{q}^2}{2mV}\ . \qquad (3.184)$$

Note that this integral, which is the first moment of the structure factor, is *independent of the potential*!

$$\int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega^n\,S(\boldsymbol{q},\omega) = \frac{1}{\hbar V}\Big\langle\hat{\boldsymbol{n}}_{\boldsymbol{q}}\Big[\overbrace{\mathcal{H},\big[\mathcal{H},\cdots[\mathcal{H},}^{n\text{ times}}\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}]\cdots\big]\Big]\Big\rangle\ . \qquad (3.185)$$

Moments with $n>1$ in general do depend on the potential. The $n=0$ moment gives

$$\begin{aligned}S(\boldsymbol{q}) \equiv \int\limits_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega^n\,S(\boldsymbol{q},\omega) &= \frac{1}{\hbar V}\big\langle\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}\big\rangle\\ &= \frac{1}{\hbar}\int\! d^3\!r\,\langle n(\boldsymbol{r})\,n(0)\rangle\,e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\ , \qquad (3.186)\end{aligned}$$

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

Compressibility Sum Rule

The isothermal compressibility is given by

$$\kappa_T = -\frac{1}{V}\frac{\partial V}{\partial n}\bigg|_T = \frac{1}{n^2}\frac{\partial n}{\partial \mu}\bigg|_T \ . \tag{3.187}$$

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

$$\langle \delta n \rangle = \chi(0,0)\,\delta\mu \quad \Longrightarrow \quad \kappa_T = \frac{1}{\hbar n^2} \lim_{\boldsymbol{q}\to 0} \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\, \frac{S(\boldsymbol{q},\omega)}{\omega} \ . \tag{3.188}$$

This is known as the *compressibility sum rule*.

3.7 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 $\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}} = \sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}$ increases the wavevector by $\boldsymbol{q}$. At $T = 0$, in order for $\langle\, n \,|\, \hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}} \,|\, \mathrm{G} \,\rangle$ to be nonzero (where $|\, \mathrm{G} \,\rangle$ 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 $\boldsymbol{k} = k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ and transferring it to a state outside the Fermi sphere with wavevector $\boldsymbol{k}+\boldsymbol{q}$. For $|\boldsymbol{q}| < 2k_{\mathrm{F}}$, the minimum excitation frequency is zero – one can always form particle-hole excitations with states adjacent to the Fermi sphere. For $|\boldsymbol{q}| > 2k_{\mathrm{F}}$, the minimum excitation frequency is obtained by taking an electron just inside the Fermi sphere with wavevector $\boldsymbol{k} = -k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ to an unfilled state outside the Fermi sphere with wavevector $\boldsymbol{k}+\boldsymbol{q}$. These cases are depicted graphically in fig. 3.2.

We therefore have

$$\omega_{\mathrm{max}}(q) = \frac{\hbar q^2}{2m} + \frac{\hbar k_{\mathrm{F}} q}{m} \tag{3.189}$$

$$\omega_{\mathrm{min}}(q) = \begin{cases} 0 & \text{if } q \le 2k_{\mathrm{F}} \\ \frac{\hbar q^2}{2m} - \frac{\hbar k_{\mathrm{F}} q}{m} & \text{if } q > 2k_{\mathrm{F}} \ . \end{cases} \tag{3.190}$$

This is depicted in fig. 3.3. Outside of the region bounded by $\omega_{\mathrm{min}}(q)$ and $\omega_{\mathrm{max}}(q)$, 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. 3.4. However, these multipair states do not couple to the ground state $|\, \mathrm{G} \,\rangle$ through a single application of the density operator $\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}$, hence they have zero oscillator strength: $\langle\, n \,|\, \hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}} \,|\, \mathrm{G} \,\rangle = 0$ for any multipair state $|\, n \,\rangle$.

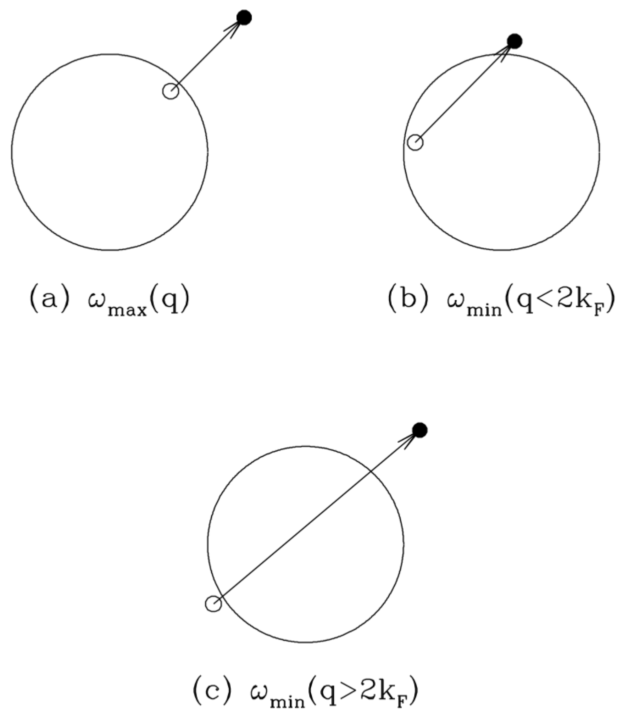

Figure 3.2: Minimum and maximum frequency particle-hole excitations in the free electron gas at $T=0$. (a) To construct a maximum frequency excitation for a given $\boldsymbol{q}$, create a hole just inside the Fermi sphere at $\boldsymbol{k}=k_{\mathrm{F}}\,\hat{\boldsymbol{q}}$ and an electron at $\boldsymbol{k}'=\boldsymbol{k}+\boldsymbol{q}$. (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 $\boldsymbol{k}'=\boldsymbol{k}+\boldsymbol{q}$.

3.7.1 Explicit $T=0$ Calculation

We start with

$$\begin{aligned} S(\boldsymbol{r},t) &= \langle n(\boldsymbol{r},t)\,n(0,0)\rangle && (3.191)\\ &= \int\!\frac{d^3k}{(2\pi)^3}\int\!\frac{d^3k'}{(2\pi)^3}\,e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\sum_{i,j}\big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i(t)}\,e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_j}\big\rangle\ . && (3.192)\end{aligned}$$

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

$$e^{A+B}=e^{A}\,e^{B}\,e^{-\frac{1}{2}[A,B]}\ , \tag{3.193}$$

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

$$e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i(t)}=e^{i\hbar\boldsymbol{k}^2t/2m}\,e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\,e^{-i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\ , \tag{3.194}$$

hence

$$S(\boldsymbol{r},t)=\int\!\frac{d^3k}{(2\pi)^3}\int\!\frac{d^3k'}{(2\pi)^3}\,e^{i\hbar\boldsymbol{k}^2t/2m}\,e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\sum_{i,j}\big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\,e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\,e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_j}\big\rangle\ . \tag{3.195}$$

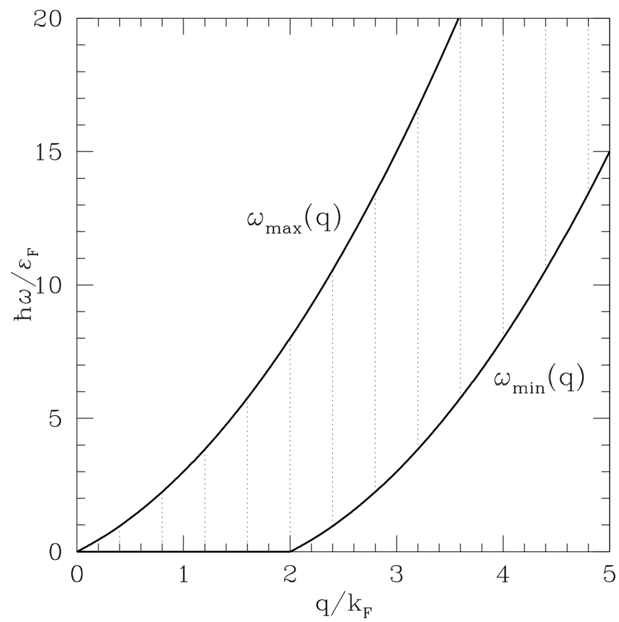

Figure 3.3: Minimum and maximum excitation frequency ω in units of $\varepsilon_{\rm F}/\hbar$ *versus* wavevector q in units of $k_{\rm F}$. Outside the hatched areas, there are no *single pair* excitations.

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

$$\begin{aligned}\Big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_i}\Big\rangle &= e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{k}' t/m}\,\Big\langle e^{i(\boldsymbol{k}-\boldsymbol{k})\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\Big\rangle \\ &= e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{k}' t/m}\,\frac{(2\pi)^3}{NV}\,\delta(\boldsymbol{k}-\boldsymbol{k}')\sum_{\boldsymbol{q}}\Theta(k_{\rm F}-q)\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\ ,\end{aligned} \tag{3.196}$$

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

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

$$\begin{aligned}\Big\langle e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}\cdot\boldsymbol{p}_i t/m}\, e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_j}\Big\rangle &= \frac{1}{N(N-1)}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'}\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-q') \\ &\quad\times\int\!\frac{d^3\!r_i}{V}\!\int\!\frac{d^3\!r_j}{V}\, e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\Big\{e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i}\, e^{i\boldsymbol{k}'\boldsymbol{r}_j} \\ &\qquad - e^{i(\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{k})\cdot\boldsymbol{r}_i}\, e^{i(\boldsymbol{q}'-\boldsymbol{q}+\boldsymbol{k}')\cdot\boldsymbol{r}_j}\Big\} \\ &= \frac{(2\pi)^6}{N(N-1)V^2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{q}'}\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-q') \\ &\quad\times e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\Big\{\delta(\boldsymbol{k})\,\delta(\boldsymbol{k}')-\delta(\boldsymbol{k}-\boldsymbol{k}')\,\delta(\boldsymbol{k}+\boldsymbol{q}'-\boldsymbol{q})\Big\}\ .\end{aligned} \tag{3.197}$$

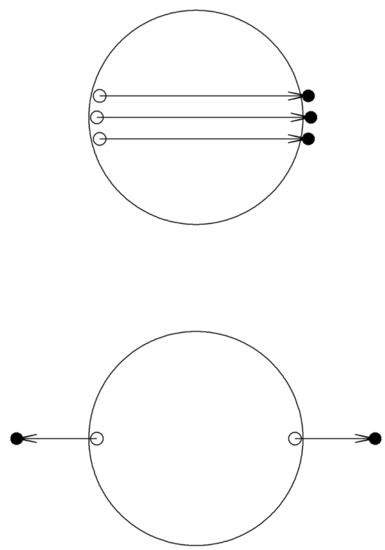

Figure 3.4: With multiple pair excitations, every part of $(\boldsymbol{q},\omega)$ space is accessible. However, these states to not couple to the ground state $\big|\mathrm{G}\big\rangle$ through a *single* application of the density operator $\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}$.

Summing over the $i=j$ terms gives

$$S_{\rm diag}(\boldsymbol{r},t)=\int\!\frac{d^3\!k}{(2\pi)^3}\;e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,e^{-i\hbar\boldsymbol{k}^2t/2m}\int\!\frac{d^3\!q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\;, \tag{3.198}$$

while the off-diagonal terms yield

$$\begin{aligned}S_{\rm off-diag}&=\int\!\frac{d^3\!k}{(2\pi)^3}\;e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\int\!\frac{d^3\!q}{(2\pi)^3}\!\int\!\frac{d^3\!q'}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-q')\\&\qquad\qquad\times(2\pi)^3\Big\{\delta(\boldsymbol{k})-e^{+i\hbar\boldsymbol{k}^2t/2m}\,e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\,\delta(\boldsymbol{q}-\boldsymbol{q}'-\boldsymbol{k})\Big\}\\&=n^2-\int\!\frac{d^3\!k}{(2\pi)^3}\;e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,e^{+i\hbar\boldsymbol{k}^2t/2m}\int\!\frac{d^3\!q}{(2\pi)^3}\Theta(k_{\rm F}-q)\,\Theta(k_{\rm F}-|\boldsymbol{k}-\boldsymbol{q}|)\,e^{-i\hbar\boldsymbol{k}\cdot\boldsymbol{q}t/m}\;,\end{aligned} \tag{3.199}$$

and hence

$$\begin{aligned}S(\boldsymbol{k},\omega)&=n^2\,(2\pi)^4\delta(\boldsymbol{k})\,\delta(\omega)+\int\!\frac{d^3\!q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\Big\{2\pi\,\delta\Big(\omega-\frac{\hbar\boldsymbol{k}^2}{2m}-\frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big)\\&\qquad\qquad-\Theta(k_{\rm F}-|\boldsymbol{k}-\boldsymbol{q}|)\,2\pi\delta\Big(\omega+\frac{\hbar\boldsymbol{k}^2}{2m}-\frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big)\Big\}\\&=(2\pi)^4n^2\delta(\boldsymbol{k})\delta(\omega)+\int\!\frac{d^3\!q}{(2\pi)^3}\,\Theta(k_{\rm F}-q)\,\Theta(|\boldsymbol{k}+\boldsymbol{q}|-k_{\rm F})\cdot2\pi\delta\Big(\omega-\frac{\hbar\boldsymbol{k}^2}{2m}-\frac{\hbar\boldsymbol{k}\cdot\boldsymbol{q}}{m}\Big).\end{aligned} \tag{3.200}$$

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

$$
\begin{aligned}
S(\boldsymbol{k},\omega) &= \frac{1}{2\pi}\int\limits_0^{k_\mathrm{F}} dq\, q^2 \int\limits_{-1}^{1} dx\, \Theta\big(\sqrt{k^2+q^2+2kqx}-k_\mathrm{F}\big)\,\delta\Big(\omega - \frac{\hbar k^2}{2m} - \frac{\hbar k q}{m}\,x\Big) \\
&= \frac{m}{2\pi\hbar k}\int\limits_0^{k_\mathrm{F}} dq\, q\, \Theta\Big(\sqrt{q^2+\frac{2m\omega}{\hbar}}-k_\mathrm{F}\Big)\int\limits_{-1}^{1} dx\, \delta\Big(x + \frac{k}{2q} - \frac{m\omega}{\hbar k q}\Big) \\
&= \frac{m}{4\pi\hbar k}\int\limits_0^{k_\mathrm{F}^2} du\, \Theta\Big(u + \frac{2m\omega}{\hbar} - k_\mathrm{F}^2\Big)\,\Theta\bigg(u - \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2\bigg) \ . \qquad (3.201)
\end{aligned}
$$

The constraints on u are

$$
k_\mathrm{F}^2 \geq u \geq \max\bigg(k_\mathrm{F}^2 - \frac{2m\omega}{\hbar}\,,\ \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2\bigg) \ . \qquad (3.202)
$$

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

The first case is

$$
k_\mathrm{F}^2 - \frac{2m\omega}{\hbar} \geq \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2 \quad \Longrightarrow \quad 0 \leq \omega \leq \frac{\hbar k_\mathrm{F} k}{m} - \frac{\hbar k^2}{2m} \ , \qquad (3.203)
$$

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

$$
\begin{aligned}
S(\boldsymbol{k},\omega) &= \frac{m}{4\pi\hbar k}\bigg\{k_\mathrm{F}^2 - \Big(k_\mathrm{F}^2 - \frac{2m\omega}{\hbar}\Big)\bigg\} \\
&= \frac{m^2\omega}{2\pi\hbar^2 k} \ . \qquad (3.204)
\end{aligned}
$$

The second case

$$
k_\mathrm{F}^2 - \frac{2m\omega}{\hbar} \leq \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2 \quad \Longrightarrow \quad \omega \geq \frac{\hbar k_\mathrm{F} k}{m} - \frac{\hbar k^2}{2m} \ . \qquad (3.205)
$$

However, we also have that

$$
\Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2 \leq k_\mathrm{F}^2 \ , \qquad (3.206)
$$

hence ω is restricted to the range

$$
\frac{\hbar k}{2m}\,|k - 2k_\mathrm{F}| \leq \omega \leq \frac{\hbar k}{2m}\,|k + 2k_\mathrm{F}| \ . \qquad (3.207)
$$

The integral in (3.201) then gives

$$
S(\boldsymbol{k},\omega) = \frac{m}{4\pi\hbar k}\bigg\{k_\mathrm{F}^2 - \Big|\frac{k}{2} - \frac{m\omega}{\hbar k}\Big|^2\bigg\} \ . \qquad (3.208)
$$

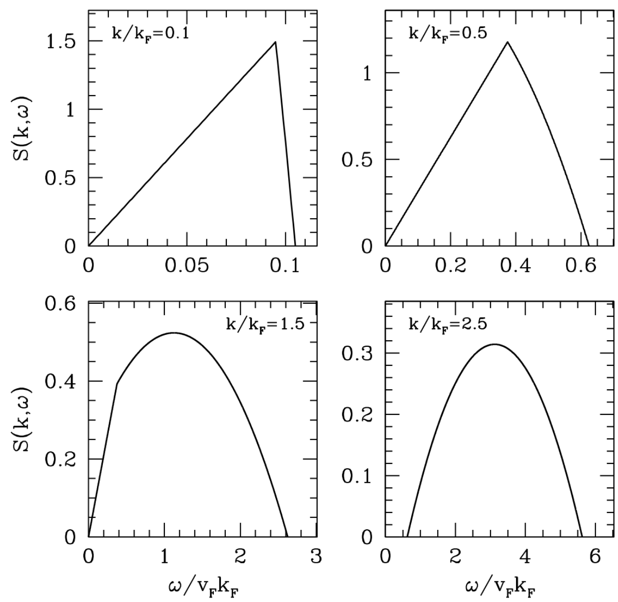

Figure 3.5: The dynamic structure factor $S(k,\omega)$ for the electron gas at various values of $k/k_{\rm F}$.

Putting it all together,

$$S(\boldsymbol{k},\omega) = \begin{cases} \frac{mk_{\rm F}}{\pi^2\hbar^2} \cdot \frac{\pi\omega}{2v_{\rm F}k} & \text{if } 0 < \omega \le v_{\rm F}k - \frac{\hbar k^2}{2m} \\ \\ \frac{mk_{\rm F}}{\pi^2\hbar^2} \cdot \frac{\pi k_{\rm F}}{4k} \left[1 - \left(\frac{\omega}{v_{\rm F}k} - \frac{k}{2k_{\rm F}}\right)^2\right] & \text{if } \left|v_{\rm F}k - \frac{\hbar k^2}{2m}\right| \le \omega \le v_{\rm F}k + \frac{\hbar k^2}{2m} \\ \\ 0 & \text{if } \omega \ge v_{\rm F}k + \frac{\hbar k^2}{2m}\ . \end{cases} \tag{3.209}$$

Integrating over all frequency gives the static structure factor,

$$S(\boldsymbol{k}) = \frac{1}{V}\big\langle n^\dagger_{\boldsymbol{k}}\, n_{\boldsymbol{k}}\big\rangle = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, S(\boldsymbol{k},\omega)\ . \tag{3.210}$$

The result is

$$S(\boldsymbol{k}) = \begin{cases} \left(\frac{3k}{4k_{\rm F}} - \frac{k^3}{16k_{\rm F}^3}\right)n & \text{if } 0 < k \le 2k_{\rm F} \\ \\ n & \text{if } k \ge 2k_{\rm F} \\ \\ Vn^2 & \text{if } k = 0\ , \end{cases} \tag{3.211}$$

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

3.8 Charged Systems: Screening and Dielectric Response

3.8.1 Definition of the Charge Response Functions

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

$$\begin{aligned}\mathcal{H}_1 &= -e\int\! d^3\!r \int\! d^3\!r'\, \frac{n(\boldsymbol{r})\,\rho_{\rm ext}(\boldsymbol{r},t)}{\big|\boldsymbol{r}-\boldsymbol{r}'\big|} \\ &= -e\int\!\frac{d^3\!k}{(2\pi)^3}\,\frac{4\pi}{\boldsymbol{k}^2}\,\hat{\boldsymbol{n}}(\boldsymbol{k})\,\hat\rho_{\rm ext}(-\boldsymbol{k},t)\ . \end{aligned} \tag{3.212}$$

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

$$\delta\hat{\boldsymbol{n}}(\boldsymbol{q},\omega) = \frac{4\pi e}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega)\,\hat\rho_{\rm ext}(\boldsymbol{q},\omega)\ . \tag{3.213}$$

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

$$\boldsymbol{\nabla}\cdot\boldsymbol{D} = 4\pi\rho_{\rm ext} \tag{3.214}$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{E} = 4\pi\big(\rho_{\rm ext} - e\,\langle\delta n\rangle\big)\ . \tag{3.215}$$

In Fourier space,

$$i\boldsymbol{q}\cdot\boldsymbol{D}(\boldsymbol{q},\omega) = 4\pi\hat\rho_{\rm ext}(\boldsymbol{q},\omega) \tag{3.216}$$

$$i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega) = 4\pi\hat\rho_{\rm ext}(\boldsymbol{q},\omega) - 4\pi e\big\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q},\omega)\big\rangle\ , \tag{3.217}$$

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

$$\frac{1}{\epsilon(\boldsymbol{q},\omega)} = \frac{i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},\omega)}{i\boldsymbol{q}\cdot\boldsymbol{D}(\boldsymbol{q},\omega)} = 1 - \frac{\delta\hat{\boldsymbol{n}}(\boldsymbol{q},\omega)}{Z\hat{\boldsymbol{n}}_{\rm ext}(\boldsymbol{q},\omega)} \tag{3.218}$$

$$= 1 - \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega)\ . \tag{3.219}$$

A system is said to exhibit *perfect screening* if

$$\epsilon(\boldsymbol{q}\to 0,\omega=0)=\infty \quad\Longrightarrow\quad \lim_{\boldsymbol{q}\to 0}\frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},0)=1\ . \tag{3.220}$$

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

$$\chi(\boldsymbol{q},\omega) = \frac{1}{\hbar V}\sum_n \frac{2\omega_{n\circ}}{\omega_{n\circ}^2-(\omega+i\epsilon)^2}\,\big|\big\langle\, n\,\big|\,\hat{\boldsymbol{n}}_{\boldsymbol{q}}\,\big|\,0\,\big\rangle\big|^2\ , \tag{3.221}$$

where we content ourselves to work at $T=0$, and where $\omega_{n\circ}\equiv\omega_n-\omega_\circ$ is the excitation frequency for the state $\big|\,n\,\big\rangle$.

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

$$i\boldsymbol{q} \cdot \langle \hat{\boldsymbol{j}}_{\text{charge}}(\boldsymbol{q}, \omega) \rangle = -ie\omega \langle \hat{\boldsymbol{n}}(\boldsymbol{q}, \omega) \rangle = i\sigma(\boldsymbol{q}, \omega)\, \boldsymbol{q} \cdot \boldsymbol{E}(\boldsymbol{q}, \omega) \ , \tag{3.222}$$

we find

$$\Big(4\pi \hat{\rho}_{\text{ext}}(\boldsymbol{q}, \omega) - 4\pi e \big\langle \delta\hat{\boldsymbol{n}}(\boldsymbol{q}, \omega) \big\rangle \Big) \sigma(\boldsymbol{q}, \omega) = -i\omega e \big\langle \delta\hat{\boldsymbol{n}}(\boldsymbol{q}, \omega) \big\rangle \ , \tag{3.223}$$

or

$$\frac{4\pi i}{\omega}\, \sigma(\boldsymbol{q}, \omega) = \frac{\big\langle \delta\hat{\boldsymbol{n}}(\boldsymbol{q}, \omega) \big\rangle}{e^{-1} \hat{\rho}_{\text{ext}}(\boldsymbol{q}, \omega) - \big\langle \delta\hat{\boldsymbol{n}}(\boldsymbol{q}, \omega) \big\rangle} = \frac{1 - \epsilon^{-1}(\boldsymbol{q}, \omega)}{\epsilon^{-1}(\boldsymbol{q}\omega)} = \epsilon(\boldsymbol{q}, \omega) - 1 \ . \tag{3.224}$$

Thus, we arrive at

$$\boxed{\frac{1}{\epsilon(\boldsymbol{q}, \omega)} = 1 - \frac{4\pi e^2}{\boldsymbol{q}^2}\, \chi(\boldsymbol{q}, \omega) \qquad , \qquad \epsilon(\boldsymbol{q}, \omega) = 1 + \frac{4\pi i}{\omega}\, \sigma(\boldsymbol{q}, \omega)} \tag{3.225}$$

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

$$\sigma(\boldsymbol{q}, \omega) = -\frac{i\omega}{\boldsymbol{q}^2}\, \frac{e^2 \chi(\boldsymbol{q}, \omega)}{1 - \frac{4\pi e^2}{\boldsymbol{q}^2} \chi(\boldsymbol{q}, \omega)} \ . \tag{3.226}$$

3.8.2 Static Screening: Thomas-Fermi Approximation

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

$$\mu \equiv \widetilde{\mu}(\boldsymbol{r}) - e\phi(\boldsymbol{r}) \ , \tag{3.227}$$

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

$$\begin{aligned} \widetilde{\mu}(\boldsymbol{r}) &\equiv \frac{\hbar^2}{2m}\, k_{\text{F}}^2(\boldsymbol{r}) = \frac{\hbar^2}{2m} \Big(3\pi^2 n + 3\pi^2 \delta n(\boldsymbol{r}) \Big)^{2/3} \\ &= \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \left\{ 1 + \frac{2}{3}\, \frac{\delta n(\boldsymbol{r})}{n} + \ldots \right\} \ , \end{aligned} \tag{3.228}$$

hence, to lowest order,

$$\delta n(\boldsymbol{r}) = \frac{3en}{2\mu}\, \phi(\boldsymbol{r}) \ . \tag{3.229}$$

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

$$\langle \delta\hat{\boldsymbol{n}}(\boldsymbol{q}, \omega = 0) \rangle = \frac{3en}{2\mu}\, \hat{\phi}(\boldsymbol{q}, \omega = 0) \ . \tag{3.230}$$

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

$$\begin{aligned} i\boldsymbol{q}\cdot\boldsymbol{E}(\boldsymbol{q},0) &= \boldsymbol{q}^2\,\hat\phi(\boldsymbol{q},0) \\ &= 4\pi\hat\rho_{\rm ext}(\boldsymbol{q},0) - 4\pi e\,\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q},0)\rangle \qquad (3.231)\\ &= 4\pi\hat\rho_{\rm ext}(\boldsymbol{q},0) - \frac{6\pi n e^2}{\mu}\,\hat\phi(\boldsymbol{q},0)\ , \qquad (3.232)\end{aligned}$$

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

$$q^2_{\rm TF} \equiv \frac{6\pi n e^2}{\mu}\ , \tag{3.233}$$

we have

$$\hat\phi(\boldsymbol{q},0) = \frac{4\pi\hat\rho_{\rm ext}(\boldsymbol{q},0)}{\boldsymbol{q}^2 + q^2_{\rm TF}}\ , \tag{3.234}$$

hence

$$e\,\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q},0)\rangle = \frac{q^2_{\rm TF}}{\boldsymbol{q}^2+q^2_{\rm TF}}\cdot\hat\rho_{\rm ext}(\boldsymbol{q},0) \quad\Longrightarrow\quad \boxed{\epsilon(\boldsymbol{q},0) = 1 + \frac{q^2_{\rm TF}}{\boldsymbol{q}^2}} \tag{3.235}$$

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

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

$$\lambda_{\rm TF} = \left(\frac{\pi}{12}\right)^{1/6}\sqrt{r_s}\,a_{\rm B} \simeq 0.800\,\sqrt{r_s}\,a_{\rm B}\ , \tag{3.236}$$

where r_s is the dimensionless free electron sphere radius, 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.* $\frac{4}{3}\,\pi\lambda^3_{\rm TF}\,n > 1$, 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 $\rho_{\rm ext}(\boldsymbol{r}) = Ze\,\delta(\boldsymbol{r})$, we have $\hat\rho_{\rm ext}(\boldsymbol{q},0) = Ze$ and

$$\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q},0)\rangle = \frac{Zq^2_{\rm TF}}{\boldsymbol{q}^2+q^2_{\rm TF}} \quad\Longrightarrow\quad \boxed{\langle\delta n(\boldsymbol{r})\rangle = \frac{Z\,e^{-r/\lambda_{\rm TF}}}{4\pi r}} \tag{3.237}$$

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

$$e\,\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q}\to 0,\omega=0)\rangle = \hat\rho_{\rm ext}(\boldsymbol{q}\to 0,\omega=0) = Ze\ . \tag{3.238}$$

3.8.3 High Frequency Behavior of $\epsilon(\boldsymbol{q},\omega)$

We have

$$\epsilon^{-1}(\boldsymbol{q},\omega) = 1 - \frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi(\boldsymbol{q},\omega) \tag{3.239}$$

and, at $T=0$,

$$\chi(\boldsymbol{q},\omega)=\frac{1}{\hbar V}\sum_j \big|\langle\, j\,|\,\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}\,|\,0\,\rangle\big|^2\left\{\frac{1}{\omega+\omega_{j0}+i\epsilon}-\frac{1}{\omega-\omega_{j0}+i\epsilon}\right\}\ , \tag{3.240}$$

where the number density operator is

$$\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}=\begin{cases}\sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i} & (1^{\text{st}}\text{ quantized})\\ \\ \sum_{\boldsymbol{k}}\psi^\dagger_{\boldsymbol{k}+\boldsymbol{q}}\,\psi_{\boldsymbol{k}} & (2^{\text{nd}}\text{ quantized: }\{\psi_{\boldsymbol{k}},\psi^\dagger_{\boldsymbol{k}'}\}=\delta_{\boldsymbol{k}\boldsymbol{k}'})\ .\end{cases} \tag{3.241}$$

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

$$\chi(\boldsymbol{q},\omega\to\infty)=-\frac{2}{\hbar V\,\omega^2}\sum_j\big|\langle\, j\,|\,\hat{\boldsymbol{n}}^\dagger_{\boldsymbol{q}}\,|\,0\,\rangle\big|^2\,\omega_{j0}=-\frac{2}{\hbar\omega^2}\int\limits_{-\infty}^{\infty}\!\frac{d\omega'}{2\pi}\,\omega'\,S(\boldsymbol{q},\omega')\ . \tag{3.242}$$

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

$$\chi(\boldsymbol{q},\omega\to\infty)=-\frac{n\boldsymbol{q}^2}{m\omega^2}\ , \tag{3.243}$$

and

$$\epsilon^{-1}(\boldsymbol{q},\omega\to\infty)=1+\frac{\omega_{\text{p}}^2}{\omega^2}\ , \tag{3.244}$$

where

$$\omega_{\text{p}}\equiv\sqrt{\frac{4\pi ne^2}{m}} \tag{3.245}$$

is the *plasma frequency*.

3.8.4 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 $\chi(\boldsymbol{q},\omega)$ from the noninteracting $\chi^0(\boldsymbol{q},\omega)$ by self-consistently adjusting the charge so that the perturbing charge density is not $\rho_{\text{ext}}(\boldsymbol{r})$, but rather $\rho_{\text{ext}}(\boldsymbol{r},t)-e\,\langle\delta n(\boldsymbol{r},t)\rangle$. Thus, we write

$$e\,\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q},\omega)\rangle=\frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^{\text{RPA}}(\boldsymbol{q},\omega)\,\hat{\rho}_{\text{ext}}(\boldsymbol{q},\omega) \tag{3.246}$$

$$=\frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^0(\boldsymbol{q},\omega)\left\{\hat{\rho}_{\text{ext}}(\boldsymbol{q},\omega)-e\,\langle\delta\hat{\boldsymbol{n}}(\boldsymbol{q},\omega)\rangle\right\}\ , \tag{3.247}$$

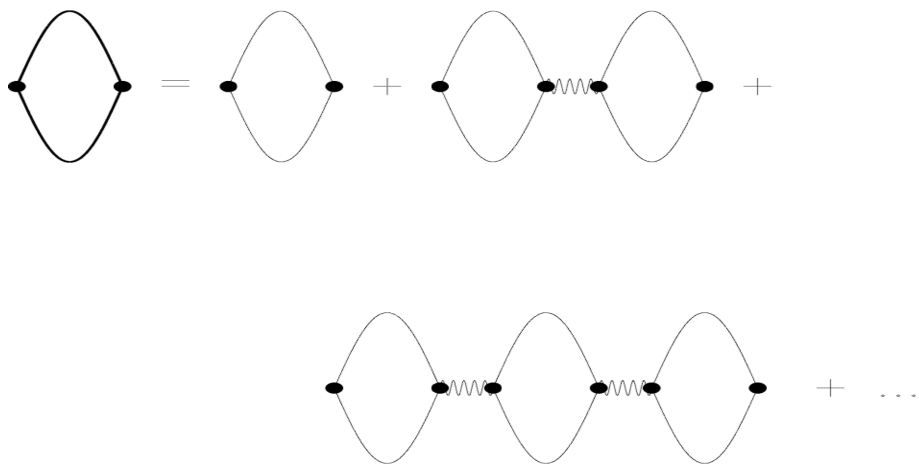

Figure 3.6: Perturbation expansion for RPA susceptibility bubble. Each bare bubble contributes a factor $\chi^0(\boldsymbol{q},\omega)$ and each wavy interaction line $\hat{v}(\boldsymbol{q})$. The infinite series can be summed, yielding eqn. 3.249.

which gives

$$\boxed{\chi^{\rm RPA}(\boldsymbol{q},\omega)=\frac{\chi^0(\boldsymbol{q},\omega)}{1+\frac{4\pi e^2}{\boldsymbol{q}^2}\chi^0(\boldsymbol{q},\omega)}} \tag{3.248}$$

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

$$\chi^{\rm RPA}(\boldsymbol{q},\omega)=\frac{\chi^0(\boldsymbol{q},\omega)}{1+\hat{v}(\boldsymbol{q})\,\chi^0(\boldsymbol{q},\omega)}\ . \tag{3.249}$$

2. Within the RPA, there is perfect screening:

$$\lim_{\boldsymbol{q}\to 0}\frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^{\rm RPA}(\boldsymbol{q},\omega)=1\ . \tag{3.250}$$

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

$$\chi^{\rm RPA}=\chi^0-\chi^0\,\hat{v}\,\chi^0+\chi^0\,\hat{v}\,\chi^0\,\hat{v}\,\chi^0-\ldots\ , \tag{3.251}$$

which has a diagrammatic interpretation, depicted in fig. 3.6. 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

$$\epsilon^{\rm RPA}(\boldsymbol{q},\omega)=1+\frac{4\pi e^2}{\boldsymbol{q}^2}\,\chi^0(\boldsymbol{q},\omega)\ . \tag{3.252}$$

5. Explicitly,

$$\begin{aligned}\mathrm{Re}\,\epsilon^{\mathrm{RPA}}(\boldsymbol{q},\omega) = 1 + \frac{q_{\mathrm{TF}}^2}{q^2}\Bigg\{\frac{1}{2} + \frac{k_{\mathrm{F}}}{4q}\Bigg[\bigg(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\mathrm{F}} q)^2}\bigg)\ln\bigg|\frac{\omega - v_{\mathrm{F}} q - \hbar q^2/2m}{\omega + v_{\mathrm{F}} q - \hbar q^2/2m}\bigg| \\ + \bigg(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\mathrm{F}} q)^2}\bigg)\ln\bigg|\frac{\omega - v_{\mathrm{F}} q + \hbar q^2/2m}{\omega + v_{\mathrm{F}} q + \hbar q^2/2m}\bigg|\Bigg]\Bigg\} \end{aligned} \tag{3.253}$$

$$\mathrm{Im}\,\epsilon^{\mathrm{RPA}}(\boldsymbol{q},\omega) = \begin{cases} \frac{\pi\omega}{2v_{\mathrm{F}} q}\cdot\frac{q_{\mathrm{TF}}^2}{q^2} & \text{if } 0 \le \omega \le v_{\mathrm{F}} q - \hbar q^2/2m \\ \frac{\pi k_{\mathrm{F}}}{4q}\Big(1 - \frac{(\omega - \hbar q^2/2m)^2}{(v_{\mathrm{F}} q)^2}\Big)\frac{q_{\mathrm{TF}}^2}{q^2} & \text{if } v_{\mathrm{F}} q - \hbar q^2/2m \le \omega \le v_{\mathrm{F}} q + \hbar q^2/2m \\ 0 & \text{if } \omega > v_{\mathrm{F}} q + \hbar q^2/2m \end{cases} \tag{3.254}$$

6. Note that

$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q},\omega\to\infty) = 1 - \frac{\omega_{\mathrm{p}}^2}{\omega^2}\ , \tag{3.255}$$

in agreement with the f-sum rule, and

$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q}\to 0,\omega = 0) = 1 + \frac{q_{\mathrm{TF}}^2}{q^2}\ , \tag{3.256}$$

in agreement with Thomas-Fermi theory.

7. At $\omega = 0$ we have

$$\epsilon^{\mathrm{RPA}}(\boldsymbol{q},0) = 1 + \frac{q_{\mathrm{TF}}^2}{q^2}\Bigg\{\frac{1}{2} + \frac{k_{\mathrm{F}}}{2q}\bigg(1 - \frac{q^2}{4k_{\mathrm{F}}^2}\bigg)\ln\bigg|\frac{q + 2k_{\mathrm{F}}}{2 - 2k_{\mathrm{F}}}\bigg|\Bigg\}\ , \tag{3.257}$$

which is real and which has a singularity at $q = 2k_{\mathrm{F}}$. This means that the long-distance behavior of $\langle\delta n(\boldsymbol{r})\rangle$ must oscillate. For a local charge perturbation, $\rho_{\mathrm{ext}}(\boldsymbol{r}) = Ze\,\delta(\boldsymbol{r})$, we have

$$\langle\delta n(\boldsymbol{r})\rangle = \frac{Z}{2\pi^2 r}\int_0^\infty dq\, q\sin(qr)\left\{1 - \frac{1}{\epsilon(\boldsymbol{q},0)}\right\}\ , \tag{3.258}$$

and within the RPA one finds for long distances

$$\langle\delta n(\boldsymbol{r})\rangle \sim \frac{Z\cos(2k_{\mathrm{F}} r)}{r^3}\ , \tag{3.259}$$

rather than the Yukawa form familiar from Thomas-Fermi theory.

3.8.5 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 $\chi^{\rm RPA}$ 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

$$\begin{aligned}\chi^0(\boldsymbol{q},t) &= \frac{i}{\hbar V}\big\langle\big[\hat{\boldsymbol{n}}(\boldsymbol{q},t),\hat{\boldsymbol{n}}(-\boldsymbol{q},0)\big]\big\rangle \qquad (3.260)\\ &= \frac{i}{\hbar V}\Big\langle\Big[\sum_{\boldsymbol{k}\sigma}\psi^\dagger_{\boldsymbol{k},\sigma}\,\psi_{\boldsymbol{k}+\boldsymbol{q},\sigma},\sum_{\boldsymbol{k}',\sigma'}\psi^\dagger_{\boldsymbol{k}',\sigma'}\,\psi_{\boldsymbol{k}'-\boldsymbol{q},\sigma'}\Big]\Big\rangle\, e^{i(\varepsilon(\boldsymbol{k})-\varepsilon(\boldsymbol{k}+\boldsymbol{q}))t/\hbar}\,\Theta(t)\ , \qquad (3.261)\end{aligned}$$

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

$$\big[AB,CD\big] = A\big\{B,C\big\}D - \big\{A,C\big\}BD + CA\big\{B,D\big\} - C\big\{A,D\big\}B \qquad (3.262)$$

we obtain

$$\chi^0(\boldsymbol{q},t) = \frac{i}{\hbar V}\sum_{\boldsymbol{k}\sigma}(f_{\boldsymbol{k}} - f_{\boldsymbol{k}+\boldsymbol{q}})\,e^{i(\varepsilon(\boldsymbol{k})-\varepsilon(\boldsymbol{k}+\boldsymbol{q}))t/\hbar}\,\Theta(t)\ , \qquad (3.263)$$

and therefore

$$\boxed{\chi^0(\boldsymbol{q},\omega) = 2\int\!\frac{d^3\!k}{(2\pi)^3}\;\frac{f_{\boldsymbol{k}+\boldsymbol{q}} - f_{\boldsymbol{k}}}{\hbar\omega - \varepsilon(\boldsymbol{k}+\boldsymbol{q}) + \varepsilon(\boldsymbol{k}) + i\epsilon}}\ . \qquad (3.264)$$

Here,

$$f_{\boldsymbol{k}} = \frac{1}{e^{(\varepsilon(\boldsymbol{k})-\mu)/k_{\rm B}T} + 1} \qquad (3.265)$$

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

$$\chi^0(\boldsymbol{q},\omega) = -\frac{k_{\rm F}^3}{3\pi^2}\cdot\frac{q^2}{m\omega^2}\left\{1 + \frac{3}{5}\left(\frac{\hbar k_{\rm F}q}{m\omega}\right)^2 + \ldots\right\}\ , \qquad (3.266)$$

so the resonance condition becomes

$$\begin{aligned}0 &= 1 + \frac{4\pi e^2}{q^2}\,\chi^0(\boldsymbol{q},\omega)\\ &= 1 - \frac{\omega_{\rm p}^2}{\omega^2}\cdot\left\{1 + \frac{3}{5}\left(\frac{v_{\rm F}q}{\omega}\right)^2 + \ldots\right\}\ . \qquad (3.267)\end{aligned}$$

This gives the dispersion

$$\omega = \omega_{\rm p}\left\{1 + \frac{3}{10}\left(\frac{v_{\rm F}q}{\omega_{\rm p}}\right)^2 + \ldots\right\}\ . \qquad (3.268)$$

Recall that the particle-hole continuum frequencies are bounded by $\omega_{\rm min}(q)$ and $\omega_{\rm max}(q)$, which are given in eqs. 3.190 and 3.189. Eventually the plasmon penetrates the particle-hole continuum, at which point it becomes heavily damped since it can decay into particle-hole excitations.