

# Response Properties of the Electronic System in Low Dimensions

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## Abstract

In this topic we will analyze how the electronic system responds to the presence of an external field. This response determines how the electrons interact with each other after the application of an external interaction. Thus, response properties are crucial to understand how a material will respond to the interaction with an external experimental probe, i.e., an electromagnetic probe, or also to a simple distortion of the lattice potential. We will make use of linear response theory within the nearly free electron model in which the response is determined by the Lindhard function. The Lindhard function will be calculated for the static case in 3D, 2D, and 1D. The impact of the static response function on the phonons will be analyzed, focusing on the different effects observed depending on the dimension of the system. The differences will be underlined. Finally, the dynamical Lindhard function will be given also for different dimensions. The impact on plasmon dispersions will be discussed.

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# 1 Linear response theory

Let's assume we have a system of electrons whose density is  $n(\mathbf{r})$  and is the solution of a general separable time independent Hamiltonian  $H_0$ . Let's assume the Hamiltonian for each electron is diagonalizable:

$$H_0|\psi_i\rangle = E_i|\psi_i\rangle. \quad (1)$$

The electronic density will therefore be

$$n(\mathbf{r}) = \sum_i f_i \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}), \quad (2)$$

where  $f_i$  is the Fermi-Dirac occupation factor of state  $i$ . In case we have a free electron gas the density will be homogeneous and the Hamiltonian will equal the kinetic energy. If suddenly there is an external time-dependent potential  $V_{ext}(\mathbf{r}', t')$  that starts acting on this electronic system, it will impose a change on the electron density. If the interaction is weak, we can adopt linear response theory and assume that the change in the density at time  $t$  and position  $\mathbf{r}$  will be

$$\delta n(\mathbf{r}, t) = \int_{-\infty}^{\infty} dt' \int d\mathbf{r}' \chi(\mathbf{r}, \mathbf{r}', t - t') V_{ext}(\mathbf{r}', t'). \quad (3)$$

$\chi(\mathbf{r}, \mathbf{r}', t - t')$  is the so-called density response function. Fourier transforming the equation above to the frequency regime, we have the following equation

$$\delta n(\mathbf{r}, \omega) = \int d\mathbf{r}' \chi(\mathbf{r}, \mathbf{r}', \omega) V_{ext}(\mathbf{r}', \omega). \quad (4)$$

From the equation above we see that the response function can be defined from

$$\chi(\mathbf{r}, \mathbf{r}', \omega) = \frac{\delta n(\mathbf{r}, \omega)}{\delta V_{ext}(\mathbf{r}', \omega)} \quad (5)$$

as well. If we want to study the ultimate effect of the interaction between the external probe on the electronic system, we need to focus on the static limit at  $\omega = 0$ :

$$\delta n(\mathbf{r}) = \int d\mathbf{r}' \chi(\mathbf{r}, \mathbf{r}') V_{ext}(\mathbf{r}'), \quad (6)$$

where we have dropped the  $\omega$  dependence for simplicity. In other words, the response function will tell us how the electronic system will respond to the presence of the external field.

The density response function also determines how the potential felt by the electrons is effectively affected by the rest of the electrons when the interaction with the external probe is turned on. Let's assume we have an electron in position  $\mathbf{r}$  and that it is independent from the rest (this is like a Hartree approximation). The interaction potential with the rest of the electrons before the probe is turned on will be

$$V(\mathbf{r}) = \int d\mathbf{r}' e^2 \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \quad (7)$$

When the external potential is switched on, the density will change as discussed above and the potential that the electron feels will be modified to

$$V'(\mathbf{r}, \omega) = V_{ext}(\mathbf{r}, \omega) + \int d\mathbf{r}' e^2 \frac{n'(\mathbf{r}', \omega)}{|\mathbf{r} - \mathbf{r}'|}, \quad (8)$$

where  $n'(\mathbf{r}, \omega)$  is the new density of the system affected by the presence of the external field. If we calculate the change in the total potential felt by the electron, we have

$$\begin{aligned} \delta V(\mathbf{r}, \omega) &= V'(\mathbf{r}, \omega) - V(\mathbf{r}) = V_{ext}(\mathbf{r}, \omega) + e^2 \int d\mathbf{r}' d\mathbf{r}'' \frac{\chi(\mathbf{r}', \mathbf{r}'', \omega)}{|\mathbf{r} - \mathbf{r}'|} V_{ext}(\mathbf{r}'', \omega) \\ &= \int d\mathbf{r}' \left[ \delta(\mathbf{r} - \mathbf{r}') + e^2 \int d\mathbf{r}'' \frac{\chi(\mathbf{r}'', \mathbf{r}', \omega)}{|\mathbf{r} - \mathbf{r}''|} \right] V_{ext}(\mathbf{r}', \omega) \\ &= \int d\mathbf{r}' \epsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega) V_{ext}(\mathbf{r}', \omega), \end{aligned} \quad (9)$$

where we have defined the inverse of the dielectric function as

$$\epsilon^{-1}(\mathbf{r}, \mathbf{r}', \omega) = \frac{\delta V(\mathbf{r}, \omega)}{\delta V_{ext}(\mathbf{r}', \omega)} = \delta(\mathbf{r} - \mathbf{r}') + e^2 \int d\mathbf{r}'' \frac{\chi(\mathbf{r}'', \mathbf{r}', \omega)}{|\mathbf{r} - \mathbf{r}''|}. \quad (10)$$

We can see that the dielectric function is *screening* the external potential due to the presence of the other electrons of the system. Screening is one of the most important concepts in material science as it is key when determining the response of the material to any external probe. Thus, the dielectric matrix determines the optical properties of materials and it is a key concept whenever we want to study the perturbation of the electronic system with respect to small change of the interactions.

## 1.1 Non-interacting response function in the static limit

Sometimes it is confusing in the literature the fact that also a non-interacting density response function is defined as

$$\chi^0(\mathbf{r}, \mathbf{r}', \omega) = \frac{\delta n(\mathbf{r}, \omega)}{\delta V(\mathbf{r}', \omega)}, \quad (11)$$

where now the functional derivative is taken with respect to the full potential  $V = V_{ee} + V_{ext}$ . Using the chain rule, we can determine the relation between  $\chi$  and  $\chi^0$ :

$$\begin{aligned} \chi(\mathbf{r}, \mathbf{r}', \omega) &= \frac{\delta n(\mathbf{r}, \omega)}{\delta V_{ext}(\mathbf{r}', \omega)} = \int d\mathbf{r}'' \frac{\delta n(\mathbf{r}, \omega)}{\delta V(\mathbf{r}'', \omega)} \frac{\delta V(\mathbf{r}'', \omega)}{\delta V_{ext}(\mathbf{r}', \omega)} \\ &= \int d\mathbf{r}'' \chi^0(\mathbf{r}, \mathbf{r}'', \omega) \left[ \delta(\mathbf{r}' - \mathbf{r}'') + \frac{\delta V_{ee}(\mathbf{r}'', \omega)}{\delta V_{ext}(\mathbf{r}', \omega)} \right]. \end{aligned} \quad (12)$$

The dependence of the electron-electron interaction on the density  $n$  yields to a self-consistent Dyson-like equation for the interacting response function  $\chi$ , which may be complicated to solve.

The non-interacting response function, however, can be easily calculated as long as we know the eigenfunctions and eigenvalues of the electronic system before the external interaction is switched on. We are assuming that that is the case. When the  $V_{ext}$  is turned on the Hamiltonian will be shifted to

$$H = H_0 + \delta V. \quad (13)$$

In order to calculate  $\chi_0$  we need to calculate the change in the density. We are going to do it on the static limit in which  $\omega = 0$ . Assuming that  $\delta V$  is small (and Hermitian), using first order perturbation theory, the eigenfunction will be shifted as

$$\delta\psi_i(\mathbf{r}) = \sum_{j \neq i} \frac{\langle \psi_j | \delta V | \psi_i \rangle}{E_i - E_j} \psi_j(\mathbf{r}). \quad (14)$$

Thus, the change in the electronic density at linear order will be

$$\begin{aligned} \delta n(\mathbf{r}) &= \sum_i f_i [\psi_i^*(\mathbf{r}) \delta\psi_i(\mathbf{r}) + \delta\psi_i^*(\mathbf{r}) \psi_i(\mathbf{r})] \\ &= \sum_i f_i \left[ \sum_{j \neq i} \frac{\langle \psi_j | \delta V | \psi_i \rangle}{E_i - E_j} \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) + \sum_{j \neq i} \frac{(\langle \psi_j | \delta V | \psi_i \rangle)^*}{E_i - E_j} \psi_j^*(\mathbf{r}) \psi_i(\mathbf{r}) \right] \\ &= \sum_{i,j \neq i} \frac{f_i - f_j}{E_i - E_j} \langle \psi_j | \delta V | \psi_i \rangle \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}) \\ &= \sum_{i,j \neq i} \frac{f_i - f_j}{E_i - E_j} \int d\mathbf{r}' \delta V(\mathbf{r}') \psi_j^*(\mathbf{r}') \psi_i(\mathbf{r}') \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}). \end{aligned} \quad (15)$$

Consequently, the non-interacting response function at the static level is

$$\chi^0(\mathbf{r}, \mathbf{r}') = \frac{\delta n(\mathbf{r})}{\delta V(\mathbf{r}')} = \sum_{i,j \neq i} \frac{f_i - f_j}{E_i - E_j} \psi_j^*(\mathbf{r}') \psi_i(\mathbf{r}') \psi_i^*(\mathbf{r}) \psi_j(\mathbf{r}). \quad (16)$$

## 2 Static response function of the free electron gas

So far we have only assumed that the Hamiltonian for each electron is separable. Here we will assume that instead we have free electrons, so that the Hamiltonian is just the kinetic energy and the unperturbed eigenfunctions are plane-waves and the eigenenergies are parabolic. The good quantum number will be the wave number  $\mathbf{k}$ . It is important to remark that in this limit the non-interacting and interacting response functions are the same,  $\chi^0 = \chi$ , because the potential is 0 before the interaction is turned on. This is sometime not obvious in the literature.

In the following we will calculate the static response function  $\chi$  (or  $\chi^0$ ) for the free electron gas in 3D, 2D, and 1D. As we will see the dimension plays a crucial role on the properties of the response functions, and this has clear physical consequences.

## 2.1 Lindhard response function in 3D

Substituting plane-waves solutions  $\psi_i(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$  in Eq. (16), where  $V$  is the volume of the solid, we see that

$$\chi^0(\mathbf{r}, \mathbf{r}') = \frac{1}{V^2} \sum_{\mathbf{k}\mathbf{k}', \mathbf{k}\neq\mathbf{k}'} \frac{f_{\mathbf{k}} - f_{\mathbf{k}'}}{E_{\mathbf{k}} - E_{\mathbf{k}'}} e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}-\mathbf{r}')}, \quad (17)$$

where  $E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$ . As we can see the response function only depends on the distance between  $\mathbf{r}$  and  $\mathbf{r}'$ . This is expected for a homogeneous medium like the electron gas. In general this is not true. Thus, we can write

$$\chi^0(\mathbf{r} - \mathbf{r}') = \frac{1}{V^2} \sum_{\mathbf{k}\mathbf{k}', \mathbf{k}\neq\mathbf{k}'} \frac{f_{\mathbf{k}} - f_{\mathbf{k}'}}{E_{\mathbf{k}} - E_{\mathbf{k}'}} e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}-\mathbf{r}')}. \quad (18)$$

It is convenient to Fourier transform the response function as

$$\chi^0(\mathbf{q}) = \int d\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \chi^0(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}', \mathbf{k}\neq\mathbf{k}'} \frac{f_{\mathbf{k}} - f_{\mathbf{k}'}}{E_{\mathbf{k}} - E_{\mathbf{k}'}} \delta_{\mathbf{q}, \mathbf{k}-\mathbf{k}'} \quad (19)$$

so that we finally obtain

$$\chi^0(\mathbf{q}) = \frac{1}{V} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}}}, \quad (20)$$

where  $\mathbf{q}$  cannot be 0. This is the so-called Lindhard response function.

In order to calculate the explicit form of the Lindhard function, we will assume that we are at 0K, which implies that

$$f_{\mathbf{k}} = 2\theta(k_F - k), \quad (21)$$

where we are assuming the spin degeneracy of the state. Then,

$$\begin{aligned} \chi^0(\mathbf{q}) &= \frac{2}{V} \frac{1}{(2\pi)^3/V} \int d\mathbf{k} \frac{\theta(k_F - k) - \theta(k_F - |\mathbf{k} - \mathbf{q}|)}{\frac{\hbar^2}{2m}(k^2 - (\mathbf{k} - \mathbf{q})^2)} \\ &= \frac{-m}{2\pi^3 \hbar^2} \int d\mathbf{k} \theta(k_F - k) \left( \frac{1}{q^2 + 2\mathbf{k} \cdot \mathbf{q}} + \frac{1}{q^2 - 2\mathbf{k} \cdot \mathbf{q}} \right). \end{aligned} \quad (22)$$

Let's perform first the integral

$$\begin{aligned} \int d\mathbf{k} \theta(k_F - k) \frac{1}{q^2 + 2\mathbf{k} \cdot \mathbf{q}} &= 2\pi \int_0^{k_F} dk k^2 \int_0^\pi d\theta \sin\theta \frac{1}{q^2 + 2kq \cos\theta} \\ &= \frac{\pi}{q} \int_0^{k_F} dk k \ln \left| \frac{q/(2k) + 1}{q/(2k) - 1} \right|. \end{aligned} \quad (23)$$

Considering the  $\mathbf{q} \rightarrow -\mathbf{q}$  exchange, we readily can see that

$$\begin{aligned} \int d\mathbf{k} \theta(k_F - k) \frac{1}{q^2 - 2\mathbf{k} \cdot \mathbf{q}} &= -\frac{\pi}{q} \int_0^{k_F} dk k \ln \left| \frac{-q/(2k) + 1}{-q/(2k) - 1} \right| \\ &= \frac{\pi}{q} \int_0^{k_F} dk k \ln \left| \frac{q/(2k) + 1}{q/(2k) - 1} \right|. \end{aligned} \quad (24)$$

Thus,

$$\begin{aligned}
\chi^0(\mathbf{q}) &= \frac{-m}{\pi^2 \hbar^2} \frac{1}{q} \int_0^{k_F} dk k \ln \left| \frac{q/(2k) + 1}{q/(2k) - 1} \right| \\
&= \frac{-m}{\pi^2 \hbar^2} \frac{1}{q} \left[ \frac{k^2}{2} \ln \left| \frac{q/(2k) + 1}{q/(2k) - 1} \right| - \int dk k^2 \left( \frac{1}{q+2k} + \frac{1}{q-2k} \right) \right]_0^{k_F} \\
&= \frac{-m}{\pi^2 \hbar^2} \frac{1}{q} \left[ \frac{k^2}{2} \ln \left| \frac{q/(2k) + 1}{q/(2k) - 1} \right| - \int dk \left( -q/2 + q^2/4 \left( \frac{1}{q+2k} + \frac{1}{q-2k} \right) \right) \right]_0^{k_F} \\
&= \frac{-m}{\pi^2 \hbar^2} \frac{1}{q} \left[ \left( \frac{k^2}{2} - \frac{q^2}{8} \right) \ln \left| \frac{q/(2k) + 1}{q/(2k) - 1} \right| + \frac{qk}{2} \right]_0^{k_F} \\
&= \frac{-m}{\pi^2 \hbar^2} \frac{1}{q} \left[ \left( \frac{k_F^2}{2} - \frac{q^2}{8} \right) \ln \left| \frac{q/(2k_F) + 1}{q/(2k_F) - 1} \right| + \frac{qk_F}{2} \right]. \tag{25}
\end{aligned}$$

This is usually rewritten as

$$\chi^0(\mathbf{q}) = \frac{-m}{\pi^2 \hbar^2} k_F F_L(q/(2k_F)), \tag{26}$$

where

$$F_L(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right|. \tag{27}$$

## 2.2 Lindhard response function in 2D

For a 2D electron gas, the Lindhard function looks in analogy as

$$\chi^0(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}}}. \tag{28}$$

A rather lengthy calculation (exercise 1) yields in this case

$$\chi^0(\mathbf{q}) = \begin{cases} \frac{-m}{\pi \hbar^2} \left( 1 - \sqrt{1 - (2k_F/q)^2} \right) & , q > 2k_F \\ \frac{-m}{\pi \hbar^2} & , q < 2k_F \end{cases}. \tag{29}$$

## 2.3 Lindhard response function in 1D

For a 1D electron gas, the Lindhard function looks in analogy as

$$\chi^0(q) = \frac{1}{L} \sum_k \frac{f_k - f_{k-q}}{E_k - E_{k-q}}. \tag{30}$$

A simpler calculation (exercise 2) yields in this case

$$\chi^0(\mathbf{q}) = \frac{-2m}{\pi \hbar^2} \frac{1}{q} \ln \left| \frac{1 + 2k_F/q}{1 - 2k_F/q} \right|. \tag{31}$$

In Fig. 2.3 the Lindhard function for the free electron gas in the 3D, 2D, and 1D cases is shown. It is clear that the results are extremely different depending on the dimension.

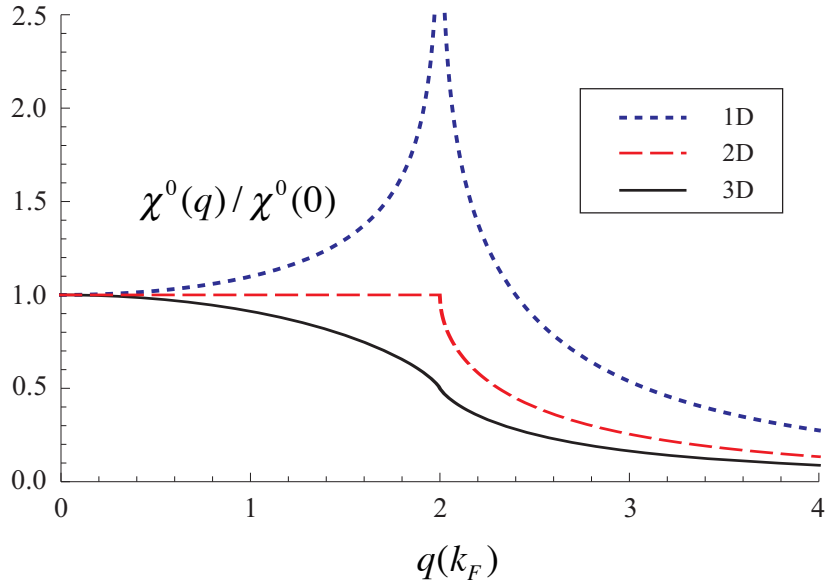


Figure 1: Response function of the free electron gas in different dimensions.

### 3 Linear response and phonon instabilities

As we can see in Fig 2.3, the  $\chi^0$  response function has singularities at  $q = 2k_F$  at all dimensions. However, the singularities are stronger for systems with reduced dimension. This has consequences on several properties that are somewhat related to the response function.

For instance phonon frequencies are affected by the static response function. When we are dealing with phonons we need to consider in the electronic Hamiltonian at least the Coulomb electron-ion interaction as well as the Coulomb ion-ion interaction:

$$H(\mathbf{R}) = T_e + V_{ei}(\mathbf{R}) + V_{ii}(\mathbf{R}), \quad (32)$$

where

$$V_{ei}(\mathbf{R}) = -\sum_{iI} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} = \sum_i V_{ext}(\mathbf{r}_i) \quad (33)$$

$$V_{ii}(\mathbf{R}) = \frac{1}{2} \sum_{IJ} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}. \quad (34)$$

Here  $\mathbf{R}$  denotes the parametric dependence of the electronic Hamiltonian on the ionic positions. The potential in which the ions move is defined by the

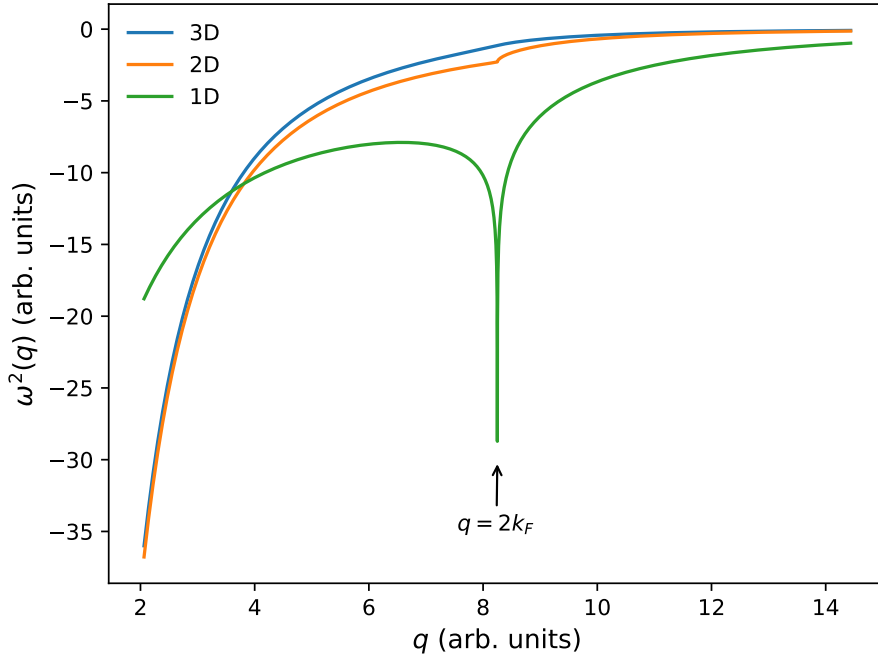


Figure 2: Solution of Eq. (40) for different dimensions, but assuming that the Coulomb potential is always the 3D and that the prefactor in the response function is the 3D one. In other words only the adimensional part of the response function is modified.

ground state energies of this Hamiltonian. These ground state electronic energies form the Born Oppenheimer potential  $V(\mathbf{R})$ . In the harmonic approximation the phonon frequencies are obtained diagonalizing the so called force-constant matrix

$$\frac{\partial^2 V(\mathbf{R})}{\partial R_I^\alpha \partial R_J^\beta}, \quad (35)$$

where  $R_I^\alpha$  is the  $\alpha$  Cartesian component of ion  $I$ . Let's first take the first derivative, which is easily considered due to Hellman-Feynman theorem:

$$\frac{\partial V(\mathbf{R})}{\partial R_J^\beta} = \langle \Psi(\mathbf{R}) | \frac{\partial H(\mathbf{R})}{\partial R_J^\beta} | \Psi(\mathbf{R}) \rangle = \frac{\partial V_{ii}(\mathbf{R})}{\partial R_J^\beta} + \int d\mathbf{r} n(\mathbf{r}) \frac{\partial V_{ext}(\mathbf{r})}{\partial R_J^\beta}. \quad (36)$$

When taking the second derivative we obtain

$$\frac{\partial^2 V(\mathbf{R})}{\partial R_I^\alpha \partial R_J^\beta} = \frac{\partial^2 V_{ii}(\mathbf{R})}{\partial R_I^\alpha \partial R_J^\beta} + \int d\mathbf{r} n(\mathbf{r}) \frac{\partial^2 V_{ext}(\mathbf{r})}{\partial R_I^\alpha \partial R_J^\beta} + \int d\mathbf{r} \frac{\partial n(\mathbf{r})}{\partial R_I^\alpha} \frac{\partial V_{ext}(\mathbf{r})}{\partial R_J^\beta}. \quad (37)$$

The first two addends are rather straightforward to calculate as they just depend on the density. The tricky part is the calculation of the last term due to



the derivative of the density. However, linear response theory allows simply to calculate that rather easily as

$$\frac{\partial n(\mathbf{r})}{\partial R_I^\alpha} = \int d\mathbf{r}' \frac{\partial n(\mathbf{r})}{\partial V_{ext}(\mathbf{r}')} \frac{\partial V_{ext}(\mathbf{r}')}{\partial R_I^\alpha} = \int d\mathbf{r}' \chi(\mathbf{r}, \mathbf{r}') \frac{\partial V_{ext}(\mathbf{r}')}{\partial R_I^\alpha}. \quad (38)$$

In this way the last term of the force constants can be written as

$$\Phi_{IJ}^{\alpha\beta} = \int d\mathbf{r} d\mathbf{r}' \chi(\mathbf{r}, \mathbf{r}') \frac{\partial V_{ext}(\mathbf{r}')}{\partial R_I^\alpha} \frac{\partial V_{ext}(\mathbf{r})}{\partial R_J^\beta}. \quad (39)$$

In this way can see that how the response function affects the phonon properties.

In order to illustrate the effect of dimensionality on the phonons, we will assume that we have a hydrogen crystal and that the response function is the one of the free electron like gas. Fourier transforming Eq. (20) we obtain

$$\Phi^{\alpha\beta}(\mathbf{q}) \sim \omega^2(\mathbf{q}) \sim v_c(\mathbf{q})^2 \chi(\mathbf{q}) q^\alpha q^\beta, \quad (40)$$

where  $\omega(\mathbf{q})$  would be the contribution of this term to the phonon frequencies. In Fig. 3 we see that depending on the dimension this force constants are more or less anomalous. As the instabilities are larger in 1D, we clearly see that the 1D lattice is much more unstable at  $q = 2k_F$ , than the higher dimension systems. Indeed, at 3D there is no subtlety at  $q = 2k_F$ . This means that the 1D system has a much stronger tendency towards lattice instabilities than higher dimension systems. Indeed Peierls already said that the 1D lattice formed by a free electron gas was unstable at  $q = 2k_F$  and it should distort opening a gap in the electronic structure. This is what it is called a Peierls transition. At higher dimensions, however, it is not so clear if the electronic response function itself is capable of making the lattice unstable at  $q = 2k_F$  or more in general for  $\mathbf{q}$  points with Fermi surface nesting. Usually, other effects like the electron-phonon coupling are needed to make a higher dimension system unstable.

## 4 Dynamic response function of the free electron gas

In Sec. 1 we obtained the general expression of the non-interacting static response function (see Eq. (16)). As we have seen, the static limit of the response function is useful to analyze the effect of interactions that do not depend on time, or that reach an equilibrium state with the interaction turned on. That is why the potential imposed by the lattice and phonons can be derived from the static response function as described in Sec. 3. However, electromagnetic probes used to measure materials are often oscillating fields that impose a potential that depends explicitly on time, or in frequency. In this case the non-interacting response function should be calculated by Eq. (11).

Let's assume that at  $t = -\infty$  the Hamiltonian of the system is  $H_0$ , who is separable and we know its eigenvalues and eigenfrequencies. Then, the time-dependent interaction is turned on so that the Hamiltonian is changed to

$$H = H_0 + \delta V(t) e^{i\omega t}, \quad (41)$$

where  $\eta$  is a small positive number that ensures that at  $t = -\infty$  we recover  $H = H_0$ . In order to calculate the time-dependent density change,  $\delta n(\mathbf{r}, t)$ , we need to solve the time-dependent Schrödinger equation

$$i\hbar \frac{\partial |\Psi_i(t)\rangle}{\partial t} = (H_0 + \delta V(t)e^{\eta t}) |\Psi_i(t)\rangle. \quad (42)$$

We can expand the true eigenfunctions of  $H$  in the basis of the eigenfunctions of the time-dependent Schrödinger equation with  $\delta V = 0$ :

$$|\Psi_i(t)\rangle = \sum_j \alpha_{ij}(t) e^{-iE_j t/\hbar} |\psi_j\rangle. \quad (43)$$

Plugging this equation into Eq. (42), we obtain the following relation:

$$i\hbar \frac{\partial \alpha_{ij}(t)}{\partial t} = \sum_k \alpha_{ik}(t) e^{i(E_j - E_k - i\hbar\eta)t/\hbar} \langle \psi_j | \delta V(t) | \psi_k \rangle. \quad (44)$$

As we want to stick to lowest linear order in the interaction, we can assume that it is possible to make a Taylor expansion to the coefficients themselves so that at linear order

$$\alpha_{ij}(t) = \delta_{ij} + \overset{(1)}{\alpha}_{ij}(t). \quad (45)$$

Substituting this in Eq. (44) and keeping only linear terms on  $\overset{(1)}{\alpha}$  and  $\delta V$ , we see that

$$i\hbar \frac{\partial \overset{(1)}{\alpha}_{ij}(t)}{\partial t} = e^{i(E_j - E_i - i\hbar\eta)t/\hbar} \langle \psi_j | \delta V(t) | \psi_i \rangle. \quad (46)$$

This differential equation can be easily solved as

$$\overset{(1)}{\alpha}_{ij}(t) = -\frac{i}{\hbar} \int_{-\infty}^t d\tau e^{i(E_j - E_i - i\hbar\eta)\tau/\hbar} \langle \psi_j | \delta V(\tau) | \psi_i \rangle, \quad (47)$$

so that at lowest order the perturbed time-dependent wave function is

$$|\Psi_i(t)\rangle = e^{-iE_i t/\hbar} |\psi_i\rangle - \frac{i}{\hbar} \sum_j \delta n(\mathbf{r}, t) = |\psi_j\rangle. \quad (48)$$

With the time-dependence of the wave functions described at linear order, we can proceed to evaluate the time-dependent change in the density:

$$\delta n(\mathbf{r}, t) = \sum_i f_i \Psi_i^*(\mathbf{r}, t) \Psi_i(\mathbf{r}, t) - \sum_i f_i \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}). \quad (49)$$

Substituting Eq. (48) here, we obtain at linear order in  $\delta V$  the following change in density:

$$\delta n(\mathbf{r}, t) = \frac{i}{\hbar} \sum_{ij} (f_i - f_j) e^{i(E_j - E_i)t/\hbar} \psi_j^*(\mathbf{r}) \psi_i(\mathbf{r}) \int_{-\infty}^t d\tau e^{-i(E_j - E_i + i\hbar\eta)\tau/\hbar} \langle \psi_i | \delta V(\tau) | \psi_j \rangle \quad (50)$$

Calculating the Fourier transform of it we obtain

$$\delta n(\mathbf{r}, \omega) = \sum_{ij} \frac{f_j - f_i}{\hbar\omega + E_j - E_i + i\hbar\eta} \langle \psi_i | \delta V(\omega) | \psi_j \rangle \psi_j^*(\mathbf{r}) \psi_i(\mathbf{r}). \quad (51)$$

We can now calculate the non-interacting response function easily following Eq. (11), which yields

$$\chi^0(\mathbf{r}, \mathbf{r}', \omega) = \sum_{ij} \frac{f_j - f_i}{\hbar\omega + E_j - E_i + i\hbar\eta} \psi_i^*(\mathbf{r}') \psi_i(\mathbf{r}') \psi_j^*(\mathbf{r}) \psi_i(\mathbf{r}) \quad (52)$$

and precisely coincides with the static non-interacting response function of Eq. (16) in the  $\omega = 0$  limit.

The dynamical non-interacting response function that we have obtained is valid for any  $H_0$  Hamiltonian that has independent electrons, in other words, which is separable. This is the case, for instance, in the free electron case, where  $H_0$  is simply the kinetic energy of the electrons and the wave functions are plane-waves, as well as in density-functional theory (DFT), where  $H_0$  is the Kohn-Sham Hamiltonian and the wave functions the Kohn-Sham states.

#### 4.1 Dynamic Lindhard response function in 3D

As mentioned above in the free electron gas we have  $\psi_i(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$  as the wave functions, where  $V$  is the total volume of the crystal and the good quantum number is the wave number. Plugging this into Eq. (52) and Fourier transforming we obtain the dynamic Lindhard function in 3D:

$$\chi^0(\mathbf{q}, \omega) = \frac{1}{V} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{\hbar\omega + E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}} + i\hbar\eta}. \quad (53)$$

Due to the presence of the small positive number  $\eta$  that ensures causality, the non-interacting response function is complex. This makes more complicated than in the static case the calculation of the sum over  $\mathbf{k}$  points. The real part of the result is the following [2]:

$$\Re \chi^0(\mathbf{q}, \omega) = \frac{k_F m}{2\pi^2 \hbar^2} \left[ -1 + \frac{4(q/k_F)^2 - q_-^4}{8(q/k_F)^3} \ln \left| \frac{1 + q_-^2/(2q/k_f)}{1 - q_-^2/(2q/k_f)} \right| - \frac{4(q/k_F)^2 - q_+^4}{8(q/k_F)^3} \ln \left| \frac{1 + q_+^2/(2q/k_f)}{1 - q_+^2/(2q/k_f)} \right| \right], \quad (54)$$

where  $q_{\pm}^2 = \hbar\omega/E_F \pm (q/k_F)^2$ . The analytic part of the imaginary is rather complex (see Ref. [2]), but it is easy to understand what its meaning is. From Eq. (53) and using the formal identity

$$\lim_{\eta \rightarrow 0} 1/(a \pm i\eta) = \mathcal{P}(1/a) \mp i\pi\delta(a), \quad (55)$$

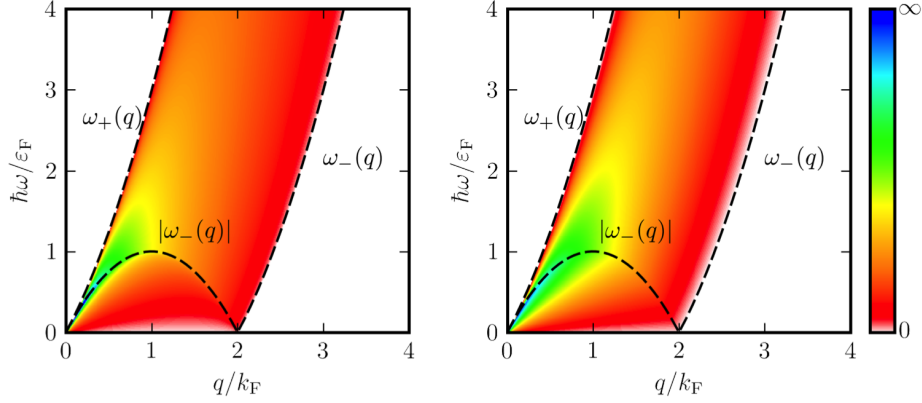


Figure 3:  $\Im\mathbf{\chi}^0(\mathbf{q}, \omega)$  for the free electron gas in 2D (left panel) and 3D (right panel). Figure taken from Ref. [1].

where  $\mathcal{P}$  denotes the principal value, we see that

$$\Im\mathbf{\chi}^0(\mathbf{q}, \omega) = -\pi \frac{1}{V} \sum_{\mathbf{k}} (f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}) \delta(\hbar\omega + E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}}) \quad (56)$$

so that it will be non-zero only when the energy transfer from the external probe,  $\hbar\omega$ , excites one electron with energy  $E_{\mathbf{k}}$  to an empty state at  $E_{\mathbf{k}-\mathbf{q}}$ , or the other way around. Due to the parabolic band dispersion, in the free electron case this is limited to

$$\frac{\hbar^2 q^2}{2m} - \frac{\hbar^2 k_F q}{m} \leq \hbar\omega \leq \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2 k_F q}{m}. \quad (57)$$

In this range the imaginary part of the Lindhard response function will be non-zero, as shown in Fig. 4.1.

## 4.2 Dynamic Lindhard response function in 2D

In the 2D case

$$\chi^0(\mathbf{q}, \omega) = \frac{1}{A} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{\hbar\omega + E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}} + i\hbar\eta}. \quad (58)$$

A tedious calculation [2] yields

$$\Re\epsilon\chi^0(\mathbf{q}, \omega) = \frac{m}{\pi\hbar^2} \left[ -1 - \text{sgn}(q_-^2) \theta(|q_-^2|/(2q/k_F) - 1) \frac{k_F}{q} \sqrt{\left| \frac{q_-^2}{2q/k_F} \right|^2 - 1} \right. \\ \left. + \text{sgn}(q_+^2) \theta(|q_+^2|/(2q/k_F) - 1) \frac{k_F}{q} \sqrt{\left| \frac{q_+^2}{2q/k_F} \right|^2 - 1} \right], \quad (59)$$

for the real part of the dynamical response function. The imaginary part is also non-zero exclusively for the region determined in Eq. (57). In Fig. 4.1 the imaginary part is shown as a color plot.

### 4.3 Dynamic Lindhard response function in 1D

In the 1D case

$$\chi^0(q, \omega) = \frac{1}{L} \sum_k \frac{f_k - f_{k-q}}{\hbar\omega + E_k - E_{k-q} + i\hbar\eta}. \quad (60)$$

A tedious calculation [2] yields

$$\Re\chi^0(q, \omega) = \frac{m}{\pi\hbar^2q} \left[ \ln \left| \frac{1 + q_-^2/(2q/k_F)}{1 - q_-^2/(2q/k_F)} \right| - \ln \left| \frac{1 + q_+^2/(2q/k_F)}{1 - q_+^2/(2q/k_F)} \right| \right], \quad (61)$$

for the real part of the dynamical response function. The imaginary part is also non-zero exclusively for the region determined in Eq. (57).

## 5 Plasmon dispersion of the free electron gas in 3D and 2D

A plasmon is a collective excitation of the electrons of the system, different from electron-hole excitations. A plasmon, consequently, can be defined as the capacity of the electron system to create an induced electric field without any external perturbation. Inverting Eq. (10) we see that, in Fourier space, we have

$$\delta V_{ext}(\mathbf{q}, \omega) = \epsilon(\mathbf{q}, \omega) \delta V(\mathbf{q}, \omega). \quad (62)$$

Thus, we can have a plasmon excitation, that is non-vanishing induced potential  $\delta V$ , if the dielectric function vanishes. In practice, we need that the real part of the dielectric function vanishes, but if the imaginary part is non-zero, the plasmon excitation will be damped and as it will decay into electron-hole excitations.

Fourier transforming Eq. (10) we obtain for the free electron gas, where dependence on the position only is on  $\mathbf{r} - \mathbf{r}'$ ,

$$\epsilon^{-1}(\mathbf{q}, \omega) = 1 + v_c(\mathbf{q})\chi(\mathbf{q}, \omega), \quad (63)$$

with  $v_C(\mathbf{q})$  the Fourier transform of the Coulomb potential. At linear order, this gives

$$\epsilon(\mathbf{q}, \omega) = 1 - v_c(\mathbf{q})\chi(\mathbf{q}, \omega). \quad (64)$$

or

$$\epsilon(\mathbf{q}, \omega) = 1 - v_c(\mathbf{q})\chi^0(\mathbf{q}, \omega). \quad (65)$$

for the free electron gas, as  $\chi^0 = \chi$  in this case. Thus, in order to obtain plasmon dispersion relations we need to solve the  $1 - v_c(\mathbf{q})\chi^0(\mathbf{q}, \omega) = 0$  equation in the free electron case.

In order to solve that equation for the 3D and 2D free electron gas, it is good to note that the Fourier transform of the Coulomb potential is the following:

$$v_c(\mathbf{q}) = \frac{4\pi e^2}{q^2} \quad (66)$$

in the 3D case, while

$$v_c(\mathbf{q}) = \frac{2\pi e^2}{q} \quad (67)$$

in the 2D case. In the 1D limit the Fourier transform of the Coulomb potential is not well defined, so we will not consider the 1D plasmon dispersion.

In the  $q \rightarrow 0$  limit (Exercise 4) for the 3D case the plasmon dispersion that is obtained is the following:

$$\omega(\mathbf{q}) = \omega_p + \frac{3v_F^2}{10\omega_p^2} q^2, \quad (68)$$

where

$$\omega_p = \sqrt{\frac{4\pi e^2 n}{m}} \quad (69)$$

is the plasma frequency of the 3D electron gas that depends on the square root of the electronic density. As we can see, at  $\mathbf{q} = 0$  long wave-length limit, there is a collective plasmonic excitation precisely at the plasma energy. This is the excitation that precisely gives color to bulk metals. Then, the plasmon shows a quadratic dispersion, until it enters into the region in which the imaginary part of the dielectric is non-zero and it decays. In the 2D case (Exercise 5) instead, there is no collective excitation that survives in the  $\mathbf{q} = 0$  long wave-length limit, but the plasmon disperses as  $\sim \sqrt{q}$  with the following equation:

$$\omega(\mathbf{q}) = \sqrt{\frac{2\pi n e^2}{m} q + \frac{3}{4} v_F^2 q^2}. \quad (70)$$

This shows that the plasmon dispersion of a free electron gas is intrinsically different depending on the dimension of the system. Since in the 2D case the dispersion is linear at very small wave number, the 2D free electron gas is often named as the “acoustic plasmon”. This has implications on the optical properties of materials, and, it is sometimes claimed, that the presence of a very low energy plasmonic excitation may play an important role in the coupling with other excitations of lower energies, like phonons. In Fig.

## References

- [1] Marco Gibertini. Ground-state properties of inhomogeneous graphene sheets, 2009. PhD thesis.
- [2] Bogdan Mihaila. Lindhard function of a d-dimensional fermi gas, 2011.

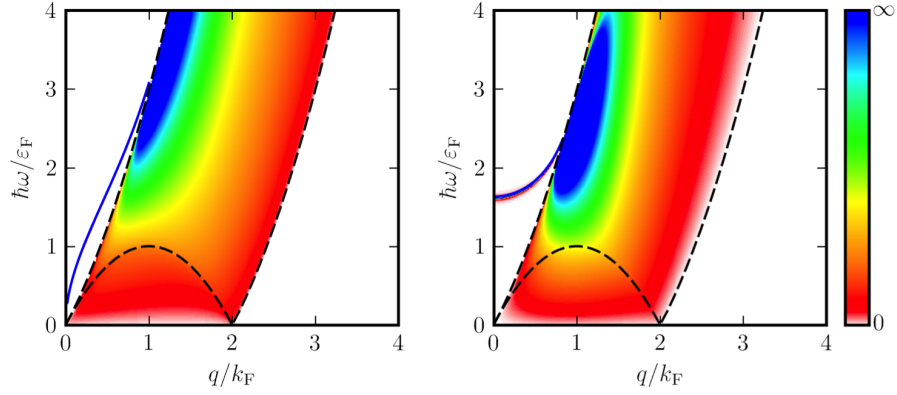


Figure 4: Plasmon dispersion together for the free electron gas in 2D (left panel) and 3D (right panel). The plasmon decays when it enters in the electron-hole excitation continuum. Figure taken from Ref. [1].

## 6 Exercises

1. Show that the Lindhard function for the 2D electron gas is the one given in Eq. (29). The following integral may be useful:

$$\int_0^{2\pi} d\phi \frac{1}{q^2 - 4k^2 \cos^2 \phi} = \begin{cases} \frac{2\pi}{|q|\sqrt{q^2 - 4k^2}} & , q > 2k \\ 0 & , q \leq 2k \end{cases}. \quad (71)$$

2. Show that the Lindhard function for the 1D electron gas is the one given in Eq. (31).
3. Discuss the singularities of the static Lindhard function in 1D, 2D, and 3D.
4. Show that the plasmon dispersion in the 3D electron gas in the long wavelength limit is given by Eq. (68).
5. Show that the plasmon dispersion in the 2D electron gas in the long wavelength limit is given by Eq. (70).