Screening and Linear Response

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Notes on Screening and Linear Response Theory for Physics 7450, Spring 2010

I. THOMAS-FERMI APPROXIMATION FOR NON-INTERACTING ELECTRONS

We are interested in the problem of how the electron density responds, when the electron gas is modified by addition of an external potential. This potential could represent, for example, the electrostatic potential of a charged impurity in a metal. Or, if it’s time-dependent, it could represent electromagnetic radiation shining on a metal. Formally, we want to consider the Hamiltonian

\[ H = H_K + H_{\text{int}} + \int d^3r U_{\text{ext}}(r) \psi_\sigma^\dagger(r) \psi_\sigma(r). \]  

(1)

Here, \( H_K \) is the kinetic energy part of the Hamiltonian, \( H_{\text{int}} \) is the Coulomb interaction between electrons, and the last term is the external potential. For now we assume \( U_{\text{ext}} \) is time-independent.

Let’s start out by neglecting interactions altogether. Then the Hamiltonian is just

\[ H_0 = H_K + \int d^3r U_{\text{ext}}(r) \psi_\sigma^\dagger(r) \psi_\sigma(r), \]  

(2)

which is a non-interacting Hamiltonian describing non-interacting fermions moving in the potential \( U_{\text{ext}}(r) \). However, for a general potential \( U_{\text{ext}} \), it is difficult to find the single-particle eigenstates.

Let’s make another simplifying assumption, which is the crucial assumption of the Thomas-Fermi approximation: we assume that \( U_{\text{ext}}(r) \) is a slowly-varying function of position – so the potential changes very slowly and smoothly in space. In this limit, at every point in space we can treat \( U_{\text{ext}}(r) \) as a constant, the effect of which is to shift the single-particle energies: \( \epsilon_k = k^2/2m \rightarrow \epsilon_k(r) = k^2/2m + U_{\text{ext}}(r) \). Note that we are making a kind of semiclassical approximation here, where we are specifying position and momentum of an electron simultaneously – this is only okay because we assume that \( U_{\text{ext}} \) changes very slowly. To calculate the density as a function of position \( n(r) \), first note that the chemical potential \( \mu \) is the same everywhere (this is always true in thermal equilibrium). When \( U_{\text{ext}} = 0 \), using the standard formulae for the non-interacting Fermi gas (with spin), we have

\[ n = \frac{(2m)^{3/2}}{3\pi^2} \mu^{3/2}. \]  

(3)

How should this formula be modified when \( U_{\text{ext}} \neq 0 \), in our slowly-varying approximation? In Eq. (3), \( \mu \) is actually the energy difference between the chemical potential, and the minimum single-particle energy (which happens to be zero). That is, it tells us how far up in energy we have to go from the bottom of the one-electron dispersion, before we hit the chemical potential. Now, in the presence of \( U_{\text{ext}} \), the minimum single-particle energy is \( U_{\text{ext}}(r) \), so we should modify the expression for the density as follows:

\[ n(r) = \frac{(2m)^{3/2}}{3\pi^2} [\mu - U_{\text{ext}}(r)]^{3/2}. \]  

(4)

This is the main result of the Thomas-Fermi approximation for non-interacting fermions. It gives the density as a very simple function of \( U_{\text{ext}}(r) \).

Note that we haven’t assumed anything about \( U_{\text{ext}} \) being small, and so the result for \( n(r) \) is a non-linear function of the applied potential. This is a rather rare case where it’s possible to get a simple analytic result for the non-linear response to a perturbation, and to get this result we relied both on the non-interacting nature of the fermions, and the assumption that the potential is slowly-varying. Often we are interested in the case of a small external potential. The two main reasons for this are first, calculation is easier (with fewer assumptions than we’ve made here), and second, the linear response to a small perturbation contains very important physical information about the unperturbed system. Because of the latter reason, if we want to think about our external perturbation as a probe of the system, small perturbations and linear response are the way to go.

With the above discussion in mind, let’s take our result above and assume \( U_{\text{ext}} \) is small, so we can expand to linear order. (Precisely, we assume \( U_{\text{ext}}(r) \ll \mu \).) The result of first-order Taylor expansion is \( n(r) = n + \delta n(r) \), where \( n \) is the unperturbed density of Eq. (3), and

\[ \delta n(r) = -\frac{(2m)^{3/2} \mu^{1/2}}{2\pi^2} U_{\text{ext}}(r) = -\frac{mk_F}{\pi^2} U_{\text{ext}}(r). \]  

(5)
II. INTERACTIONS AND SCREENING

So far we haven’t discussed the effect of interactions. A reasonable way to take this into account is to make the Hartree approximation, since the major effect of the external potential is to make the background density non-uniform – we should be able to capture this in the Hartree approximation, where we will have \( n \to n(r) \). Let’s write the density operator as follows,

\[
\hat{n}(r) = n + \delta n(r) + [\hat{n}(r) - n - \delta n(r)],
\]

where as usual the term in brackets is to be treated as a small fluctuation part. It is actually most useful to write this in the form

\[
\hat{n}(r) - n = \delta n(r) + [\hat{n}(r) - n - \delta n(r)],
\]

since the interaction part of the Hamiltonian depends explicitly on \( \hat{n}(r) - n \). We are interested in how the electrons respond to \( \delta n(r) \), and not in any of the constant terms in the mean-field Hamiltonian. So, making the usual approximation of dropping the term quadratic in the fluctuations, and keeping only the non-constant terms (i.e. those involving operators), we have

\[
H_{\text{int}} \to \frac{e^2}{2} \int d^3r d^3r' \left[ \frac{\delta n(r)\hat{n}(r') + \delta n(r')\hat{n}(r)}{|r - r'|} \right]
\]

\[
= \frac{e^2}{2} \int d^3r d^3r' \left[ \frac{\delta n(r')\hat{n}(r)}{|r - r'|} \right] = \int d^3r U_H(r)\hat{n}(r),
\]

\[
\text{where}
\]

\[
U_H(r) = \frac{e^2}{2} \int d^3r' \frac{\delta n(r')}{|r - r'|}
\]

is called the Hartree potential. This just expresses the very simple physics that the electrons feel a Coulomb potential from their own inhomogeneous charge density (which is, in mean-field theory, treated as a number and not an operator).

Then the mean-field Hamiltonian is

\[
H_{MF} = H_K + \int d^3r U_{\text{tot}}(r)\hat{n}(r),
\]

\[
\text{where}
\]

\[
U_{\text{tot}}(r) = U_H(r) + U_{\text{ext}}(r).
\]

Making again the Thomas-Fermi approximation, we can quickly redo the analysis above to find

\[
\delta n(r) = \frac{m k_F}{\pi^2} U_{\text{tot}}(r).
\]

The difference from before is the presence of \( U_{\text{tot}} \) on the right-hand side, which itself depends on \( \delta n \). We can solve for \( \delta n \) if we want, but let’s defer this to a bit later, when we discuss how to go beyond the Thomas-Fermi approximation.

Instead, let’s consider a situation of physical interest, where \( U_{\text{ext}}(r) \) comes from some external charges (by external we just mean that they are some other charges than the electrons themselves). A good example is a charged impurity in a metal. Therefore we can write \( U_{\text{ext}}(r) = -e\phi_{\text{ext}}(r) \), where \( \phi_{\text{ext}}(r) \) is the electrostatic potential generated by the external charges. Because the electron density changes in response to this perturbation, the non-uniform electron density also contributes to the electrostatic potential, and so the true potential \( \phi(r) \) is not the same as \( \phi_{\text{ext}}(r) \); instead, \( U_{\text{tot}}(r) = -e\phi(r) \).

Let’s understand how to compute \( \phi(r) \), which we can do using Gauss’ Law

\[
-\nabla^2 \phi = 4\pi \delta \rho_{\text{el}}(r) + 4\pi \rho_{\text{ext}}(r).
\]

Here \( \delta \rho_{\text{el}} \) is the deviation of the electron density from its uniform value, and \( \rho_{\text{ext}}(r) \) is the external charge density that gives rise to \( \phi_{\text{ext}}(r) \). We have made the assumption that \( \phi(r) \) is a constant (say, zero), in the absence of any external charges – this has to be correct since in that case the system is electrically neutral and homogeneous.

Now, \( \delta \rho_{\text{el}}(r) = -e\delta n(r) \), so using Eq. (13) we have

\[
\delta \rho_{\text{el}}(r) = \frac{me^2 k_F}{\pi^2}\phi(r) = -\frac{k_F}{\pi^2 a_0} \phi(r) = -\frac{k_F^2}{4\pi} \phi(r),
\]
where $a_0$ is the Bohr radius (remember that we’re working in units where $\hbar = 1$), and we have introduced the new wavevector scale $k_s \sim \sqrt{k_F/a_0}$. Plugging this into Gauss’ Law for $\delta \rho_{el}$, we have
\[ (-\nabla^2 + k_s^2) \phi = 4\pi \rho_{ext}(r). \] (16)

Let’s suppose that $\rho_{ext}(r) = q\delta(r)$, which is just a point charge $q$ at the origin. In this case, Gauss’ Law is solved by the potential
\[ \phi(r) = 4\pi q \int \frac{d^3 k}{(2\pi)^3} \frac{e^{ik\cdot r}}{k^2 + k_s^2} = \frac{q}{|r|} e^{-k_s|r|}. \] (17)
(The $k$-integral can be done by going to spherical coordinates and using contour integration on the radial integral.) This is a screened Coulomb potential, which decays exponentially on a length scale $\ell_s = 1/k_s$, the screening length. So we see that, apparently, the electron gas is very effective at screening out the electrostatic potential of a charged impurity.

However, a question arises here, which is whether it was really legitimate to make the Thomas-Fermi approximation in this case. The potential $U_{ext}(r)$ is definitely not slowly-varying here near $r = 0$. To address this question we need to understand how to go beyond the Thomas-Fermi approximation.

### III. LINEAR RESPONSE BEYOND THOMAS-FERMI, AND FOR A TIME-DEPENDENT POTENTIAL

Let’s go back to the original setup for the electron gas in an external potential. We now also allow for the external potential to be time-dependent, and we have
\[ H = H_K + H_{int} + \int d^3r \, U_{ext}(r, t) \dot{n}(r). \] (18)

Let’s consider the linear-response of the density to this perturbation. That is, we are interested in the quantity
\[ \delta n(r, t) = (\dot{n}(r, t)) - n, \] (19)
to linear order in $U_{ext}$. Here, $\dot{n}(r, t)$ is the density operator in the Heisenberg picture. On very general grounds we can write
\[ \delta n(r, t) = \int d^3r'\int dt' \chi(r - r', t - t') U_{ext}(r', t'), \] (20)
where the function $\chi$ is called the density response function. This is almost the most general form we could write down under the assumption that $\delta n$ depends linearly on $U_{ext}$. The only simplification that is made is that $\chi$ depends only on the differences $r - r'$ and $t - t'$. This has to be true for the following reason: since this expression is the linear term in the response to $U_{ext}$, $\chi$ can only depend on properties of the unperturbed system, with no external potential. Because the unperturbed system is translation invariant in both space and time, $\chi$ can only depend on the differences. Actually it also has to be true that $\chi = 0$ if $t - t' < 0$, which is the statement of causality: the density response at time $t$ cannot depend on the behavior of the potential at later times $t'$. So far we are not saying anything about how to calculate $\chi$ – that will come a bit later, but the basic idea is just to do perturbation theory in $U_{ext}$.

It is often convenient to work in Fourier space for both position and time, defining for example the Fourier transform of the density by
\[ \delta n(r, t) = \int \frac{d^3 k}{(2\pi)^3} \int \frac{d\omega}{2\pi} e^{i k \cdot r} e^{-i\omega t} \delta n(k, \omega). \] (21)

Defining Fourier transforms of the other functions the same way, in Fourier space Eq. (20) becomes
\[ \delta n(k, \omega) = \chi(k, \omega) U_{ext}(k, \omega). \] (22)

The more complicated integral form on the right-hand side of Eq. (20) – known as a convolution – just becomes a simple product in Fourier space. This expresses an important piece of physics, which is that in a space- and time-translation invariant system, in linear response, a Fourier mode of the external potential at a given $k$ and $\omega$ can only induce a density response at the same $k$ and $\omega$. Responses at other $k$ and $\omega$ can only occur as a nonlinear effect.
There is a general framework, which we will develop in a bit, to calculate $\chi$ even for interacting systems. However, for interacting systems, this framework only tells what mathematical object to calculate if we want to know $\chi$ – it certainly will not allow us to calculate it exactly. So, first, let’s see how we can use the Hartree approximation to relate $\chi$ to the density response function of the non-interacting system. After doing that, we will set up our general framework, and use it to calculate the non-interacting $\chi$.

Let’s consider the non-interacting system we get starting with $H$ [in Eq. (18)], and dropping the interaction term. Let’s call the response function in this case $\chi_0$, so that the density response to the external potential is

$$\delta n(k, \omega) = \chi_0(k, \omega) U_{\text{ext}}(k, \omega).$$  

Next, let’s consider the interacting Hamiltonian, but we make the Hartree approximation for the interaction term. We want to make a time-dependent Hartree approximation – all we do is make the same mean-field guess as before, just letting $\delta n$ be time-dependent:

$$\hat{n}(r) = n + \delta n(r, t) + [\hat{n} - n - \delta n(r, t)].$$  

If we proceed as above when we worked out the Hartree potential, everything goes exactly the same way as before:

$$H_{\text{int}} \rightarrow \int d^3r U_H(r, t) \hat{n}(r),$$

and

$$U_H(r, t) = e^2 \int d^3r' \frac{\delta n(r', t)}{|r - r'|}.$$  

Again the mean-field Hamiltonian is

$$H_{\text{MF}} = H_K + \int d^3r U_{\text{tot}}(r, t),$$

where $U_{\text{tot}}(r, t) = U_H(r, t) + U_{\text{ext}}(r, t)$. Therefore, the Hartree approximation tells us that

$$\delta n(k, \omega) = \chi_0(k, \omega) U_{\text{tot}}(k, \omega) = \chi_0(k, \omega) [U_H(k, \omega) + U_{\text{ext}}(k, \omega)].$$  

If we use the result that the Fourier transform of the $1/|r|$ Coulomb potential is $4\pi/|k|^2$, then the Hartree potential can be written as:

$$U_H(k, \omega) = \frac{4\pi e^2}{|k|^2} \delta n(k, \omega).$$

Plugging this in above allows us to solve for $\delta n$:

$$\delta n(k, \omega) = \frac{\chi_0(k, \omega)}{1 - \frac{4\pi e^2}{|k|^2} \chi_0(k, \omega)} U_{\text{ext}}(k, \omega).$$

So what we’ve shown is that, in the Hartree approximation,

$$\chi(k, \omega) = \frac{\chi_0(k, \omega)}{1 - \frac{4\pi e^2}{|k|^2} \chi_0(k, \omega)}.$$  

This will be useful once we know how to calculate $\chi_0(k, \omega)$!

**IV. GENERAL LINEAR-RESPONSE THEORY**

Let’s now set up a general framework for calculating response functions. We will consider the following very general Hamiltonian:

$$H = H_0 - \int d^3r \lambda(r, t) \hat{A}(r) \equiv H_0 + H'(t).$$
Here $H_0$ is the Hamiltonian of the unperturbed system. The only thing we assume about $H_0$ is that it is time-independent – it could be a very complicated interacting Hamiltonian, as long as it has no time-dependence. The second term $H'(t)$ is the external perturbation (in general time-dependent). Clearly the example of a time-dependent potential (coupled to the density) can be written in this form. Another important example is a time- and space-dependent Zeeman magnetic field, where the operator $\hat{A}(r)$ would be the spin density.

For simplicity, we will study this problem at zero temperature. Our approach will be to do time-dependent perturbation theory in $H'$. We assume that the system is in $|\psi_0\rangle$, the ground state of $H_0$, at a time $t_0$. At the end of the calculations, we will take $t_0 \to -\infty$; the system is in its ground state in the far past, and then we turn on the perturbation. The state of the system at a time $t$ is

$$|\psi(t)\rangle = U(t,t_0)|\psi_0\rangle,$$

where

$$U(t,t_0) = T \exp \left( -i \int_{t_0}^t dt' H(t') \right)$$

is the evolution operator for the Hamiltonian $H(t)$ (all time-dependence is in $H'(t)$). Here, $T$ is the time-ordering symbol. We are interested in the expectation value of an observable $\hat{B}(r)$ at time $t > t_0$. In particular, we’re interested in the change in this expectation value induced by the perturbation:

$$\delta \langle \hat{B}(r,t) \rangle \equiv \langle \psi(t)|\hat{B}(r)|\psi(t)\rangle - \langle \psi_0|\hat{B}(r)|\psi_0\rangle = \langle \psi_0| \left[ \hat{B}(r,t) - \hat{B}(r) \right] |\psi_0\rangle.$$

Here, $\hat{B}(r,t)$ is the Heisenberg picture operator defined by

$$\hat{B}(r,t) = U(t_0,t)\hat{B}(r)U(t,t_0).$$

We are interested in expanding in to first order $H'$, since we assume the external perturbation is small. Before we can easily do this, we need to do some formal manipulations on the expression for $\langle \psi_0|\hat{B}(r,t)|\psi_0\rangle$:

$$\langle \psi_0|\hat{B}(r,t)|\psi_0\rangle = \langle \psi_0|U(t_0,t)\hat{B}(r)U(t,t_0)|\psi_0\rangle$$

$$= \langle \psi_0|U(t_0,t)e^{-iH_0t}\left[ e^{iH_0t}\hat{B}(r)e^{-iH_0t} \right] e^{iH_0t}U(t,t_0)|\psi_0\rangle$$

$$= \langle \psi_0|U(t_0,t)e^{-iH_0t}\hat{B}_1(r,t)e^{iH_0t}U(t,t_0)|\psi_0\rangle. \quad (37)$$

In the last line we defined

$$\hat{B}_1(r,t) = e^{iH_0t}\hat{B}(r)e^{-iH_0t},$$

which is referred to as an operator in the interaction picture. In this case, the interaction picture is the same as the Heisenberg picture, but for the unperturbed Hamiltonian $H_0$. Continuing with the manipulations above, and letting $E_0$ be the ground state energy of $H_0$, we write

$$\langle \psi_0|\hat{B}(r,t)|\psi_0\rangle = \langle \psi_0|U(t_0,t)e^{-iH_0t}\hat{B}_1(r,t)e^{iH_0t}U(t,t_0)|\psi_0\rangle$$

$$= e^{iE_0t_0} \langle \psi_0|U(t_0,t)e^{-iH_0t}\hat{B}_1(r,t)e^{iH_0t}U(t,t_0)|\psi_0\rangle e^{-iE_0t_0}$$

$$= \langle \psi_0|e^{iH_0t_0}U(t_0,t)e^{-iH_0t}\hat{B}_1(r,t)e^{iH_0t}U(t,t_0)e^{-iH_0t_0}\rangle \langle \psi_0|$$

$$= \langle \psi_0|U_1(t_0,t)\hat{B}_1(r,t)U_1(t,t_0)|\psi_0\rangle, \quad (41)$$

where in the last line we defined the interaction picture evolution operator

$$U_1(t,t_0) = e^{iH_0t}U(t,t_0)e^{-iH_0t_0}. \quad (42)$$

The whole reason for these manipulations is that $U_1(t,t_0)$ turns out to have a simple and convenient form – although it is not at all clear yet that this will be true. To find the form of $U_1$, we will show that it satisfies a simple first-order differential equation, and we will write down the unique solution to this equation. First, note that

$$\frac{d}{dt} U(t,t_0) = -iH(t)U(t,t_0). \quad (43)$$
The fact that we have a time-ordered exponential is crucial here – otherwise this result is not true. The easiest way to see that it is true with the time-ordering symbol is to note that, inside the time-ordering operation, all the operators commute with one another, so we can use the usual rules of algebra for numbers and forget that \( H(t) \) is a matrix. Then, we just have to bring \( H(t) \) outside of the time-ordering symbol. But since \( t \) is later than all the other times involved, \( T \) automatically brings it out on the left for us.

Now consider the first time-derivative of \( U_I \), which will give us our differential equation:

\[
\frac{dU_I(t, t_0)}{dt} = -H_0U_I(t, t_0) + e^{iH_0t}H(t)U(t, t_0)e^{-iH_0t_0}
\]

\[
= -H_0e^{iH_0t}U(t, t_0)e^{-iH_0t_0} + e^{iH_0t}H(t)U(t, t_0)e^{-iH_0t_0}
\]

\[
= e^{iH_0t}[H(t) - H_0]U(t, t_0)e^{-iH_0t_0}
\]

\[
= e^{iH_0t}H'(t)U(t, t_0)e^{-iH_0t_0}
\]

\[
= [e^{iH_0t}H'(t)e^{-iH_0t}]e^{iH_0t}U(t, t_0)e^{-iH_0t_0}
\]

\[
= H'_I(t)U_I(t, t_0).
\]

Here we have

\[
H'_I(t) = e^{iH_0t}H'(t)e^{-iH_0t} = -\int d^3\lambda(r, t)\hat{A}_I(r, t).
\]

The unique solution to this differential equation (which satisfies the boundary condition \( U_I(t_0, t_0) = 1 \)) is

\[
U_I(t, t_0) = T\exp\left(-i\int_{t_0}^t dt' H_I(t')\right).
\]

This expression is very useful, because it will easily allow us to expand to first order in \( H' \):

\[
U_I(t, t_0) \approx 1 - i\int_{t_0}^t dt' H_I(t').
\]

To evaluate \( \delta(\hat{B}(r, t)) \), we will also need

\[
U_I(t_0, t) = [U_I(t, t_0)]^\dagger \approx 1 + i\int_{t_0}^t dt' H_I(t').
\]

We have

\[
\langle \hat{B}(r, t) \rangle = \langle \psi_0 | U_I(t_0, t)\hat{B}_I(r, t)U_I(t, t_0) | \psi_0 \rangle
\]

\[
\approx \langle \psi_0 | \left[ 1 + i\int_{t_0}^t dt' H_I(t') \right]\hat{B}_I(r, t) \left[ 1 - i\int_{t_0}^t dt' H_I(t') \right] | \psi_0 \rangle
\]

\[
\approx \langle \psi_0 | \hat{B}_I(r, t) | \psi_0 \rangle + i\int_{-\infty}^t dt' \langle \psi_0 | H'_I(t'), \hat{B}_I(r, t) | \psi_0 \rangle
\]

\[
= \langle \psi_0 | \hat{B}(r) | \psi_0 \rangle - i\int_{-\infty}^t dt' \int d^3\lambda(r', t')\langle \psi_0 | \hat{A}_I(r', t'), \hat{B}_I(r, t) | \psi_0 \rangle
\]

\[
= \langle \psi_0 | \hat{B}(r) | \psi_0 \rangle + i\int_{-\infty}^t dt' \int d^3\lambda(r', t')\langle \psi_0 | \hat{B}_I(r, t), \hat{A}_I(r', t') | \psi_0 \rangle.
\]

Therefore we can write

\[
\delta(\hat{B}(r, t)) = \int_{-\infty}^\infty dt' \int d^3 r' \chi_{BA}(r - r', t - t')\lambda(r', t'),
\]

where

\[
\chi_{BA}(r - r', t - t') \equiv i\Theta(t - t')\langle \psi_0 | \hat{B}_I(r, t), \hat{A}_I(r', t') | \psi_0 \rangle.
\]
Here we have assumed that $\chi_{BA}$ only depends on $r$, $r'$ and $t$, $t'$ via their differences, which will be true if $H_0$ is time-independent and invariant under spatial translations. Notice also the $\Theta$-function in the definition of $\chi$, which enforces the fact that the range of the $t'$-integral is from $-\infty$ to $t$.

Now that we’re done with this calculation, we usually don’t use the interaction picture anymore. Instead when we write a time-dependent operator, normally we mean the Heisenberg picture operator for $H_0$. So we will drop the $I$’s on the operators above and write

$$\chi_{BA}(r - r', t - t') = i\Theta(t - t') \langle \psi_0 | \hat{B}(r, t), \hat{A}(r', t') | \psi_0 \rangle. \quad (64)$$

**V. DENSITY RESPONSE FUNCTION FOR NON-INTERACTING FERMIons**

Let’s calculate $\chi_0(q, \omega)$ for non-interacting fermions using the expression we derived above. In this case we have $\hat{A}(r) = \hat{B}(r) = \hat{n}(r)$, and $\lambda(r, t) = -U_{\text{ext}}(r, t)$. Therefore,

$$\chi_0(r - r', t - t') = -i\Theta(t - t') \langle \psi_0 | [\hat{n}(r, t), \hat{n}(r', t')] | \psi_0 \rangle. \quad (65)$$

Note the presence of the minus sign, which is different from Eq. (64) above – this is because $\lambda(r, t) = -U_{\text{ext}}(r, t)$. As usual, we can make progress by going to Fourier space, and writing

$$\hat{n}(r, t) = \frac{1}{V} \sum_{\sigma} \sum_{k, k'} e^{-i(k-k') \cdot r} \psi^\dagger_\sigma(k, t) \psi_\sigma(k', t). \quad (66)$$

We need to deal with these Heisenberg picture creation and annihilation operators, which we have not encountered before. Fortunately, for non-interacting fermions, it is simple to solve the Heisenberg equation of motion and find the time-dependence. In general

$$\frac{d}{dt} \psi_\sigma(k) = i[H, \psi_\sigma(k)]. \quad (67)$$

Using the fact that

$$H = \sum_{k, \sigma} \epsilon_k \psi^\dagger_\sigma(k) \psi_\sigma(k), \quad (68)$$

we can calculate the commutator to find $[H, \psi_\sigma(k)] = -\epsilon_k \psi_\sigma(k)$, and so

$$\frac{d}{dt} \psi_\sigma(k) = -i\epsilon_k \psi_\sigma(k), \quad (69)$$

with the solution

$$\psi(k, t) = e^{-i\epsilon_k t} \psi(k). \quad (70)$$

(The same result for $\psi_\sigma^\dagger(k, t)$ is given by taking the Hermitian conjugate of both sides above.)

Putting this into our expression for the Heisenberg picture density operator, we have

$$\hat{n}(r, t) = \frac{1}{V} \sum_{\sigma} \sum_{k, k'} e^{-i(k-k') \cdot r} e^{i(\epsilon_k - \epsilon_{k'}) t} \psi^\dagger_\sigma(k) \psi_\sigma(k'). \quad (71)$$

Now if we plug this back into the expression for $\chi_0$, we should be able to make some progress, using our experience evaluating expectation values containing creation and annihilation operators. We have

$$\chi_0(r - r', t - t') = -\frac{i\Theta(t - t')}{V^2} \sum_{\sigma, \sigma'} \sum_{k, k'} \sum_{q, q'} e^{-i(k-k') \cdot r} e^{i(\epsilon_k - \epsilon_{k'}) t} e^{-i(q-q') \cdot r} e^{i(\epsilon_q - \epsilon_{q'}) t'} \langle \psi_0 | \left[ \psi^\dagger_\sigma(k) \psi_\sigma(k'), \psi^\dagger_{\sigma'}(q) \psi_{\sigma'}(q') \right] | \psi_0 \rangle. \quad (72)$$

One way to proceed from here is to calculate the commutator – this can be done using only the anticommutation relations for the creation/annihilation operators. The idea is to take the first term in the commutator, and then bring the two operators in $\psi^\dagger_{\sigma'}(q) \psi_{\sigma'}(q')$ over to the left, one by one. This will leave a term that cancels out the second
term in the commutator, and two other terms resulting from the right-hand side of the anticommutation relations. The result is:

\[
\left[\psi_\sigma^\dagger(k)\psi_\sigma(k'), \psi_\sigma^\dagger(q)\psi_\sigma(q')\right] = \delta_{\sigma\sigma'} \left[\delta_{kq} \psi_\sigma^\dagger(k)\psi_\sigma(q') - \delta_{qk} \psi_\sigma^\dagger(q)\psi_\sigma(k')\right].
\] (73)

Taking the expectation value of this we get

\[
\langle \psi_0 | \left[\psi_\sigma^\dagger(k)\psi_\sigma(k'), \psi_\sigma^\dagger(q)\psi_\sigma(q')\right] | \psi_0 \rangle = \delta_{\sigma\sigma'} \delta_{kq} \delta_{qk} \left[\Theta(k_F - |k|) - \Theta(k_F - |q|)\right].
\] (74)

Let’s plug this back into the expression for \(\chi_0\). The sum over spins can be done by noting that \(\sum_{\sigma\sigma'} \delta_{\sigma\sigma'} = 2\). So we have

\[
\chi_0(r - r', t - t') = \frac{-2i\Theta(t - t')}{V^2} \sum_k \sum_q e^{-i(k-q)(r-r')} e^{i(\epsilon_k - \epsilon_q)(t-t')} \left[\Theta(k_F - |k|) - \Theta(k_F - |q|)\right].
\] (75)

Note that we have now shown by direct calculation that \(\chi_0\) is only a function of the differences \(r - r'\) and \(t - t'\).

To simply things further it is much better to work with the Fourier transform,

\[
\chi_0(Q, \omega) = \int d^3r \int_{-\infty}^{\infty} dt e^{-iQ\cdot r} e^{i\omega t} \chi_0(r, t).
\] (76)

Plugging in Eq. (75), we see that doing the integral over \(r\) gives a Kronecker delta – specifically it gives \(V \delta_{q,k+Q}\). The integral over \(t\) requires a bit more discussion. Because of the \(\Theta\)-function, we need to evaluate

\[
\int_0^\infty dt e^{i(\omega + \epsilon_k - \epsilon_q)t}.
\] (77)

This integral isn’t well-defined due to the oscillatory integrand. In order to do it, we give \(\omega\) a small positive imaginary part,

\[
\omega \rightarrow \omega + i\delta,
\] (78)

where \(\delta > 0\) is an infinitesimal quantity. This makes the integrand decay exponentially for \(t \rightarrow \infty\), and we can use usual formulae to get

\[
\int_0^\infty dt e^{i(\omega + i\delta + \epsilon_k - \epsilon_q)t} = \frac{i}{\omega + i\delta + \epsilon_k - \epsilon_q}.
\] (79)

Doing both the \(r\) and \(t\) integrals as discussed, and renaming \(Q \rightarrow q\), we find the final result for \(\chi_0\):

\[
\chi_0(q, \omega) = \frac{2}{V} \sum_k \frac{\left[\Theta(k_F - |k|) - \Theta(k_F - |k + q|)\right]}{\omega + i\delta + (\epsilon_k - \epsilon_{k+q})}
\] (80)

\[
= \int \frac{d^3k}{4\pi^3} \frac{\left[\Theta(k_F - |k|) - \Theta(k_F - |k + q|)\right]}{\omega + i\delta + (\epsilon_k - \epsilon_{k+q})}.
\] (81)

The apparently ad hoc procedure of making \(\omega\) slightly imaginary actually has some important physics behind it. Let’s consider a simple case of linear response, where \(\lambda(r, t) = Re e^{-i\omega t}\). (The reason for the minus sign in the exponential is that, by convention, \(e^{-i\omega t}\) is the \(+\omega\) Fourier component – so this choice of \(\lambda\) gives a response at \(\omega\) and not \(-\omega\).) When we do linear response we always say that the system starts out in the unperturbed ground state in the far past, when \(t \rightarrow -\infty\). But how can this be true if the perturbation is always present at full strength for all \(t\)? The way to resolve this is in fact to make \(\omega \rightarrow \omega + i\delta\) just as we did before. This makes the perturbation turn off very slowly in the far past (infinitely slowly in the limit \(\delta \rightarrow 0^+\)), which is needed to make the linear response problem well-defined.
VI. PLASMONS

VII. PROPAGATION OF ELECTROMAGNETIC WAVES IN METALS

VIII. SCREENING OF CHARGED IMPURITIES REVISITED

IX. DISSIPATION

Let’s now return to our more abstract treatment of linear response theory, not focused on the electron gas in particular. That is, consider again the Hamiltonian

$$H = H_0 - \int d^3r \lambda(r,t) \hat{A}(r) = H_0 + H'(t).$$

(82)

We certainly know that, if we drive a system with an external oscillating force, the system can absorb energy – this is what we mean by dissipation. Using our general Hamiltonian, we would like to calculate the energy dissipated (for a small perturbation, as always), and show that it can be related simply to the response function $\chi_{AA}$.

To do this, we will need to first prove a general theorem. Let $H(t)$ be the Hamiltonian, which may depend explicitly on time. Let $G(t)$ be some other operator, which may also depend explicitly on time. Let $|\psi(t)\rangle$ be a solution of the time-dependent Schrödinger equation. Then:

$$\frac{d}{dt} \langle \psi(t)|G(t)\rangle \psi(t)\rangle = i\langle \psi(t)|[H(t), G(t)]\rangle \psi(t)\rangle + \langle \psi(t)|\psi(t)\rangle \frac{\partial G}{\partial t} \psi(t).$$

(83)

Note that the last term vanishes if there is no explicit time-dependence in $G$. To prove this, calculate the derivative:

$$\frac{d}{dt} \langle \psi(t)|G(t)\rangle \psi(t)\rangle = \left( \frac{d}{dt} \langle \psi(t)\rangle \right) G(t) \rangle \psi(t)\rangle + \langle \psi(t)|[H(t), G(t)]\rangle \psi(t)\rangle + \langle \psi(t)|\partial G/\partial t \rangle \psi(t)\rangle$$

(84)

Using the time-dependent Schrödinger equation,

$$\frac{d}{dt} \langle \psi(t)\rangle = -iH(t) \langle \psi(t)\rangle,$$

(85)

And, taking the Hermitian conjugate of both sides,

$$\frac{d}{dt} \langle \psi(t)| = i\langle \psi(t)|H(t).$$

(86)

Plugging these in proves the theorem.

We will use this theorem in the special case $G(t) = H(t)$, in which case the commutator vanishes and

$$\frac{d}{dt} \langle \psi(t)|H(t)\rangle \psi(t)\rangle = \langle \psi(t)|\partial H/\partial t \rangle \psi(t)\rangle = -\int d^3r \langle \psi(t)|\hat{A}(r)\rangle \langle \psi(t)|\hat{A}(r)\rangle \frac{\partial \lambda(r,t)}{\partial t}.$$}

(87)

But we can also write

$$\frac{d}{dt} \langle \psi(t)|H(t)\rangle \psi(t)\rangle = \frac{d}{dt} \langle \psi(t)|H_0\rangle \psi(t)\rangle + \frac{d}{dt} \langle \psi(t)|H'(t)\rangle \psi(t)\rangle.$$}

(88)

The first term on the right hand side is the quantity we are interested in, the power $P$ deposited into the system. That is,

$$P = \frac{d}{dt} \langle \psi(t)|H_0\rangle \psi(t)\rangle.$$}

(89)

How do we know this is the right definition? Let’s suppose we start in the ground state, turn on the perturbation for some amount of time, and then turn it off again. If the initial energy is $E_0$, the energy change (after turning off the perturbation) is

$$W = \langle \psi(t \rightarrow \infty)|H_0|\psi(t \rightarrow \infty)\rangle - E_0 = \int_{-\infty}^{\infty} dt \ P.$$}

(90)
This is the work done (hence the symbol $W$), and we can really interpret $P$ as power deposited. Using Eq. (87) and Eq. (88), we can write

$$ P = \frac{d}{dt} \int d^3r \lambda(r, t) \langle \psi(t) | \hat{A}(r) | \psi(t) \rangle - \int d^3r \langle \psi(t) | \hat{A}(r) | \psi(t) \rangle \frac{\partial \lambda(r, t)}{\partial t}, $$

(91)

$$ = \int d^3r \lambda(r, t) \frac{d}{dt} \langle \hat{A}(r) \rangle_t, $$

(92)

where $\langle \hat{A}(r) \rangle_t \equiv \langle \psi(t) | \hat{A}(r) | \psi(t) \rangle$. The expression Eq. (92) looks a lot like the familiar equation $P = Fv$ for the power dissipated when a particle is moving with velocity $v$ in a force $F$. Here, $\lambda$ is analogous to $F$, and $(d/dt)\langle \hat{A}(r) \rangle_t$ is analogous to $v$. (In fact, if we went through the same manipulations for a single quantum particle coupled to an external time-varying force, we would get $P = Fv$.)

Since we assume the perturbation is small, starting from Eq. (92), we can use linear response theory to calculate $P$ and $W$:

$$ W = \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \int d^3r d^3r' \lambda(r, t) \frac{d}{dt} \left[ \chi_{AA}(r - r', t - t') \right] \lambda(r', t') $$

(93)

$$ = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega (i\omega) \lambda(-k, -\omega) \chi_{AA}(k, \omega) \lambda(k, \omega) $$

(94)

$$ = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega (i\omega) |\chi_{AA}(k, \omega)|^2 \lambda(k, \omega)^2. $$

(95)

In the last line we used the fact that $\lambda(k, \omega)^* = \lambda(-k, -\omega)$, since $\lambda(r, t)$ is real. Making the change of variables $\omega \rightarrow -\omega$ and $k \rightarrow -k$, we have

$$ W = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega (i\omega) |\chi_{AA}(k, -\omega)|^2 \lambda(k, \omega)^2 $$

(96)

$$ = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega (i\omega) \chi_{AA}^*(k, \omega)|\lambda(k, \omega)|^2. $$

(97)

Adding Eq. (95) and Eq. (97), and dividing by two, we have

$$ W = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega (i\omega) \left[ |\chi_{AA}(k, \omega)|^2 - \chi_{AA}^*(k, \omega) |\lambda(k, \omega)|^2 \right] $$

(98)

$$ = \int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega \omega \text{Im} \chi_{AA}(q, \omega)|\lambda(q, \omega)|^2. $$

(99)

This is an important result. It tells us that, if we apply some kind of external drive to the system, and measure the energy absorbed, it gives a measurement of the imaginary part of the response function. As an example of this, think back to the response function for plasmons, where $\text{Im} \chi(q, \omega)$ was a delta function peaked at $\omega = \omega_p$. So the plasmon mode only absorbs energy from an oscillating external potential when the driving frequency is right on resonance. A more experimentally relevant (but more complicated) example is absorption of electromagnetic radiation.

This form for $W$ also implies that

$$ \text{Im} \chi_{AA}(q, \omega) > 0, \quad \omega > 0 $$

(100)

$$ \text{Im} \chi_{AA}(q, \omega) < 0, \quad \omega < 0. $$

(101)

This is needed for stability. At zero temperature, this is clearly true because $W$ must be positive. This is also true at finite temperature, where $W < 0$ would violate the third law of thermodynamics – I leave it as an exercise to understand why. (I am assuming here that temperature is positive, so that entropy is an increasing function of energy.)

**X. SPECTRAL REPRESENTATION**

There is a way of writing $\text{Im} \chi_{AA}$, which shows that it tells us rather directly about the *excitation spectrum* of the system. To derive this form, we need to go through some formal manipulations, which mostly consist of adding
complete sets of eigenstates of $H_0$. To prepare for that let the index $n$ label $|\psi_n\rangle$, the many-body eigenstates of $H_0$, with energies $E_n$. Suppose $E_0$ is the ground state energy of $H_0$, and $|\psi_0\rangle$ is the ground state.

We want to work with the general expression for $\chi(q, \omega)$:

$$\chi_{AA}(q, \omega) = i \int d^3r \int_0^\infty d(t - t') e^{-iq(r-r')} e^{i(\omega + i\delta)(t-t')} \langle \psi_0 | \hat{A}(r, t) \hat{A}(r', t') | \psi_0 \rangle. \tag{102}$$

This notation in the integration measures means we integrate over the variables $r - r'$ and $t - t'$. The first simplification is that we want to integrate over $r$ and $r'$ separately rather than just the difference. Since the integrand only depends on $r - r'$, doing this just multiplies the result by an extra factor of volume. Therefore,

$$\chi_{AA}(q, \omega) = \frac{i}{V} \int d^3r \int d^3r' \int_0^\infty d(t - t') e^{-iq(r-r')} e^{i(\omega + i\delta)(t-t')} \langle \psi_0 | \hat{A}(r, t) \hat{A}(r', t') | \psi_0 \rangle \tag{103}$$

$$= \frac{i}{V} \int_0^\infty d(t - t') e^{i(\omega + i\delta)(t-t')} \langle \psi_0 | \hat{A}(q, t) \hat{A}(-q, t') | \psi_0 \rangle. \tag{104}$$

This allows us to work with the Fourier transformed operators

$$\hat{A}(q, t) = \int d^3r e^{-iqr} \hat{A}(r, t). \tag{105}$$

The factor of $1/V$ in front, which looks a bit unpleasant, is a consequence of our Fourier transform convention and hence of the normalization of $\hat{A}(q, t)$. If we wanted to get rid of it, we could change the normalization of $\hat{A}(q, t)$ accordingly – we’d multply its definition by a factor of $1/\sqrt{V}$ – but for our purposes here there is no need to do this. Since $\hat{A}(r)$ is Hermitian, we have

$$\hat{A}(-q) = [\hat{A}(q)]^\dagger. \tag{106}$$

Now we break the commutator into the two terms and insert a complete set of states:

$$\chi_{AA}(q, \omega) = \frac{i}{V} \int_0^\infty d(t - t') e^{i(\omega + i\delta)(t-t')} \langle \psi_0 | \hat{A}(q, t) \hat{A}(-q, t') - \hat{A}(-q, t') \hat{A}(q, t) | \psi_0 \rangle \tag{107}$$

$$= \frac{i}{V} \int_0^\infty d(t - t') e^{i(\omega + i\delta)(t-t')} \sum_n \langle \psi_0 | \hat{A}(q, t) \psi_n \rangle \langle \psi_n | \hat{A}(-q, t') \psi_0 \rangle - \langle \psi_0 | \hat{A}(-q, t') \psi_n \rangle \langle \psi_n | \hat{A}(q, t) \psi_0 \rangle. \tag{108}$$

To simplify further, we use the fact that

$$\hat{A}(q, t) = e^{iH_0t} \hat{A}(q) e^{-iH_0t}. \tag{109}$$

So we have

$$\chi_{AA}(q, \omega) = \frac{i}{V} \sum_n \int_0^\infty d(t - t') e^{i(\omega + i\delta)(t-t')} \left( e^{-i(E_0 - E_n)(t-t')} \langle \psi_0 | \hat{A}(q) \psi_n \rangle \langle \psi_n | \hat{A}(-q) \psi_0 \rangle - e^{-i(E_0 - E_n)(t-t')} \langle \psi_0 | \hat{A}(-q) \psi_n \rangle \langle \psi_n | \hat{A}(q) \psi_0 \rangle \right). \tag{110}$$

Now we can do the time-integral to get

$$\chi_{AA}(q, \omega) = \frac{1}{V} \sum_n \left[ \frac{-1}{\omega + i\delta + (E_0 - E_n)} \left| \langle \psi_n | \hat{A}(-q) \psi_0 \rangle \right|^2 + \frac{1}{\omega + i\delta - (E_0 - E_n)} \left| \langle \psi_n | \hat{A}(q) \psi_0 \rangle \right|^2 \right]. \tag{111}$$

The imaginary part comes entirely from the infinitesimal $i\delta$. We use the identity

$$\text{Im} \frac{1}{a + i\delta} = \text{Im} \frac{a - i\delta}{a^2 + \delta^2} = \frac{-\delta}{a^2 + \delta^2} = -\pi \delta(a), \tag{112}$$

where the last equality holds as $\delta \to 0$. From this we get

$$\text{Im} \chi_{AA}(q, \omega) = \frac{\pi}{V} \sum_n \left\{ \left| \langle \psi_n | \hat{A}(-q) \psi_0 \rangle \right|^2 \delta[\omega - (E_n - E_0)] - \left| \langle \psi_n | \hat{A}(q) \psi_0 \rangle \right|^2 \delta[\omega + (E_n - E_0)] \right\}. \tag{113}$$
This is the desired result, and is referred to as the spectral representation of Im $\chi_{AA}$. Since $E_n \geq E_0$, the first term vanishes for $\omega < 0$, and the second term vanishes for $\omega > 0$. This clearly shows that Im $\chi_{AA}$ is positive for $\omega > 0$ and negative for $\omega < 0$; we argued above that this had to be the case, based on stability of the ground state. To get a better feeling for the meaning of this expression, let’s focus on $\omega > 0$, where we have

$$\text{Im } \chi_{AA}(q, \omega > 0) = \frac{\pi}{V} \sum_n \left| \langle \psi_n | \hat{A}(-q) | \psi_0 \rangle \right|^2 \delta[\omega - (E_n - E_0)].$$

(114)

We can think about this expression in the following way. We take the state created by acting on the ground state with $\hat{A}(-q)$. Then, we compute the squared overlap of this state with eigenstates $|\psi_n\rangle$. The delta function tells us we should focus on only those eigenstates with exactly the right energy so that $\omega = E_n - E_0$. Then we add up all the overlaps. So Im $\chi_{AA}$ gives a “weight” for the total overlap of $\hat{A}(-q)|\psi_0\rangle$, with all eigenstates of the specified energy. This gives useful information about the excitation spectrum – for example, if $\hat{A}(-q)|\psi_0\rangle$ is an eigenstate, then we have a delta function peak in Im $\chi_{AA}$ as a function of $\omega$. If $\hat{A}(-q)|\psi_0\rangle$ isn’t an exact eigenstate, but corresponds to an excitation that decays with some lifetime, then instead of a delta function peak there will be a broadened peak, where the width tells us about the decay rate.

It is also instructive to think about the quantum numbers carried by the state $\hat{A}(-q)|\psi_0\rangle$. If momentum is conserved, then this state carries a momentum $q$. (Why?) This means that, by momentum conservation, the overlap with $|\psi_n\rangle$ can only be nonzero for eigenstates with the same momentum $q$. So we get very specific information about the spectrum of eigenstates carrying momentum $q$. Similar statements hold whenever $\hat{A}$ carries some other conserved quantum number (e.g. particle number, spin, etc).

Recall the form we found for Im $\chi$ of the density response function at the plasmon pole – it was a delta function. This is another way of seeing that we should think about the plasmon as a well-defined excitation of the system – it just corresponds to an excited energy eigenstate.

**XI. FLUCTUATION-DISSIPATION THEOREM**

Somewhat surprisingly, the imaginary part of the response function is related to the correlation function:

$$C_{AA}(r - r', t - t') = \langle \psi_0 | \hat{A}(r, t) \hat{A}(r', t') | \psi_0 \rangle. \quad (115)$$

The correlation function can be thought of as giving information about the fluctuations of the observable $\hat{A}$ in the ground state. Indeed, when $t = t'$, $C_{AA}$ measures the equilibrium fluctuations, with no dynamics involved. This is very different physically from Im $\chi_{AA}$, which we have seen measures the energy dissipated in the system by an external force coupled to $\hat{A}$. Another reason the correlation function is interesting is that, in many cases, it can be directly measured in a scattering experiment – we will see this below.

To expose this relationship, we shall work out a spectral representation for $C_{AA}$. We have

$$C_{AA}(r - r', t - t') = \sum_n \langle \psi_0 | \hat{A}(r, t) | \psi_n \rangle \langle \psi_n | \hat{A}(r', t') | \psi_0 \rangle \quad (116)$$

$$= \sum_n e^{-i(E_n - E_0)(t - t')} \langle \psi_0 | \hat{A}(r) | \psi_n \rangle \langle \psi_n | \hat{A}(r') | \psi_0 \rangle. \quad (117)$$

To proceed, we take the Fourier transform:

$$C_{AA}(q, \omega) = \int d^3r \int_0^\infty dt \int d^3r' \int_0^\infty dt' e^{-i\omega(t - t') e^{i\omega(t - t')}} C_{AA}(r - r', t - t') \quad (118)$$

$$= \frac{1}{V} \int d^3r d^3r' \int_0^\infty dt \int_0^\infty dt' e^{-i\omega(t - t') e^{i\omega(t - t')}} C_{AA}(r - r', t - t') \quad (119)$$

$$= \frac{1}{V} \int_0^\infty dt \int_0^\infty dt' \sum_n e^{i\omega(E_n - E_0)(t - t')} \langle \psi_0 | \hat{A}(q) | \psi_n \rangle \langle \psi_n | \hat{A}(-q) | \psi_0 \rangle \quad (120)$$

$$= \frac{2\pi}{V} \sum_n \left| \langle \psi_n | \hat{A}(-q) | \psi_0 \rangle \right|^2 \delta[\omega - (E_n - E_0)]. \quad (121)$$

Note that this is only nonzero for $\omega \geq 0$. Comparing this to the result for Im $\chi_{AA}$, we have the desired result:

$$C_{AA}(q, \omega) = 2\Theta(\omega) \text{Im } \chi_{AA}(q, \omega). \quad (122)$$
This is a special case of the fluctuation-dissipation theorem. It is actually true much more generally (including for other kinds of dynamics besides quantum dynamics). It is also true for quantum systems at finite temperature, where the form changes a bit. Stated without proof, the finite-temperature result is:

\[
C_{AA}(q, \omega) = \frac{2}{1 - e^{-\omega/k_B T}} \text{Im} \chi_{AA}(q, \omega).
\]  

(123)

XII. MEASURING THE CORRELATION FUNCTION BY SCATTERING

Here we explain how the correlation function \(C_{AA}(q, \omega)\), and hence also \(\text{Im} \chi_{AA}(q, \omega)\), can be measured via a scattering experiment. We want to consider a single particle with position \(r_p\) (and momentum \(k_p\), that interacts with our large many-body system via an interaction \(H_{\text{int}}\). A good example of such a particle would be a neutron – scattering of neutrons is a very important probe of a variety of solid state systems. The particle’s energy is \(\epsilon_p(k_p)\). We assume that the particle starts in a momentum eigenstate \(|k_{pi}\rangle\), and the large system starts in the ground state \(|0\rangle\). So the initial state of the combined system is

\[
|i\rangle = |\psi_0\rangle|k_{pi}\rangle,
\]

and the initial energy is \(E_i = E_0 + \epsilon_p(k_{pi})\). (We will follow the convention where the first ket (or bra) is the state of the many-particle system, and the second one represents the state of the particle.)

The particle scatters off the large system, so that the system’s final state is an eigenstate \(|n\rangle\), and the particle’s final state is \(|k_{pf}\rangle\). So the combined final state is

\[
|f\rangle = |\psi_n\rangle|k_{pf}\rangle,
\]

and \(E_f = E_n + \epsilon_p(k_{pf})\). After the scattering event we collect the particle in a detector that measures \(k_{pf}\). (Note that we also assume we know \(k_{pi}\), because we controlled the properties of the incoming particle.)

Now, we assume that the interaction \(H_{\text{int}}\) between particle and system is small, so that we can treat the scattering event in perturbation theory. Therefore we can use Fermi’s golden rule, which gives us the following expression for the transition rate:

\[
T(k_{pi}, k_{pf}) = 2\pi \sum_n \left|\langle \psi_n | k_{pf} | H_{\text{int}} | \psi_0 | k_{pi}\rangle\right|^2 \delta[\epsilon_p(k_{pi}) - \epsilon_p(k_{pf}) - (E_n - E_0)].
\]

(126)

Here we sum over the final states of the many-body system \(|n\rangle\), because we have no way of detecting this state in our detector – so what we can measure is the total transition rate from the initial state \(|i\rangle\), to all final states where the particle has momentum \(k_{pf}\).

To go further we need to assume something about the interaction \(H_{\text{int}}\). We assume it has the following form:

\[
H_{\text{int}} = \int d^3 r \delta(r_p - r) \hat{A}(r) = \hat{A}(\hat{r}_p).
\]

(127)

(Note that \(\hat{r}_p\) is an operator here – it measures the position of the scattered particle.) To justify why this is a good form for the interaction, it’s helpful to consider some examples. For scattering of neutrons off whatever particles that make up the many-body system, a good choice for \(A\) would be \(A(r) = V_0 \hat{n}(r)\), where \(\hat{n}(r)\) is the density operator. This says that the neutron interacts with the other particles via a delta function potential. This is clearest if we remember that the first-quantized form of the density operator is

\[
\hat{n}(r) = \sum_{i=1}^{N} \delta(r - \hat{r}_i),
\]

(128)

so that

\[
H_{\text{int}} = V_0 \sum_{i=1}^{N} \delta(\hat{r}_p - \hat{r}_i).
\]

(129)

Another example would be if scattered particle interacted with the other particles via a potential \(V(r)\). In that case, we would choose

\[
\hat{A}(r) = \int d^3 r' V(r - r') \hat{n}(r').
\]

(130)
Following the manipulations above in this case leads to

$$ H_{\text{int}} = \sum_{i=1}^{N} V(\hat{r}_p - \hat{r}_i). \quad (131) $$

Note that $\hat{A}(r)$ need not involve only the density operator. For example, if the scattering particle has a magnetic moment (like the neutron does), then $\hat{A}(r)$ could also involve the spin density. Anyway, the examples above should be enough to justify that Eq. (127) is a reasonable form. Let’s now simplify the expression for the transition rate. We need to evaluate the following matrix element:

$$ \langle n | \langle k_p | H_{\text{int}} | \psi_0 \rangle | k_{pf} \rangle = \frac{1}{V} \int d^3r d^3r' e^{-i k_{pf} \cdot r} e^{i k_{pi} \cdot r'} \langle \psi_n | \langle r | \hat{A}(\hat{r}_p) | \psi_0 \rangle | r' \rangle $$

$$ = \frac{1}{V} \int d^3r d^3r' e^{-i k_{pf} \cdot r} e^{i k_{pi} \cdot r'} \delta(r - r') \langle \psi_n | \hat{A}(r) | \psi_0 \rangle $$

$$ = \frac{1}{V} \int d^3r e^{i q \cdot r} \langle \psi_n | \hat{A}(r) | \psi_0 \rangle $$

$$ = \frac{1}{V} \langle \psi_n | \hat{A}(-q) | \psi_0 \rangle. \quad (135) $$

Starting in the second line above, the expectation values are taken in states of the many-body system only. We have defined the momentum transfer $q = k_{pi} - k_{pf}$. With this simplification, the transition rate becomes

$$ T(q, \omega) = \frac{2\pi}{V^2} \sum_n \left| \langle \psi_n | \hat{A}(-q) | \psi_0 \rangle \right|^2 \delta \left[ \omega - (E_n - E_0) \right] = V C_{AA}(q, \omega). \quad (136) $$

Here we defined the energy transfer $\omega = \epsilon_p(k_{pi}) - \epsilon_p(k_{pf})$. This is the desired result – it tells us that the transition rate (and hence the scattering cross section, which is what is actually measured) is proportional to $C_{AA}(q, \omega)$. 