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Calculation of optical response function of inhomogeneous Fermi systems in the local density approximation

SH. FARAMARZI*, EZZEDDIN MOHAJERANI[a], HOSEIN AGHAHOSENI
Amir Kabir University of Technology, Department of Physics, Hafez Street, Tehran, Iran
[a]*University of Shahid Beheshti, Laser Research Institute, Evin Street, Tehran, Iran*

It is calculated the longitudinal dielectric function and optical response function of the valence electrons (metalic electrons) as a Fermi system in the local density approximation.

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1. Introduction

The study of the optical and electronic properties of many-electron systems is one of the noticeable subjects of current research in nonlinear optics, nanophotonics, spintronic, condensed matter and plasma physics.

A lot of experimental and theoretical works have been devoted to the study of photon interaction with the valance electrons of free and embedded simple metal clusters (metallic electrons) as Fermi systems. In the following atomic units are used unless otherwise specified and k_B is the Boltzman's constant. a_0 =0.529 Å is the Bohr radius and e denotes the absolute electron charge.

2. Calculation of longitudinal dielectric function in Fermi systems

The longitudinal dielectric function of an electron gas in quantum mechanical treatment of electrons was obtained by Lindhard [5].

$$\varepsilon^l(q,\omega) = 1 + \frac{2m^2\omega_0^2}{\hbar^2 q^2}\sum_n \frac{f(E_n)}{N}\left(\frac{1}{q^2 + 2\vec{q}.\vec{q}_n - \frac{2m}{\hbar}\left(\omega + \frac{i\gamma}{\hbar}\right)} + \frac{1}{q^2 - 2\vec{q}.\vec{q}_n + \frac{2m}{\hbar}\left(\omega + \frac{i\gamma}{\hbar}\right)}\right) \quad (1)$$

If $N = \sum_n f(E_n)$ is the total number of electrons, $\omega_0 = \left(\frac{4\pi e^2 n_0}{m}\right)^{\frac{1}{2}}$ is the classical resonance frequency of the gas and n_0 is the equilibrium particle density.

We assume that the damping is equal to zero, $\gamma = 0$, so one gets:

$$\varepsilon^l(q,\omega) = 1 + \frac{2m^2\omega_0^2}{\hbar^2 q^2}\sum_n \frac{f(E_n)}{N}\left(\frac{1}{q^2 + 2\vec{q}.\vec{q}_n - \frac{2m}{\hbar}\omega} + \frac{1}{q^2 - 2\vec{q}.\vec{q}_n + \frac{2m}{\hbar}\omega}\right) \quad (2)$$

by using ω_0^2 in the Eq. (2) one obtains :

$$\varepsilon^l(q,\omega) = 1 + \frac{2m}{\hbar^2 q^2}\frac{4\pi e^2}{v}\sum_n f(E_n)\left(\frac{1}{q^2 + 2\vec{q}.\vec{q}_n - \frac{2m}{\hbar}\omega} + \frac{1}{q^2 - 2\vec{q}.\vec{q}_n + \frac{2m}{\hbar}\omega}\right) \quad (3)$$

For $L \to \infty$ one has

$$\sum_n = \sum_{n_x}\sum_{n_y}\sum_{n_z} \to \int dn_x \int dn_y \int dn_z \quad (4)$$

By using the relation between the momentum and the wave vector $\vec{p} = \hbar\vec{q}$ with $|\vec{q}| = \frac{n\pi}{L}$ we have:

$$p_x = \frac{2\pi\hbar}{L}n_x \qquad p_y = \frac{2\pi\hbar}{L}n_y \qquad p_z = \frac{2\pi\hbar}{L}n_z \quad (5)$$

So:

$$dn_x = \frac{L}{2\pi\hbar}dp_x \quad dn_y = \frac{L}{2\pi\hbar}dp_y \quad dn_z = \frac{L}{2\pi\hbar}dp_z \quad (6)$$

and

$$dn_x\, dn_y\, dn_z = \left(\frac{L}{2\pi\hbar}\right)^3 dp_x\, dp_y\, dp_z \quad (7)$$

By using Eq. (7), the Eq.(3) can be rewritten as:

$$\varepsilon^l(q,\omega) = 1 + \frac{2m}{\hbar^2}\frac{4\pi e^2}{q^2}(2\pi\hbar)^{-3}\int d^3\vec{p}\, f(E_n)\left\{\frac{1}{q^2 + 2\vec{q}.\vec{q}_n - \frac{2m}{\hbar}\omega} + \frac{1}{q^2 - 2\vec{q}.\vec{q}_n + \frac{2m}{\hbar}\omega}\right\} \quad (8)$$

Where $f(E_n) = \frac{1}{e^{\beta(\varepsilon_n - \mu)} + 1} = n_F(p)$ is the Fermi-Dirac function which depends on momentum $\vec{p}$ only through the electronic energy $\varepsilon_p = \frac{p^2}{2m} = \frac{\hbar^2 q^2}{2m}$, $\beta = \frac{1}{k_B T_e}$ and μ_F is the Fermi chemical potential .

We can rewrite the Eq. (8) as:

$$\varepsilon^l(q,\omega) = 1 + 2.\frac{4\pi e^2}{q^2}(2\pi\hbar)^{-3}\int d^3\vec{p}\, n_F(\vec{p}) \left\{\frac{1}{\frac{\hbar^2}{2m}(\vec{q}+\vec{q}_n)^2 - \frac{\hbar^2 q_n^2}{2m} - \hbar\omega} + \frac{1}{\frac{\hbar^2}{2m}(\vec{q}-\vec{q}_n)^2 - \frac{\hbar^2 q_n^2}{2m} + \hbar\omega}\right\} \quad (9)$$

By using:

$$\begin{cases} \frac{\hbar^2}{2m}(\vec{q}_n \pm \vec{q})^2 = \varepsilon_{\vec{p}\pm\hbar\vec{q}} \\ \frac{\hbar^2}{2m} q_n^2 = \varepsilon_{\vec{p}} \end{cases} \quad (10)$$

one has

$$\varepsilon^l(q,\omega) = 1 + 2.\frac{4\pi e^2}{q^2}(2\pi\hbar)^{-3}\int d^3\vec{p}\, n_F(\vec{p}) \left\{\frac{1}{\varepsilon_{\vec{p}+\hbar\vec{q}} - \varepsilon_{\vec{p}} - \hbar\omega} + \frac{1}{\varepsilon_{\vec{p}-\hbar\vec{q}} - \varepsilon_{\vec{p}} + \hbar\omega}\right\} \quad (11)$$

We displace $\vec{p} \equiv \vec{p} - \hbar\vec{q}$ in the second term of Eq. (11) so:

$$\varepsilon^l(q,\omega) = 1 + 2.\frac{4\pi e^2}{q^2}(2\pi\hbar)^{-3}\int \left\{\frac{n_F(\vec{p})}{\varepsilon_{\vec{p}+\hbar\vec{q}} - \varepsilon_{\vec{p}} - \hbar\omega} + \frac{n_F(\vec{p}+\hbar\vec{q})}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\hbar\vec{q}} + \hbar\omega}\right\} d^3\vec{p} \quad (12)$$

and then:

$$\varepsilon^l(q,\omega) = 1 + 2.\frac{4\pi e^2}{q^2}(2\pi\hbar)^{-3}\int \left\{\frac{n_F(\vec{p}) - n_F(\vec{p}+\hbar\vec{q})}{\varepsilon_{\vec{p}+\hbar\vec{q}} - \varepsilon_{\vec{p}} - \hbar\omega}\right\} d^3\vec{p} \quad (13)$$

Again, we displace momentum $\vec{p} \equiv \vec{p} + \hbar\vec{k}$ in Eq. (13):

$$\varepsilon^l(q,\omega) = 1 - 2.\frac{4\pi e^2}{q^2}(2\pi\hbar)^{-3}\int \left\{\frac{n_F(\vec{p}) - n_F(\vec{p}+\hbar\vec{q})}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\hbar\vec{q}} - \hbar\omega}\right\} d^3\vec{p} \quad (14)$$

we can rewrite the Eq. (14) as:

$$\varepsilon^l(q,\omega) = 1 - V(\vec{q})\chi_0(\vec{q},\omega) \quad (15)$$

where

$$V(q) = \frac{4\pi e^2}{q^2}$$

$$\chi_0(\vec{q},\omega) = 2.(2\pi\hbar)^{-3}\int \left\{\frac{n_F(\vec{p}) - n_F(\vec{p}+\hbar\vec{q})}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\hbar\vec{q}} - \hbar\omega}\right\} d^3\vec{p} \quad (16)$$

are respectively, the Fourier transform of the Coulomb energy potential and the non-interacting retarded density correlation function.

The Eq. (16) can be rewritten as:

$$\chi_0(\vec{q},\omega) = \lim_{\eta\to 0}(2\pi\hbar)^{-3}.2.\int \left\{\frac{n_F(\vec{p}) - n_F(\vec{p}+\hbar\vec{q})}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\hbar\vec{q}} - \hbar\omega - i\eta}\right\} d^3\vec{p} \quad (17)$$

By using the usual rule (Plemelj formula)

$$\lim_{\eta\to 0}\left(\frac{1}{z - i\eta}\right) = P\frac{1}{z} + i\pi\delta(z)$$

one obtains the imaginary part of the longitudinal dielectric function from Eq.(14)

$$\varepsilon_l''(\vec{q};\omega) = \frac{V(q)}{4\pi^2\hbar^3}\int [\delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\hbar\vec{q}} + \hbar\omega) - \delta(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\hbar\vec{q}} - \hbar\omega)] n_F(\vec{p}) d^3\vec{p} \quad (18)$$

by using $n_F(\vec{p})$ in equation (18) we have:

$$\varepsilon_l''(\vec{q};\omega) = \frac{mV(q)}{\pi\hbar^4 q}\int_{p-}^{p+} \frac{pdp}{e^{\beta(\varepsilon_p - \mu_F)} + 1} \quad (19)$$

where:

$$p_\pm = \frac{m}{\hbar q}\left|\varepsilon_q \pm \hbar\omega\right|$$

By calculating the integral in Eq. (19) one gets the imaginary part of the longitudinal dielectric function of a Fermi system at a definite temperature $T_e \neq 0$ [12]:

$$\varepsilon_l''(\vec{q};\omega) = \frac{m^2 V(q)}{2\pi\hbar^4\beta q}\ln\left[\frac{1 + e^{-\beta(\varepsilon_- - \mu_F)}}{1 + e^{-\beta(\varepsilon_+ - \mu_F)}}\right] \quad (20)$$

where

$$\varepsilon_\pm = \frac{p_\pm^2}{2m}$$

For $T_e = 0$ one has:

$$\varepsilon_l''(\bar{q};\bar{\omega}) = \frac{\bar{\kappa}\bar{Y}}{\bar{k}}\begin{cases} \bar{\omega}; & 0 \le \bar{\omega} \le 2\bar{q} - \bar{q}^2; \quad \bar{q} \prec 2 \\ 1 - \frac{1}{4}\left[\bar{q} - (\bar{\omega}/\bar{q})\right]^2; & 2\bar{q} - \bar{q}^2 \le \bar{\omega} \le 2\bar{q} + \bar{q}^2; \bar{q} < 2 \\ 0; & \bar{\omega} \succ 2\bar{q} + \bar{q}^2; \quad \bar{q} \prec 2 \\ 1 - \frac{1}{4}\left[\bar{q} - (\bar{\omega}/\bar{q})\right]^2; & \bar{q}^2 - 2\bar{q} \le \bar{\omega} \le 2\bar{q} + \bar{q}^2; \quad \bar{q} > 2 \end{cases}$$

(21)

with the dimensionless quantities: $\bar{q} = \frac{q}{q_F}$, $\bar{\omega} = \frac{\hbar\omega}{E_F}$, $\bar{Y} = \frac{E_{pot}}{E_{kin}} = (\frac{e^2}{r_s})/(\frac{\hbar^2 q^2}{2m})$ and

$\overline{\kappa} = \frac{1}{2\chi}$ with $\chi = \left[\frac{4}{9\pi}\right]^{\frac{1}{3}}$. This result is normally found in textbooks [2,9].

This result can be rewritten as (see also Fig. 1of [12] and Fig. 12.9 of [9])

$$\varepsilon_l''(\overline{q};\overline{\omega}) = \frac{\overline{\kappa}\overline{Y}}{\overline{q}} \begin{cases} 1-\frac{1}{4}[\overline{q}-(\overline{\omega}/\overline{q})]^2; & -1+\sqrt{1+\overline{\omega}} \le \overline{q} \le 1-\sqrt{1-\overline{\omega}}; \quad \overline{\omega} < 1 \\ \overline{\omega}; & 1-\sqrt{1-\overline{\omega}} \le \overline{q} \le 1+\sqrt{1-\overline{\omega}}; \quad \overline{\omega} \prec 1 \\ 1-\frac{1}{4}[\overline{q}-(\overline{\omega}/\overline{q})]^2; & 1+\sqrt{1-\overline{\omega}} \le \overline{q} \le 1+\sqrt{1+\overline{\omega}}; \quad \overline{\omega} < 1 \\ 1-\frac{1}{4}[\overline{q}-(\overline{\omega}/\overline{q})]^2; & -1+\sqrt{1+\overline{\omega}} \le \overline{q} \le 1+\sqrt{1+\overline{\omega}}; \quad \overline{\omega} > 1 \end{cases} \tag{22}$$

3. Calculation of response function

Optical response of the valence electrons is treated quantum-mechanically.Within the so-called local density approximation we have the imaginary part of the response function [12] as:

$$\mathrm{Im}\left[\chi^0(R;\omega)\right] = \frac{4\pi}{R}\int_0^\infty \mathrm{Im}\left[\chi^0(q;\omega)\right]\sin(qR)dq \tag{23}$$

with:

$$\mathrm{Im}\left[\chi^0(q;\omega)\right] = -\frac{\varepsilon_l''(\overline{q};\overline{\omega})}{V(q)} \tag{24}$$

where $V(q) = \frac{4\pi e^2}{q^2}$ is the Fourier transform of the coulomb energy potential .

So we can rewrite the Eq. (23) as:

$$\mathrm{Im}\left[\chi^0(R;\omega)\right] = -\frac{1}{\mathrm{Re}^2}\int_0^\infty \varepsilon_l''(\overline{q};\overline{\omega})q^2\sin(qR)dq \tag{25}$$

by using Eq.(22) in the Eq.(25) one has:

$$Im\left[\chi^0(R;\omega)\right] = -\frac{\overline{\kappa}\overline{Y}}{Re^2}\left\{\begin{aligned} & k_F^3\int_{-1+\sqrt{1+\overline{\omega}}}^{1-\sqrt{1-\overline{\omega}}}\overline{q}\left[1-\frac{1}{4}\left(\overline{q}-\frac{\overline{\omega}}{\overline{q}}\right)^2\right]\sin(k_F R\overline{q})d\overline{q} \\ & + k_F^3\int_{1-\sqrt{1-\overline{\omega}}}^{1+\sqrt{1-\overline{\omega}}}\overline{q}\,\overline{\omega}\sin(k_F R\overline{q})d\overline{q} \\ & + k_F^3\int_{1+\sqrt{1-\overline{\omega}}}^{1+\sqrt{1+\overline{\omega}}}\overline{q}\left[1-\frac{1}{4}\left(\overline{q}-\frac{\overline{\omega}}{\overline{q}}\right)^2\right]\sin(k_F R\overline{q})d\overline{q} \end{aligned}\right\}$$

$$\overline{\omega} < 1 \tag{26}$$

By some calculations we can get the following result for the imaginary part of the response function (for $\overline{\omega} < 1$):

$$\mathrm{Im}\left[\chi^0(R;\omega)\right] = -\frac{\overline{\kappa}\overline{Y}}{\mathrm{Re}^2}k_F^3\,\frac{1}{2}\sin(k_F R\overline{q})\left\{\begin{aligned} & \left(\sqrt{1+\overline{\omega}}-\sqrt{1-\overline{\omega}}\right)(3+2\overline{\omega}) + \left((1-\overline{\omega})^{\frac{3}{2}}-(1+\overline{\omega})^{\frac{3}{2}}\right) + \\ & \frac{1}{2}\overline{\omega}^2\ln\left(\frac{\left(\sqrt{1-\overline{\omega}}+1\right)\left(\sqrt{1+\overline{\omega}}-1\right)}{\left(1+\sqrt{1+\overline{\omega}}\right)\left(1-\sqrt{1-\overline{\omega}}\right)}\right) + \overline{\omega}\left(1-\overline{\omega}+4\sqrt{1-\overline{\omega}}\right) \end{aligned}\right\}$$

$$\overline{\omega} < 1 \tag{27}$$

By using Eq. (22) one has the Eq. (25) for $\overline{\omega} \succ 1$ as:

$$\mathrm{Im}\left[\chi^0(R;\omega)\right] = -\frac{\overline{\kappa}\overline{Y}}{\mathrm{Re}^2}k_F^3\int_{-1+\sqrt{1+\overline{\omega}}}^{1+\sqrt{1+\overline{\omega}}}\overline{q}\left[1-\frac{1}{4}\left(\overline{q}-\frac{\overline{\omega}}{\overline{q}}\right)^2\right]\sin(k_F R\overline{q})d\overline{q}$$

$$\overline{\omega} > 1 \tag{28}$$

So the result for the imaginary part of the response function (for $\overline{\omega} > 1$) is:

$$\mathrm{Im}\left[\chi^0(R;\omega)\right] = -\frac{\overline{\kappa}\overline{Y}}{\mathrm{Re}^2}k_F^3\,\frac{1}{2}\sin(k_F R\overline{q})\left\{\sqrt{1+\overline{\omega}}(3+\overline{\omega}) - (1+\overline{\omega})^{\frac{3}{2}} + \frac{1}{2}\overline{\omega}^2\ln\left(\frac{\sqrt{1+\overline{\omega}}-1}{\sqrt{1+\overline{\omega}}+1}\right)\right\}$$

$$\overline{\omega} > 1 \tag{29}$$

4. Conclusion

In this paper we have calculated the imaginary part of longitudinal dielectric function and also the imaginary part of the optical response function for a quantum many electron systems. These results can be used in nanophotonics for the study of optical properties of nanometals and the optical response of simple metal clusters.

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*Corresponding author: f7611913@cic.aut.ac.ir