Chapter 5

Collective excitations

After we have discussed the structure of one-particle excitations with the one-particle Green's function, we consider here other processes that, although in principle included in the exact one-particle Green's function, have a different character since they are determined by the collective response of the electronic system to external excitation. The following discussion is restricted to the limit of weak external potential, and hence to the so-called *linear response theory*.

5.1 Linear response theory

We study here the response of a periodic solid to an external potential that leads to an additional term $H^{ext}(t)$ in general time dependent in the total Hamiltonian of the system H^T. The system on which the external potential acts is described by a Hamiltonian H, which we assume to be time independent. If $H^{ext}(t)$ is small enough, we can treat it perturbatively, in a frame similar to the one we developed for the one-particle Green's function.

We start with the Schrödinger picture we introduced in Sec. 4.4.1, where

$$ i\hbar \frac{\partial}{\partial t} \mid \Psi_S(t) > = H^T \mid \Psi_S(t) > , \tag{5.1} $$

with the difference, that we now have from the start a time dependent Hamiltonian

$$ H^T(t) = H + H^{ext}(t) . \tag{5.2} $$

Nevertheless, we can still define a time evolution operator, such that

$$ \mid \Psi_S(t) > = U_S^T(t, t_0) \mid \Psi_S(t_0) > , \tag{5.3} $$

and replacing this into Schrödinger's equation, we have quite generally,

$$ i\hbar \frac{\partial}{\partial t} U_S^T(t, t_0) = H^T(t) U_S^T(t, t_0) . \tag{5.4} $$

If the Hamiltonian were time independent, then the solution of this equation is (4.263). However, in our case it is definitively time dependent, as shown by (5.2).

Using the same reasoning we made to reach the solution (4.274) of the Schrödinger-like equation for the evolution operator in the interaction picture, we can also have a formal solution here

$$U_S^T(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, H^T(t') \, U_S^T(t', t_0) \,, \tag{5.5}$$

with the difference, that we are still in the Schrödinger picture, and the Hamiltonian in the integral is the full Hamiltonian. However, in order to have an explicit solution for $U_S^T(t, t_0)$, we take a different path. Since the evolution operator for the dynamics determined by H fulfills

$$i\hbar \frac{\partial}{\partial t} U_S(t, t_0) = H \, U_S(t, t_0) \,, \tag{5.6}$$

we propose the following form for $U_S^T(t, t_0)$:

$$U_S^T(t, t_0) = U_S(t, t_0) \, \tilde{U}(t, t_0) \,. \tag{5.7}$$

Inserting this form into (5.4), we have

$$i\hbar \frac{\partial}{\partial t} \left[U_S(t, t_0) \, \tilde{U}(t, t_0) \right] = \left[H + H^{ext}(t) \right] U_S(t, t_0) \, \tilde{U}(t, t_0) \,, \tag{5.8}$$

that due to (5.6) reduces to

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t} \tilde{U}(t, t_0) &= U_S^\dagger(t, t_0) \, H^{ext}(t) \, U_S(t, t_0) \, \tilde{U}(t, t_0) \\
&\equiv \tilde{H}^{ext}(t) \, \tilde{U}(t, t_0) \,.
\end{aligned}
\tag{5.9}
$$

Again, the formal solution has the form (5.5), that up to first order in the perturbation reduces to

$$\tilde{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, \tilde{H}^{ext}(t') \,. \tag{5.10}$$

Inserting this into (5.7) we arrive at the final solution for the evolution operator of the complete problem,

$$
\begin{aligned}
U_S^T(t, t_0) &= U_S(t, t_0) \\
&\quad - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, \underbrace{U_S(t, t_0)}_{=U_S(t, t') \, U_S(t', t_0)} U_S^\dagger(t', t_0) \, H^{ext}(t') \, U_S(t', t_0) \\
&= U_S(t, t_0) - \frac{i}{\hbar} \int_{t_0}^{t} dt' \, U_S(t, t') \, H^{ext}(t') \, U_S(t', t_0) \,.
\end{aligned}
\tag{5.11}
$$

At this point it is convenient to set $t_0 = 0$, and we assume as an initial condition $| \, \Psi_S(t = 0) >$ to be an eigenstate (in general the ground-state) of the system. Furthermore, we assume that $H^{ext}(t)$ is switched on at a time $0 < \tilde{t}_0 < t$. Here one

says that we have causal boundary conditions in time. Then, the state at time t is given by

$$
\begin{aligned}
\mid \Psi_S(t) > \; = \; & \exp\left(-\frac{i}{\hbar}Ht\right) \mid \Psi_S(t=0) > \\
& -\frac{i}{\hbar}\int_{\tilde{t}_0}^{t} \mathrm{d}t' \, \exp\left[-\frac{i}{\hbar}H\left(t-t'\right)\right] H^{ext}(t') \\
& \qquad\qquad \times \exp\left(-\frac{i}{\hbar}Ht'\right) \mid \Psi_S(t=0) > \; .
\end{aligned} \tag{5.12}
$$

Once we have the state, we can calculate expectation values of different operators. Let us conisder an operator $\hat{O}$, and its expectation value

$$
\begin{aligned}
< \hat{O}(t) >_{H^T} \; = \; & < \Psi_S(t) \mid \hat{O} \mid \Psi_S(t) > \\
= \; & < \Psi_S(0) \mid \mathrm{e}^{iH\,t/\hbar} \, \hat{O}\, \mathrm{e}^{-iH\,t/\hbar} \mid \Psi_S(0) > \\
& +\frac{i}{\hbar}\int_{\tilde{t}_0}^{t} \mathrm{d}t' < \Psi_S(0) \mid \mathrm{e}^{iH\,t'/\hbar}\, H^{ext}(t')\, \mathrm{e}^{iH(t-t')/\hbar} \\
& \qquad\qquad\qquad \times \hat{O}\, \mathrm{e}^{-iH\,t/\hbar} \mid \Psi_S(0) > \\
& -\frac{i}{\hbar}\int_{\tilde{t}_0}^{t} \mathrm{d}t' < \Psi_S(0) \mid \mathrm{e}^{iH\,t/\hbar}\, \hat{O}\, \mathrm{e}^{-iH(t-t')/\hbar} \\
& \qquad\qquad\qquad \times H^{ext}(t')\mathrm{e}^{-iH\,t'/\hbar} \mid \Psi_S(0) > \\
= \; & < \Psi_H \mid \hat{O}_H(t) \mid \Psi_H > \\
& +\frac{i}{\hbar}\int_{\tilde{t}_0}^{t} \mathrm{d}t' < \Psi_H \mid \left[H_H^{ext}(t'), \hat{O}_H(t)\right] \mid \Psi_H > \, ,
\end{aligned} \tag{5.13}
$$

where we used (4.284), i.e. $\mid \Psi_H > = \mid \Psi_S(t=0) >$, and (4.282) that gives the relation between operators in the Heisenberg and the Schrödinger picture. Furthermore, only linear contributions in H^{ext} are taken into account. We arrived then, at the general result in linear response theory, that the causal linear response to an external perturbation leads to a change of an observable in the ground-state given by

$$
\begin{aligned}
\delta < \hat{O}(t) > \; = \; & < \hat{O}(t) >_{H^T} - < \hat{O}(t) >_H \\
= \; & \frac{i}{\hbar}\int_{\tilde{t}_0}^{t} \mathrm{d}t' < \Psi_0 \mid \left[H_H^{ext}(t'), \hat{O}_H(t)\right] \mid \Psi_0 > \; .
\end{aligned} \tag{5.14}
$$

5.1.1 Density-density response function, and dielectric function

A case that is particularly important is that of the response of an electronic system to a perturbation that couples to the charge-density of the system. In that case, we have

$$
H^{ext}(t) = \int \mathrm{d}^3x \, \hat{n}_H\left(\boldsymbol{x}, t\right) \varphi^{ext}\left(\boldsymbol{x}, t\right) \; . \tag{5.15}
$$

The external potential $\varphi^{ext}\left(\boldsymbol{x}, t\right)$ could result from a probe external to the system or could be given by the ions in a solid, such that the response of the electronic system

would directly determine the properties of phonons in the system. Inserting the coupling above into (5.14) for $\hat{O} = \hat{n}$, we have the change in the density distribution in the solid that results from applying φ^{ext},

$$
\begin{aligned}
\delta < \hat{n}\left(\boldsymbol{x}, t\right) > \quad = \quad & \frac{i}{\hbar} \int_{\tilde{t}_0}^{t} \mathrm{d}t' \int \mathrm{d}^3 x' \\
& \times < \Psi_0 \mid \left[\hat{n}_H\left(\boldsymbol{x}', t'\right), \hat{n}_H\left(\boldsymbol{x}, t\right)\right] \mid \Psi_0 > \varphi^{ext}\left(\boldsymbol{x}', t'\right) \; . \; (5.16)
\end{aligned}
$$

By introducing the response function of the system as a generalized susceptibility, relating the change in density to the external potential in the form

$$
\delta < \hat{n}\left(\boldsymbol{x}, t\right) > \quad = \quad \int_{-\infty}^{\infty} \mathrm{d}t' \int \mathrm{d}^3 x' \chi\left(x, x'\right) \varphi^{ext}\left(x'\right), \tag{5.17}
$$

we have that the density-density correlation function is directly connected with the linear response function of the system

$$
\chi\left(x, x'\right) \quad = \quad -\frac{i}{\hbar} \theta\left(t - t'\right) \frac{< \Psi_0 \mid \left[\tilde{n}_H\left(\boldsymbol{x}, t\right), \tilde{n}_H\left(\boldsymbol{x}', t'\right)\right] \mid \Psi_0 >}{< \Psi_0 \mid \Psi_0 >}, \tag{5.18}
$$

where we introduced the notation

$$
\tilde{n}_H\left(\boldsymbol{x}, t\right) \equiv \hat{n}_H\left(\boldsymbol{x}, t\right) - < \hat{n}_H\left(\boldsymbol{x}, t\right) > , \tag{5.19}
$$

in order to make explicit the fact that the density-density correlation function measures the fluctuations around the ground-state density profile in the system. Due to the fact that c-numbers commute, this change can be trivially made. The θ-function had to be introduced explicitly after extending the domain of integration over time. It makes explicit the fact that we are dealing with a *retarded* correlation function. Finally, we should add that a normalization was introduced for the ground-state. We see that in this way, a structure can be reached for general correlation functions in the system that is very similar to the one already obtained for the one-particle Green's function. However, there we have seen that in order to be able to evaluate the expectation values appearing in perturbation theory, Wick's theorem was necessary, and for it to be applicable, we need to have a time ordered product. Therefore, in order to make full contact with the diagrammatic expansion, an associated correlation function with a time-ordered product should be introduced.

In the following we discuss several aspects of the density-density correlation function related to screening in electronic systems.

Screening and dielectric function

Some of the most important concepts can be already discussed in the frame of the non-interacting system. We will therefore consider first the Fermi gas, where we can calculate the density-density correlation function exactly. In this case, we can proceed as we did in the case of the one-particle Green's function and use Lehmann's

representation. As previously, we assume in the following that the ground-state is normalized such that $< \Psi_0 \mid \Psi_0 >= 1$ and, hence,

$$\chi(x, x') = -\frac{i}{\hbar} \theta(t - t') < \Psi_0 \mid [n_H(\boldsymbol{x}, t), n_H(\boldsymbol{x}', t')] \mid \Psi_0 > , \quad (5.20)$$

where we go back to the operators without the substraction of $< \hat{n}_H(\boldsymbol{x}, t) >$. We consider the complete set of eigenstates $\{\mid \Psi_n >\}$ of the Hamiltonian and insert them between the operators at different times. Since we have a commutator, let us concentrate on one of the products. The other product can be obtained at the end by interchanging $x \leftrightarrow x'$. We have then

$$< \Psi_0 \mid n_H(\boldsymbol{x}, t) \, n_H(\boldsymbol{x}', t') \mid \Psi_0 >$$
$$= \sum_n < \Psi_0 \mid \mathrm{e}^{iHt/\hbar} \sum_\alpha \hat{\psi}_\alpha^\dagger(\boldsymbol{x}) \, \hat{\psi}_\alpha(\boldsymbol{x}) \, \mathrm{e}^{-iHt/\hbar} \mid \Psi_n >$$
$$\times < \Psi_n \mid \mathrm{e}^{iHt'/\hbar} \sum_\beta \hat{\psi}_\beta^\dagger(\boldsymbol{x}') \, \hat{\psi}_\beta(\boldsymbol{x}') \, \mathrm{e}^{-iHt'/\hbar} \mid \Psi_0 >$$
$$= \sum_n \mathrm{e}^{-i(E_n - E_0)(t - t')/\hbar} \sum_{\alpha, \beta} < \Psi_0 \mid \hat{\psi}_\alpha^\dagger(\boldsymbol{x}) \, \hat{\psi}_\alpha(\boldsymbol{x}) \mid \Psi_n >$$
$$\times < \Psi_n \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}') \, \hat{\psi}_\beta(\boldsymbol{x}') \mid \Psi_0 >, (5.21)$$

and for the other product

$$< \Psi_0 \mid n_H(\boldsymbol{x}', t') \, n_H(\boldsymbol{x}, t) \mid \Psi_0 >$$
$$= \sum_n \mathrm{e}^{+i(E_n - E_0)(t - t')/\hbar} \sum_{\alpha, \beta} < \Psi_0 \mid \hat{\psi}_\alpha^\dagger(\boldsymbol{x}') \, \hat{\psi}_\alpha(\boldsymbol{x}') \mid \Psi_n >$$
$$\times < \Psi_n \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}) \, \hat{\psi}_\beta(\boldsymbol{x}) \mid \Psi_0 > . (5.22)$$

We have to consider further the θ-function, as we did in Sec. 4.4.3 for the one-particle Green's function. We do not repeat the calculation and arguments here but give the final result for the Fourier transformed correlation function:

$$\chi(\boldsymbol{x}, \boldsymbol{x}'; \omega)$$
$$= \sum_{\substack{n \\ \alpha, \beta}} \left[\frac{< \Psi_0 \mid \hat{\psi}_\alpha^\dagger(\boldsymbol{x}) \, \hat{\psi}_\alpha(\boldsymbol{x}) \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}') \, \hat{\psi}_\beta(\boldsymbol{x}') \mid \Psi_0 >}{\hbar\omega - (E_n - E_0) + i\eta} \right.$$
$$\left. - \frac{< \Psi_0 \mid \hat{\psi}_\alpha^\dagger(\boldsymbol{x}') \, \hat{\psi}_\alpha(\boldsymbol{x}') \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\beta^\dagger(\boldsymbol{x}) \, \hat{\psi}_\beta(\boldsymbol{x}) \mid \Psi_0 >}{\hbar\omega + (E_n - E_0) + i\eta} \right] . (5.23)$$

Until now we did no assumption about the system, such that the expressions above are valid in general. It is convenient at this point to consider the further development for the Fermi gas. In this case, we can express the field operators in terms of creation and annihilation operators in momentum space.

$$\hat{\psi}_\alpha(\boldsymbol{x}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} f_{\boldsymbol{k}\alpha} \exp(i\boldsymbol{k} \cdot \boldsymbol{x}) \quad\quad (5.24)$$

$$\hat{\psi}_\beta^\dagger(\boldsymbol{x}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} f_{\boldsymbol{k}\beta}^\dagger \exp(-i\boldsymbol{k} \cdot \boldsymbol{x}) . \quad\quad (5.25)$$

Then, for the matrix elements in (5.23), we have

$$< \Psi_0 \mid \hat{\psi}_\alpha^\dagger (\boldsymbol{x}) \, \hat{\psi}_\alpha (\boldsymbol{x}) \mid \Psi_n >< \Psi_n \mid \hat{\psi}_\beta^\dagger (\boldsymbol{x}') \, \hat{\psi}_\beta (\boldsymbol{x}') \mid \Psi_0 >$$

$$= \frac{1}{V^2} \sum_{\boldsymbol{k}_1,...,\boldsymbol{k}_4} \exp\left[-i\left(\boldsymbol{k}_1 - \boldsymbol{k}_2\right) \cdot \boldsymbol{x}\right] \exp\left[-i\left(\boldsymbol{k}_3 - \boldsymbol{k}_4\right) \cdot \boldsymbol{x}'\right]$$

$$\times < \Psi_0 \mid f_{\boldsymbol{k}_1\alpha}^\dagger f_{\boldsymbol{k}_2\alpha} \mid \Psi_n >< \Psi_n \mid f_{\boldsymbol{k}_3\beta}^\dagger f_{\boldsymbol{k}_4\beta} \mid \Psi_0 > \ . \quad (5.26)$$

Since $\mid \Psi_0 >$ is the ground-state of the Fermi gas, we have the following relationships and conditions:

$$\begin{aligned}
\boldsymbol{k}_4 &\equiv \boldsymbol{k} \,, & \text{with} \quad \mid \boldsymbol{k} \mid &< \ k_F \,, \\
\boldsymbol{k}_3 &\equiv \boldsymbol{k}' \,, & \text{with} \quad \mid \boldsymbol{k}' \mid &> \ k_F \,, \\
\boldsymbol{k}_2 &= \boldsymbol{k}_3 \,, & & \\
\boldsymbol{k}_1 &= \boldsymbol{k}_4 \,, & &
\end{aligned} \qquad (5.27)$$

where we do not consider the case $\boldsymbol{k} = \boldsymbol{k}'$ that would give the expectation value of the density in the ground-state, that should be substracted as we mentioned before. Inserting these relationships into (5.26), we have

$$\begin{aligned}
(5.26) &= \frac{\delta_{\alpha\beta}}{V^2} \sum_{\boldsymbol{k},\boldsymbol{k}'} \exp\left[-i\left(\boldsymbol{k} - \boldsymbol{k}'\right) \cdot \left(\boldsymbol{x} - \boldsymbol{x}'\right)\right] \theta\left(k_F - k\right) \theta\left(k' - k_F\right) \\
&= \frac{\delta_{\alpha\beta}}{V^2} \sum_{\boldsymbol{k},\boldsymbol{q}} \exp\left[i\boldsymbol{q} \cdot \left(\boldsymbol{x} - \boldsymbol{x}'\right)\right] \theta\left(k_F - k\right) \theta\left(\mid \boldsymbol{k} + \boldsymbol{q} \mid - k_F\right) \,, \quad (5.28)
\end{aligned}$$

where in the last line we just made a change of variables. From the relationships above, we can also determine the energies of the excited states E_n. They correspond to the energy of an electron-hole pair, i.e.

$$E_n = E_0 + \epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}} \,, \qquad (5.29)$$

such that, after Fourier transforming in space we have

$$\begin{aligned}
\chi^{(0)}(\boldsymbol{q}, \omega) &= \frac{1}{V} \sum_{\boldsymbol{k},\alpha} \left[\frac{\theta\left(\mid \boldsymbol{k} + \boldsymbol{q} \mid - k_F\right) \theta\left(k_F - k\right)}{\hbar\omega - \left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}\right) + i\eta} \right. \\
&\qquad\qquad \left. - \frac{\theta\left(\mid \boldsymbol{k} - \boldsymbol{q} \mid - k_F\right) \theta\left(k_F - k\right)}{\hbar\omega + \left(\epsilon_{\boldsymbol{k}-\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}\right) + i\eta} \right] \\
&= \frac{2}{V} \sum_{\boldsymbol{k}} \left[\frac{\theta\left(\mid \boldsymbol{k} + \boldsymbol{q} \mid - k_F\right) \theta\left(k_F - k\right)}{\hbar\omega - \left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}\right) + i\eta} \right. \\
&\qquad\qquad \left. - \frac{\theta\left(k - k_F\right) \theta\left(k_F - \mid \boldsymbol{k} + \boldsymbol{q} \mid\right)}{\hbar\omega - \left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}\right) + i\eta} \right] \\
&= \frac{2}{V} \sum_{\boldsymbol{k}} \left[\frac{\theta\left(k_F - k\right) - \theta\left(k_F - \mid \boldsymbol{k} + \boldsymbol{q} \mid\right)}{\hbar\omega - \left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}\right) + i\eta} \right] \,, \qquad (5.30)
\end{aligned}$$

where in the second equality we explicitly set a factor 2 due to the summation over spin and made a change of variables in the $\boldsymbol{k}$-summation. In the last equality we used the fact that $\theta(x) = 1 - \theta(-x)$. The superscript (0) makes evident that we are dealing with the non-interacting case. Equation (5.30) determines the linear response of the Fermi gas to an external potential of the form

$$\varphi^{ext}\left(\boldsymbol{x}, t\right) = \varphi_0 \, \exp\left[i\left(\boldsymbol{q} \cdot \boldsymbol{x} - \omega t\right)\right] \; . \tag{5.31}$$

By comparing the form of the susceptibility χ with the one-particle Green's function in the Lehmann representation in eq. (4.316) or in eq. (4.321), we see that the difference between the time ordered product and the retarded propagator is given by the sign of the infinitesimal factor $i\eta$. In the case of the retarded function, all the poles are in the lower half of the complex ω-plane, whereas for the time ordered product, only one piece should have the poles in the lower half and the other should have them in the upper half. Therefore, we can construct a density-density correlation function with a time ordered product by reversing the sign of $i\eta$ in the second term in (5.30), or what is the same by the relation

$$\begin{aligned}
\mathrm{Re}\chi^{(T)} &= \mathrm{Re}\chi^{(R)} \, , \\
\mathrm{Im}\chi^{(T)} \, \mathrm{sgn}\omega &= \mathrm{Im}\chi^{(R)} \, .
\end{aligned} \tag{5.32}$$

where the superscripts T and R refer to a time ordered and a retarded correlation function, respectively. This means, we can also have a diagrammatic representation of the response function we calculated for the Fermi gas. In this case, we have a time ordered product that we can reduce to a product of contractions, as follows.
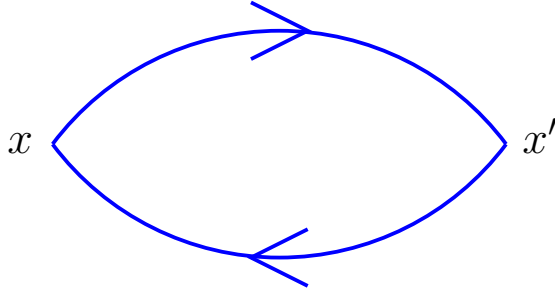

Figure 5.1: Diagram for the density response function of the Fermi gas.

$$\begin{aligned}
&< \Psi_0 \mid T\left[\tilde{n}_H\left(x\right) \tilde{n}_H\left(x'\right)\right] \mid \Psi_0 > \\
&\quad = < \Psi_0 \mid T\left[n_H\left(x\right) n_H\left(x'\right)\right] \mid \Psi_0 > - < \Psi_0 \mid n_H\left(x\right) \mid \Psi_0 >< \Psi_0 \mid n_H\left(x'\right) \mid \Psi_0 > \\
&\quad = < \Psi_0 \mid T\left[\hat{\psi}^{\dagger}_{H\alpha}\left(x\right) \hat{\psi}_{H\alpha}\left(x\right) \hat{\psi}^{\dagger}_{H\alpha}\left(x'\right) \hat{\psi}_{H\alpha}\left(x'\right)\right] \mid \Psi_0 > \\
&\qquad - < \Psi_0 \mid \hat{\psi}^{\dagger}_{H\alpha}\left(x^+\right) \hat{\psi}_{H\alpha}\left(x\right) \mid \Psi_0 >< \Psi_0 \mid \hat{\psi}^{\dagger}_{H\alpha}\left(x'^+\right) \hat{\psi}_{H\alpha}\left(x'\right) \mid \Psi_0 > \\
&\quad = iG^{(0)}_{\alpha\alpha}\left(x, x^+\right) iG^{(0)}_{\beta\beta}\left(x', x'^+\right) - iG^{(0)}_{\alpha\beta}\left(x, x'\right) iG^{(0)}_{\beta\alpha}\left(x', x\right) - < n\left(\boldsymbol{x}\right) >< n\left(\boldsymbol{x}'\right) > \\
&\quad = \left(2s + 1\right) G^{(0)}\left(x, x'\right) G^{(0)}\left(x', x\right) \; . \tag{5.33}
\end{aligned}$$

Here we used the convention that a summation is understood for repeated spin indices. Figure 5.1 shows the corresponding Feynman diagram.

Until now we considered the electrons as non-interacting particles. Although to consider the full effect of interaction is as a difficult problem as in the case of the one-particle Green's function, we can still consider the consequences of the Coulomb interaction on an average manner. From Poisson's equation in electrodynamics, we know that a change in the electronic density will lead to a corresponding induced potential.

$$\nabla^2 \, \Phi_{ind} = -4\pi \, e \, \delta < n\left(\boldsymbol{x}, t\right) > \ . \tag{5.34}$$

Since we are in the linear regime, the induced potential should have the same wavelength and frequency as the external potential,

$$\Phi_{ind}\left(\boldsymbol{x}, t\right) \ = \ \Phi_0 \, \exp\left[i\left(\boldsymbol{q} \cdot \boldsymbol{x} - \omega t\right)\right] \ . \tag{5.35}$$

This means that

$$\nabla^2 \, \Phi_{ind} = -\boldsymbol{q}^2 \Phi_{ind} \ , \tag{5.36}$$

such that

$$\Phi_0 \ = \ \frac{4\pi e}{q^2} \, \chi^{(0)}\left(\boldsymbol{q}, \omega\right) \, \varphi_0 \ . \tag{5.37}$$

Due to the presence of the induced potential, the potential acting on the system is the superposition of the external and the induced one.

$$\varphi^{total}\left(\boldsymbol{x}, t\right) = \Phi_{ind}\left(\boldsymbol{x}, t\right) + \varphi^{ext}\left(\boldsymbol{x}, t\right) \ . \tag{5.38}$$

Again this potential should have the form

$$\varphi_{total}\left(\boldsymbol{x}, t\right) \ = \ \varphi \, \exp\left[i\left(\boldsymbol{q} \cdot \boldsymbol{x} - \omega t\right)\right] \ . \tag{5.39}$$

Since this potential will also lead to a change of the density distribution, we should insert φ instead of φ_0 in (5.37), obtaining thus a self-consistent equation for the total potential.

$$\varphi = \varphi_0 + \frac{4\pi e}{q^2} \, \chi^{(0)}\left(\boldsymbol{q}, \omega\right) \, \varphi \ , \tag{5.40}$$

This equation can be solved as follows

$$\varphi = \frac{\varphi_0}{\varepsilon\left(\boldsymbol{q}, \omega\right)} \ , \tag{5.41}$$

with

$$\varepsilon\left(\boldsymbol{q}, \omega\right) = 1 - \frac{4\pi e}{q^2} \, \chi^{(0)}\left(\boldsymbol{q}, \omega\right) \ . \tag{5.42}$$

The last quantity is the dielectric function that in general describes the screening of an external potential by a polarizable medium. In the present case, where the density response is just the one due to non-interacting electrons, but the Coulomb interaction is considered on a macrosocopic level, as dictated by classical electrodynamics, one speaks of the time dependent Hartree approximation or Linhard function.

In order to discuss some of the properties of the dielectric function, let us rewrite $\chi^{(0)}$ from eq. (5.30), as follows

$$\chi^{(0)}\left(\boldsymbol{q},\omega\right) = \frac{2}{V}\sum_{\boldsymbol{k}}\left[\frac{n^0\left(\epsilon_{\boldsymbol{k}}\right) - n^0\left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}}\right)}{\hbar\omega - \left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}\right) + i\eta}\right]\ , \tag{5.43}$$

where

$$n^0\left(\epsilon_{\boldsymbol{k}}\right) = \frac{1}{\exp\left[\beta\left(\epsilon_{\boldsymbol{k}} - \mu\right)\right] + 1} \tag{5.44}$$

is the Fermi-Dirac distribution. We introduce this generalization for the non-interacting case just to make clear the following facts. Let us consider the limit $\omega = 0$ and $\boldsymbol{q} \to 0$. In this limit, we have for the numerator of (5.43)

$$n^0\left(\epsilon_{\boldsymbol{k}}\right) - n^0\left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}}\right) \rightarrow -\frac{\partial n^0\left(\epsilon_{\boldsymbol{k}}\right)}{\partial\epsilon_{\boldsymbol{k}}}\boldsymbol{\nabla}_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}\cdot\boldsymbol{q}$$

$$= \frac{\partial n^0\left(\epsilon_{\boldsymbol{k}}\right)}{\partial\mu}\boldsymbol{\nabla}_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}\cdot\boldsymbol{q}\ . \tag{5.45}$$

On the other hand, we have for the denominator

$$\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}} \rightarrow \boldsymbol{\nabla}_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}\cdot\boldsymbol{q}\ . \tag{5.46}$$

Putting the results above together, we have

$$\varepsilon\left(\boldsymbol{q}\to 0,\omega = 0\right) = 1 + \frac{4\pi e}{q^2}\frac{\partial}{\partial\mu}\underbrace{2\sum_{k}n^0\left(\epsilon_{\boldsymbol{k}}\right)}_{=N}\ , \tag{5.47}$$

where N is the number of particles in the system. This form leads us to the *Thomas-Fermi dielectric constant*, an approximation appropriate for static, long wavelength potentials. From (5.47) we see that there is a length squared

$$\kappa_0^2 = 4\pi e\frac{\partial N}{\partial\mu}\ , \tag{5.48}$$

such that the screened potential can be expressed as

$$\varphi = \frac{\varphi_0}{1 + \frac{\kappa_0^2}{q^2}} \tag{5.49}$$

Let us consider an external potential due to a probe charge Q. Then, we have in direct space

$$\varphi^{ext}\left(\boldsymbol{x}\right) = \frac{Q}{\mid \boldsymbol{x} \mid} , \tag{5.50}$$

and in momentum space

$$\varphi_0\left(\boldsymbol{q}\right) = \frac{4\pi Q}{\boldsymbol{q}^2} . \tag{5.51}$$

Inserting this last result into (5.49), we have

$$\varphi\left(\boldsymbol{q}\right) = \frac{4\pi Q}{\boldsymbol{q}^2 + \kappa_0^2} , \tag{5.52}$$

such that

$$\varphi^{total}\left(\boldsymbol{x}\right) \;\; = \;\; \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{4\pi Q}{\boldsymbol{q}^2 + \kappa_0^2} \exp\left(i\boldsymbol{q}\cdot\boldsymbol{x}\right) = \frac{Q}{\mid \boldsymbol{x} \mid} \exp\left(-\kappa_0 \mid \boldsymbol{x} \mid\right) . \tag{5.53}$$

The Thomas-Fermi approximation leads to a screened Coulomb potential, where κ_0^{-1} is the *screening length*.

Susceptibility and polarization

The susceptibility is defined generally by the relation (5.17), that for a homogeneous system or a model on a lattice becomes

$$\delta < \hat{n}\left(\boldsymbol{q},\omega\right) > \;\; = \;\; \chi\left(\boldsymbol{q},\omega\right) \varphi^{ext}\left(\boldsymbol{q},\omega\right) . \tag{5.54}$$

On the other hand, as discussed above, we can express the total potential as the sum of the external and the induced one

$$\begin{aligned}
\varphi^{total}\left(\boldsymbol{q},\omega\right) \;\; &= \;\; \varphi^{ext}\left(\boldsymbol{q},\omega\right) + \frac{4\pi e}{q^2}\chi\left(\boldsymbol{q},\omega\right)\varphi^{ext}\left(\boldsymbol{q},\omega\right) \\
&= \;\; \left[1 + \frac{4\pi}{q^2}\chi\left(\boldsymbol{q},\omega\right)\right]\varphi^{ext}\left(\boldsymbol{q},\omega\right) ,
\end{aligned} \tag{5.55}$$

where now we assume that $\delta < \hat{n}\left(\boldsymbol{q},\omega\right) >$ is the total change in electronic density due to the external potential, taking into account all induction effects. Then, comparing with (5.41), we have

$$\varepsilon^{-1}\left(\boldsymbol{q},\omega\right) = 1 + \frac{4\pi e}{q^2}\chi\left(\boldsymbol{q},\omega\right) . \tag{5.56}$$

Both ε^{-1} and χ describe the total potential given the external one and are therefore, response functions. There is another quantity that can be defined relating the

response to the total potential. This quantity is called the *polarization propagator* $P(\boldsymbol{q}, \omega)$.

$$\delta < \hat{n}(\boldsymbol{q}, \omega) > \quad = \quad P(\boldsymbol{q}, \omega) \, \varphi^{total}(\boldsymbol{q}, \omega) \ . \tag{5.57}$$

This is the quantity that defined in general for interacting systems reduces to $\chi^{(0)}$ for a non-interacting one. As we have already seen in (5.40),

$$\varphi^{total}(\boldsymbol{q}, \omega) = \varphi^{ext} + \frac{4\pi e}{q^2} P(\boldsymbol{q}, \omega) \, \varphi^{total}(\boldsymbol{q}, \omega) \ , \tag{5.58}$$

leading to the general form

$$\varepsilon(\boldsymbol{q}, \omega) = 1 - \frac{4\pi e}{q^2} P(\boldsymbol{q}, \omega) \ . \tag{5.59}$$

By comparing this equation with (5.56), we can relate the suceptibility with the polarization propagator. The result is

$$\begin{aligned} \chi(\boldsymbol{q}, \omega) \quad &= \quad \frac{P(\boldsymbol{q}, \omega)}{1 - \frac{4\pi e}{q^2} P(\boldsymbol{q}, \omega)} \\ &= \quad P + PvP + PvPvP + \cdots \ , \end{aligned} \tag{5.60}$$

where

$$v(\boldsymbol{q}) = \frac{4\pi e}{\boldsymbol{q}^2} \tag{5.61}$$

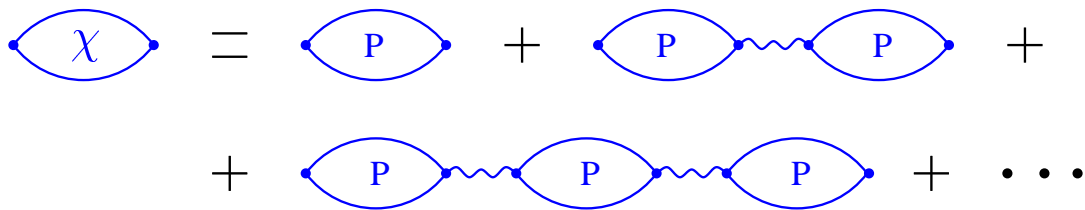is the Coulomb interaction.   Figure 5.2 gives a diagrammatic representation of

Figure 5.2: Diagrammatic representation of the integral equation for the suscepti-bility .

the geometric series that determines the susceptibility in terms of the polarization propagator. In the case that $P = \chi^{(0)}$, it is called the *random phase approximation* (RPA). The same equation can be written as an integral equation by noticing that

$$\chi = P\varepsilon^{-1} = P(1 + v\chi) = P + Pv\chi \ . \tag{5.62}$$

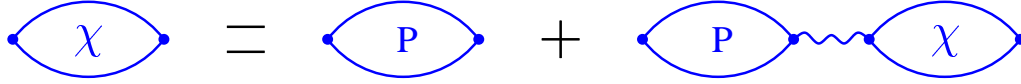The corresponding diagrammatic representation is shown in Fig. 5.3 The equation

Figure 5.3: Self-consistent equation for the susceptibility in terms of the polarization propagator.

and diagrams above can be seen as follows. The external potential polarizes the medium. Due to the Coulomb interaction, the induced charge leads to a modified potential that in turn produces a modified induced charge density. With the introduction of the polarization propagator we have a general frame to discuss screening processes beyond the non-interacting Fermi gas.

Friedel sum-rule and Friedel oscillations

We can consider now the effect of a stationary point charge Ze in an electron gas taking into account the interaction fully. In this case the external potential is given by

$$\varphi^{ext}\left(\boldsymbol{q},\omega\right) \;=\; \frac{4\pi Ze}{q^2}\,\delta(\omega)\;, \tag{5.63}$$

such that the induced charge density is

$$\rho_{ind}\left(\boldsymbol{x}\right) \;=\; \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\,\chi\left(\boldsymbol{q},\omega=0\right)\frac{4\pi Ze}{q^2}\,\exp\left(-i\boldsymbol{q}\cdot\boldsymbol{x}\right)\;. \tag{5.64}$$

Using (5.60), we have

$$\chi\left(\boldsymbol{q},\omega=0\right)\frac{4\pi}{q^2} \;=\; \frac{P\left(\boldsymbol{q},\omega=0\right)}{\frac{q^2}{4\pi}-P\left(\boldsymbol{q},\omega=0\right)}\;. \tag{5.65}$$

Then, the total induced charge is

$$\begin{aligned} Q_{ind} &= \int \mathrm{d}^3 x\,\rho_{ind}\left(\boldsymbol{x}\right) \\ &= -Ze\,\frac{P\left(\boldsymbol{q}=0,\omega=0\right)}{P\left(\boldsymbol{q}=0,\omega=0\right)} = -Ze\;, \end{aligned} \tag{5.66}$$

since $P\left(\boldsymbol{q}=0,\omega=0\right)$ is regular. Therefore, Friedel's sum rule shows that in a metallic system, a point charge is completely screened on large distances. By a direct calculation, it can be shown furthermore, that due to the presence of a sharp Fermi surface, the induced charge presents oscillations with a wavevector $2k_F$, such that

$$\rho_{ind}\left(\boldsymbol{x}\right) \longrightarrow\sim \frac{\cos(2k_F\mid\boldsymbol{x}\mid)}{\mid\boldsymbol{x}\mid^3}\;. \tag{5.67}$$

These are called *Friedel oscillations*.

5.1.2   Collective excitations: plasmons

Recalling again the relation between the induced charge density and the external perturbation (5.54),

$$\rho_{ind}\left(\boldsymbol{q},\omega\right) \;=\; \chi\left(\boldsymbol{q},\omega\right)\varphi^{ext}\left(\boldsymbol{q},\omega\right)\;, \tag{5.68}$$

and the fact that as was discussed in Sec. 5.1.1, the density-density response function will have poles at suitable energies and momenta, as shown by eq. (5.23), we see that at those energies and momenta, the system will have an eigenmode for the charge degrees of freedom, since even with an infinitesimal corresponding external perturbation, a finite response is obtained. That is, in general, the poles of the linear response functions correspond to collective excitations of the system.

Without going into the details of the structure of $\chi\left(\boldsymbol{q},\omega\right)$, we can discuss one of the collective modes of an electronic system, namely plasmons. Since as shown in (5.56), a divergence in $\chi\left(\boldsymbol{q},\omega\right)$ implies a vanishing of $\varepsilon\left(\boldsymbol{q},\omega\right)$, instead of looking for the poles of $\chi\left(\boldsymbol{q},\omega\right)$, we will focus on the zeros of $\varepsilon\left(\boldsymbol{q},\omega\right)$. In the RPA, we have

$$\varepsilon\left(\boldsymbol{q},\omega\right) \;=\; 1-\frac{4\pi e}{q^2}\,\chi^{(0)}\left(\boldsymbol{q},\omega\right)\;, \tag{5.69}$$

with $\chi^{(0)}\left(\boldsymbol{q},\omega\right)$ given by (5.43):

$$\chi^{(0)}\left(\boldsymbol{q},\omega\right) \;=\; \frac{2}{V}\sum_{\boldsymbol{k}}\left[\frac{n^0\left(\epsilon_{\boldsymbol{k}}\right)-n^0\left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}}\right)}{\hbar\omega-\left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{\boldsymbol{k}}\right)+i\eta}\right]\;. \tag{5.70}$$

Plasmons being an eigenmode of metallic systems, should lie at rather high energies since at energies comparable to the plasmon energy, the system should absorb and not reflect, as most metals do in the range of visible light. We will therefore assume that at the energies of interest, $\hbar\omega \gg \epsilon_{\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{\boldsymbol{k}}$, $\forall\,\boldsymbol{k}$ and for $\boldsymbol{q}\sim 0$. With this in mind, we rewrite $\chi^{(0)}$ as follows

$$\begin{aligned}
\chi^{(0)}\left(\boldsymbol{q},\omega\right) \;&=\; \frac{2}{V}\sum_{\boldsymbol{k}}\left[\frac{n^0\left(\epsilon_{\boldsymbol{k}}\right)}{\hbar\omega-\left(\epsilon_{\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{\boldsymbol{k}}\right)+i\eta}-\frac{n^0\left(\epsilon_{\boldsymbol{k}}\right)}{\hbar\omega-\left(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}-\boldsymbol{q}}\right)+i\eta}\right]\\
&=\; \frac{2}{V}\sum_{\boldsymbol{k}}n^0\left(\epsilon_{\boldsymbol{k}}\right)\frac{\epsilon_{\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{\boldsymbol{k}}+\epsilon_{\boldsymbol{k}-\boldsymbol{q}}-\epsilon_{\boldsymbol{k}}}{\left(\hbar\omega\right)^2\left[1+\frac{a}{\hbar\omega}+\frac{b}{\left(\hbar\omega\right)^2}\right]}\;.
\end{aligned} \tag{5.71}$$

For $\boldsymbol{q}\sim 0$ we can make the following expansion

$$\epsilon_{\boldsymbol{k}\pm\boldsymbol{q}} \simeq \epsilon_{\boldsymbol{k}}\pm\boldsymbol{\nabla}_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}\cdot\boldsymbol{q}+\frac{1}{2}\frac{\partial^2\epsilon_{\boldsymbol{k}}}{\partial k_\alpha\,\partial k_\beta}\,q_\alpha q_\beta\;, \tag{5.72}$$

such that

$$(5.71) \;=\; \frac{1}{\left(\hbar\omega\right)^2}\frac{2}{V}\sum_{\boldsymbol{k}}n^0\left(\epsilon_{\boldsymbol{k}}\right)\frac{\partial^2\epsilon_{\boldsymbol{k}}}{\partial k_\alpha\,\partial k_\beta}\,q_\alpha q_\beta\;. \tag{5.73}$$

Due to inversion symmetry, $\epsilon_{\boldsymbol{k}} = \epsilon_{-\boldsymbol{k}}$, and hence

$$\sum_{\boldsymbol{k}} n^0 \left(\epsilon_{\boldsymbol{k}} \right) \frac{\partial^2 \epsilon_{\boldsymbol{k}}}{\partial k_\alpha \, \partial k_\beta} = 0 \tag{5.74}$$

for $\alpha \neq \beta$. Let us assume further that we have a cubic symmetry, such that

$$\frac{\partial^2 \epsilon_{\boldsymbol{k}}}{\partial k_\alpha^2} = \frac{\partial^2 \epsilon_{\boldsymbol{k}}}{\partial k^2} \tag{5.75}$$

does not depend on the direction. For a parabolic band

$$\epsilon_{\boldsymbol{k}} = \frac{\hbar^2 \boldsymbol{k}^2}{2m^*} , \tag{5.76}$$

where we introduced the *effective mass m^**, we have

$$\frac{\partial^2 \epsilon_{\boldsymbol{k}}}{\partial k^2} = \frac{\hbar^2}{m^*} . \tag{5.77}$$

Furthermore, $2 \sum_k n^0 \left(\epsilon_{\boldsymbol{k}} \right) = n$, where n is the electronic density in the system. Putting everything together, we have finally

$$\varepsilon \left(\boldsymbol{q}, \omega \right) = 1 - \frac{\omega_p^2}{\omega^2} , \tag{5.78}$$

where

$$\omega_p = \sqrt{\frac{4\pi n e^2}{m^{*2}}} \tag{5.79}$$

is the *plasma frequency.*   A further expansion in powers of $\boldsymbol{q}$ up to fourth order
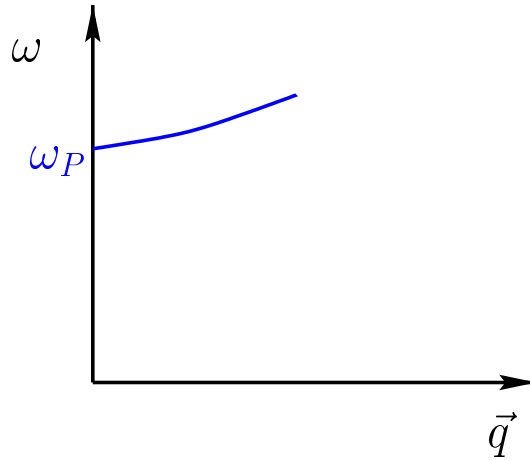

Figure 5.4: Plasmon dispersion for small wavevector $\boldsymbol{q}$.

leads to a dispersion of the form

$$\omega_p\left(\boldsymbol{q}\right) = \omega_p\left(1 + \frac{3}{10}\frac{q^2 v_F^2}{\omega_p^2}\right) \, , \tag{5.80}$$

where v_F is the Fermi velocity.

As already seen in electrodynamics, the dielectric function is related to the complex refractive index as follows

$$\kappa = \sqrt{\varepsilon} \, . \tag{5.81}$$

This means recalling (5.78) that for $\omega < \omega_p$, the refractive index is purely imaginary, and hence, a metal shows total reflexion. On the contrary, for $\omega > \omega_p$, the metal can transmit, thus becoming transparent for high enough frequencies (usually in the ultraviolet region).

We restricted ourselves in this section to metals. However, other collective excitations can be found in semiconductors like excitons, that correspond to bound electron-hole pairs. Due to lack of time we defer these subjects to elective lectures.