Microscopic Response

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Outline

- Introduction
- Dielectric Response Function
- Density Response Function
- Response in surfaces: An introduction.
- Conclusions

Introduction

Plasmons: Simplest Model

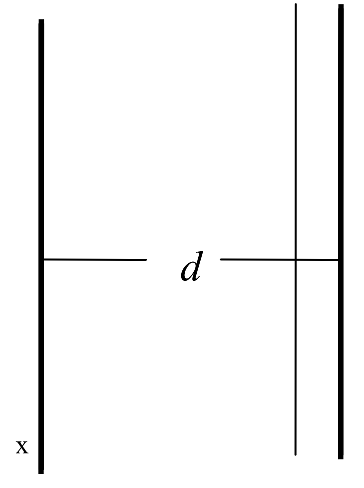
$$E(x) = -4\pi Nex, \qquad x << d : \text{ Thickness of the a slab}$$

Surface charge on the either end of the condensed is Nex

An electron inside the slab obeys the equation of motion:

$$m\ddot{x} = eE(x) = -4\pi Ne^2 x$$

$$\ddot{x} + \omega_p^2 x = 0, \qquad \omega_p^2 = \frac{4\pi Ne^2}{m}$$

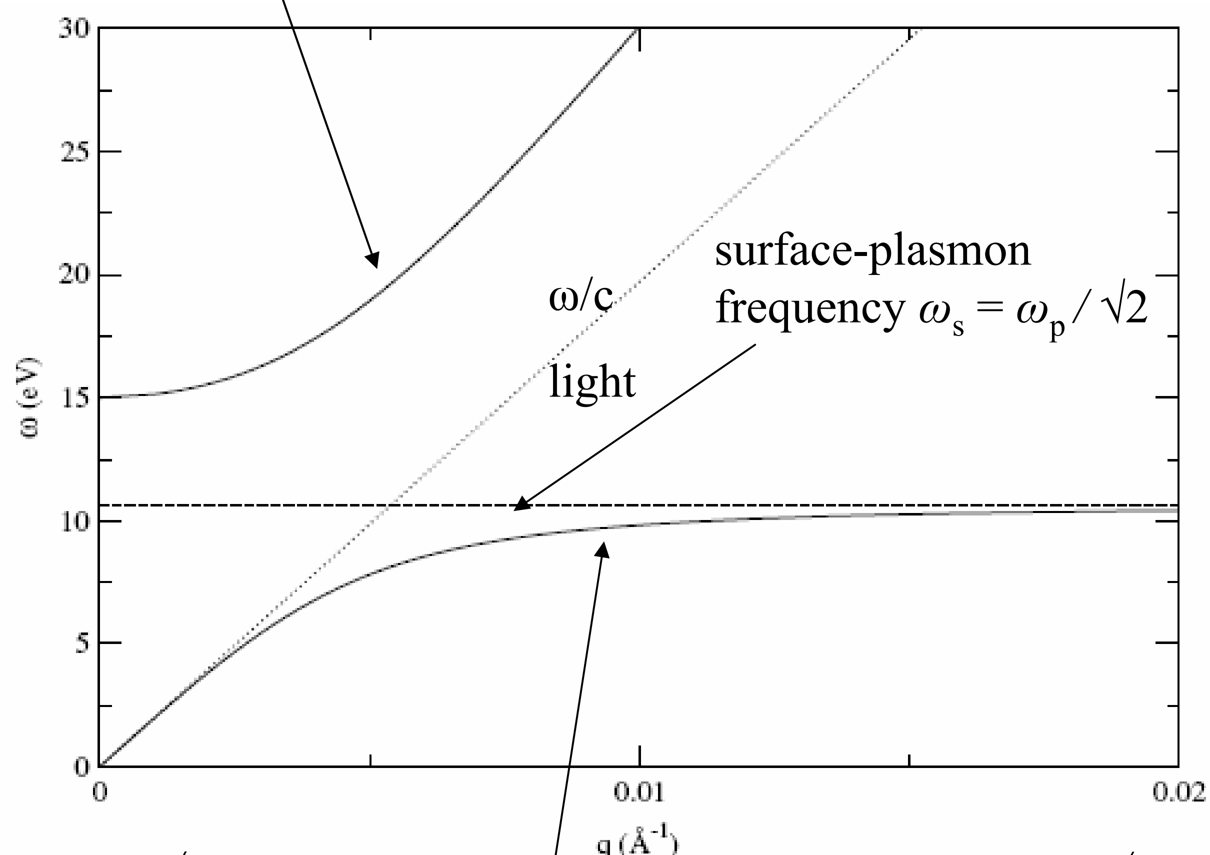


The slab will oscilate at frequency ω_p

Neglects random motion of electrons and is valid only in the limit of very long wavelength oscilations

Dispersion relation

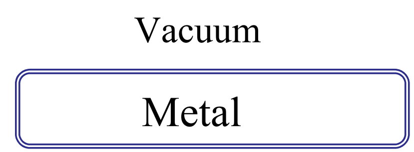
the dispersion of light in the solid



$q < \omega_s / c$
retarded

surface-plasmon polariton

$q >> \omega_s / c$
nonretarded



$$q(\omega) = \frac{\omega}{c} \sqrt{\frac{\omega^2 - \omega_p^2}{2\omega^2 - \omega_p^2}}$$

$\omega_p = 15$ eV:

Dielectric Response Function

D(**r**,t)$\rightarrow$ $Div\vec{D}(\vec{r},t) = 4\pi z\rho_e(\vec{r},t)$ (1)

$z\rho_e$(**r**,t): Density of external charge

$\mathbf{E}_p$(**r**,t)$\rightarrow$ $Div\vec{E}_p(\vec{r},t) = 4\pi e\langle\delta n(\vec{r},t)\rangle$ (2)

e‹δn(**r**,t)›:Density of polariced charge

The electric field inside of the sistem:

E(**r**,t)=**D**(**r**,t) + $\mathbf{E}_p$(r,t) (3)

then

$$Div\vec{E}(\vec{r},t) = 4\pi\left[z\rho_e(\vec{r},t) + e\langle\delta n(\vec{r},t)\rangle\right] \quad (4)$$

Let us take the Fourier transform in space and time of (1) , (4):

$$i\vec{q}.\vec{D}(\vec{q},\omega) = 4\pi z\rho_e(\vec{q},\omega) \quad (5)$$

$$i\vec{q}.\vec{E}(\vec{q},\omega) = 4\pi\left[z\rho_e(\vec{q},\omega) + e\langle\delta n(\vec{q},\omega)\rangle\right] \quad (6)$$

In linear response theory the relation between the displacement and electric field when the medium is homogeneous and isotropic can be written as:

$$\vec{D}(\vec{r},t) = \int \varepsilon(\vec{r}-\vec{r}\,',t-t')E(\vec{r}\,',t')d^3\vec{r}dt' \qquad (7)$$

Non local.

For external fields sufficiently weak the Fourier transform of the relation between **D** and **E** is:

$$\vec{E}(\vec{q},\omega) = \frac{\vec{D}(\vec{q},\omega)}{\varepsilon(\vec{q},\omega)} \qquad (8)$$

With the relations (5), (6) and (8) is possible to obtain:

$$\varepsilon(\vec{q},\omega) = 1 + \frac{4\pi i e\langle \delta n(\vec{q},\omega)\rangle}{\vec{q}.\vec{E}(\vec{q},\omega)} \tag{9}$$

$$\frac{1}{\varepsilon(\vec{q},\omega)} - 1 = -\frac{4\pi i e\langle \delta n(\vec{q},\omega)\rangle}{\vec{q}.\vec{D}(\vec{q},\omega)} \tag{10}$$

In absence of an external charge, (5) and (6) can be written as:

$$\varepsilon(\vec{q},\omega)\vec{q}.\vec{E}(\vec{q},\omega) = 0 \tag{11}$$

$$i\vec{q}.\vec{E}(\vec{q},\omega) = 4\pi e\langle \delta n(\vec{q},\omega)\rangle \tag{12}$$

Two solutions:

$$\vec{q}.\vec{E}(\vec{q},\omega) = 0 \qquad \rightarrow \langle \delta n(\vec{q},\omega)\rangle = 0$$

But for frequencies ω_q such that:

$\varepsilon(\vec{q},\omega_q) = 0$ Free oscilations of the charge density

In the presence of the test charge, the response of the sistem can be expressed as:

$$\varepsilon(\vec{q},\omega) = 1 - \frac{4\pi e^2}{q^2}\chi(\vec{q},\omega)$$

$$\chi(\vec{q},\omega) = \frac{\langle \delta n(\vec{q},\omega)\rangle}{\varphi_{tot}(\vec{q},\omega)}$$:Density response function

χ depends only on the sistem properties in absence of the test Charge.

Density-response function

- N interacting electrons

External perturbation $\qquad \phi^{\mathrm{ext}}(\vec{r},\omega)$

$$\delta n(\vec{r},\omega) = \int d\vec{r}\,'\chi(\vec{r},\vec{r}\,';\omega)\phi^{ext}(\vec{r},\omega)$$

Inducen electron density

$$\chi(\vec{r},\vec{r}\,',\omega) = \sum_n \rho^*_{n0}(\vec{r})\rho_{0n}(\vec{r}\,')\left[\frac{1}{E_0 - E_n + \hbar(\omega + i\eta)} - \frac{1}{E_0 + E_n + \hbar(\omega + i\eta)}\right]$$

*χ(**r**, **r**; ω)* represents the so-called density-response function of the many-electron system

$$\rho_{0n}(\vec{r}) = \langle \Psi_0 \left| \rho(\vec{r}) - \rho_0(\vec{r}) \right| \Psi_n \rangle$$

Ψ_n interacting electron sistem wavefunction

It’s not possible to calculate

<u>RPA</u> approximation (time dependence-Hartree approx)

$$\chi(\vec{r},\vec{r}',\omega) \rightarrow \chi^0(\vec{r},\vec{r}',\omega)\left[\phi^{ext}(\vec{r},\omega) + \delta\phi^H(\vec{r},\omega)\right]$$

$$\delta\phi^H(\vec{r},\omega) = \int d\vec{r}'v(\vec{r},\vec{r}')\delta n(\vec{r}',\omega); v(\vec{r},\vec{r}') : \text{bare coulomb interaction}$$

$$\delta n(r,\omega) = \int d\vec{r}'\chi^0(r,r',\omega)x\left[\phi^{ext}(r,r',\omega) + \int d\vec{r}''v(r',r'')\delta n(r'',\omega)\right]$$

Then is possible to obtain Dyson-type equation for the *interacting* density-response function:

$$\chi(\vec{r},\vec{r}\,',\omega) = \chi^0(\vec{r},\vec{r}\,',\omega) + \int d\vec{r}_1 \int d\vec{r}_2 \chi^0(\vec{r},\vec{r}_1,\omega) v(\vec{r}_1,\vec{r}_2) \chi(\vec{r}_2,\vec{r}\,',\omega)$$

Where $\chi^0(r,r',\omega)$ denotes the density-response function of noninteracting Hartree electrons:

$$\chi^0(\vec{r},\vec{r}\,',\omega) = \frac{2}{\Omega} \sum_{i,j} (f_i - f_j) \frac{\psi_i(\vec{r})\psi_j^*(\vec{r})\psi_j(\vec{r}\,')\psi_i^*(\vec{r}\,')}{\omega - \varepsilon_j + \varepsilon_i + i\eta}$$

f_i are Fermi-Dirac ocupation factors, Which at zero temperature take the form $f_i = \theta(\varepsilon_F - \varepsilon_i)$, ε_F is the Fermi energy and the single particule state and energy ψ_i, ε_i are eigenfunctions and eigenvalues of Hartree Hamiltonian, The poles of the χ are given by:

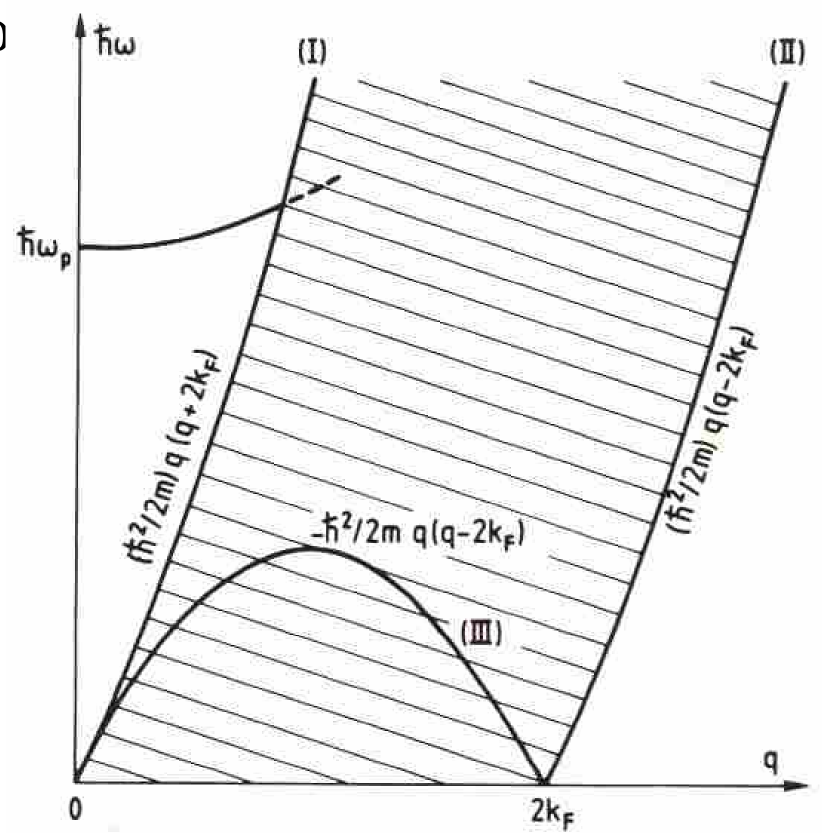
$$\hbar\omega = \pm(E_{k+q} - E_k) = \pm(\frac{\hbar^2 \vec{q}.\vec{k}}{m} + \frac{\hbar^2 q^2}{2m})$$

And, physically correspond to the creation and annihilation of the electron-hole pair with energy $\hbar\omega$

For a fixed value of **q** this leads to:

$$-\frac{\hbar^2}{2m} q(q + 2K_f) < \hbar\omega < -\frac{\hbar^2}{2m} q(q - 2K_f)$$

$$\frac{\hbar^2}{2m} q(q - 2K_f) < \hbar\omega < -\frac{\hbar^2}{2m} q(q + 2K_f)$$

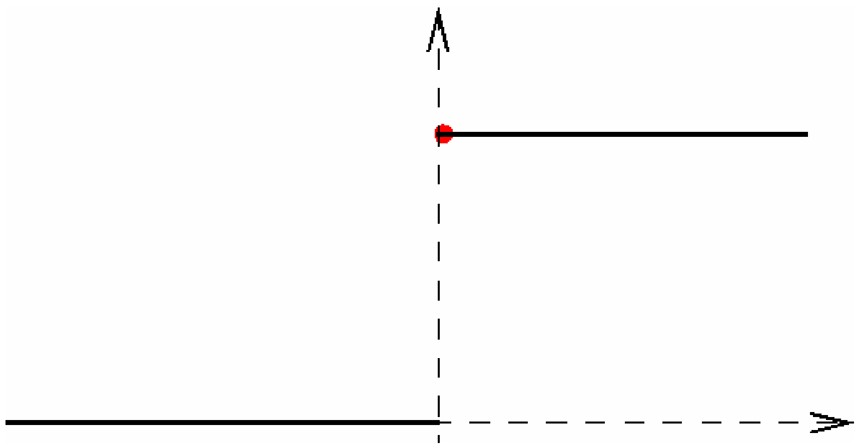


Bulk Plasmon dispersion curve; the hatched area shows the region wrere the plasmons decay into electron-hole pair excitations.

Surfaces Response: *Jellium surface*

In the case of a free-electron gas bounded by a semi-infinite positivebackground of density

$$n_+(z) = \begin{cases} \bar{n}, & z \leqslant 0, \\ 0, & z > 0, \end{cases}$$



Another key quantity in the description of electronic excitations in a many-electron system is the complex screened interaction *W(**r**, **r**;ω)*:

$$W(r, r'; \omega) = v(r, r') + \int \mathrm{d}r_1 \int \mathrm{d}r_2 v(r, r_1)\, \chi(r_1, r_2; \omega)\, v(r_2, r')$$

Where *v(**r**,**r**')* is the bare Coulomb potential translationally invariance in the plane of the surface allows one to define the 2D Fourier transform $W(z, z'; q,\omega)$ which can be obtained as follows:

$$W(z,z';\vec{q},\omega) = v(z,z';\vec{q}) + \int dz_1 \int dz_2 v(z,z_1,\vec{q})\chi(z_1,z_2;\vec{q})v(z_2,z';\vec{q})$$

where $v(z, z'; \mathbf{q})$ is the 2D Fourier transform of the bare Coulomb interaction $v(\mathbf{r}, \mathbf{r})$:

$$v(z, z'; q) = \frac{2\pi}{q} \mathrm{e}^{-q|z-z'|},$$

and $\chi(z, z'; q,\omega)$ denotes the 2D Fourier transform of the interacting density-response function $\chi(\mathbf{r}, \mathbf{r}; \omega)$.

In the framework of TDDFT the density response function can be written as:

$$\chi(z, z'; q, \omega) = \chi^0(z, z'; q, \omega) + \int \mathrm{d}z_1 \int \mathrm{d}z_2\, \chi^0(z, z_1; q, \omega) \times \{v(z_1, z_2; q) + f_{\mathrm{xc}}[n_0](z_1, z_2; q, \omega)\}\, \chi(z_2, z'; q, \omega),$$

where $\chi_0(z, z'; q,\omega)$ denote the 2D Fourier transforms of the noninteracting density-response function $\chi_0(\mathbf{r}, \mathbf{r}; \omega)$ and $f_{xc}[n_0](z, z'; \mathbf{q},\omega)$ is asociated with exchange-correlation energy.

noting that the single-particle orbitals $\psi_i(\mathbf{r})$ now take the form:

$$\psi_{\boldsymbol{k},i}(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_\parallel}\, \psi_i(z),$$

It’s possible to find:

$$\chi^0(z,z',\vec{q},\omega)=\frac{2}{A}\sum_{i,j}\psi_i(z)\psi_j^*(z)\psi_j(z')\psi_i^*(z')\sum_k \frac{f_{k,i}-f_{k+q,j}}{E_{k,i}-E_{k+q,j}+\omega+i\eta}$$

where $E_{k,i}=\varepsilon_i+\frac{k^2}{2}$

Conclusions

- In the non retarded region the many body interaction are very important.
- The response of the sistem of interacting many electrons to an external potential can be describing by ε, χ.
- This formalism can give information about the excititation states of many body interacting sistems.
- It`s possible to study the dispersion relation of mny diferent sistems
- The physical means of the poles can be diferent depend

References

[1] Rep. Prog. Phys. 70 (2007) 1–87; J M Pitarke, V M Silkin, E V Chulkov, P M Echenique.

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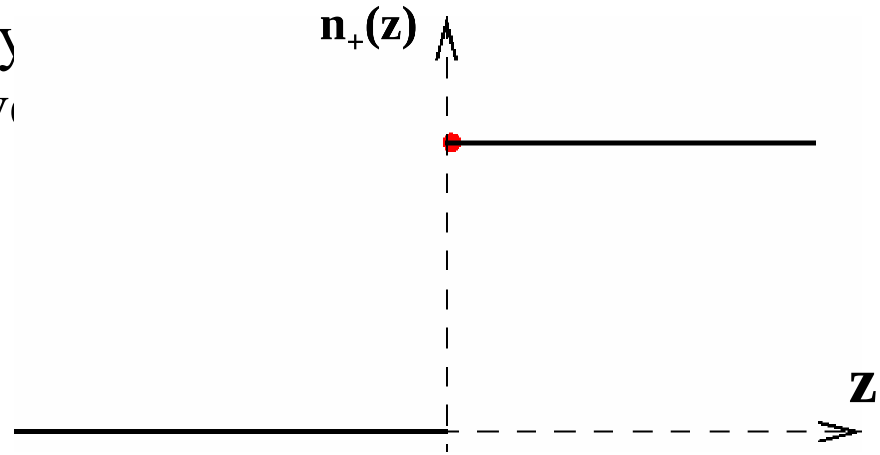
Semi-infinite Jellium model

- The ion cores are remplaced by uniform background of positive charge



$$n^+(r) = \begin{cases} \overline{n}, & z \le 0 \\ 0, & z > 0 \end{cases}$$

Spatial average of the ion charge distribution