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Dynamical equation determining plasmon energy spectrum in a metallic slab

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Abstract

On the basis of general principles of electrodynamics and quantum theory we have elaborated the quantum field theory of plasmons in the plane metallic slab with a finite thickness by applying the functional integral technique. A hermitian scalar field φ was used to describe the collective oscillations of the interacting electron gas in the slab and the effective action functional of the system was established in the harmonic approximation. The fluctuations of this scalar field φ around the background one φ_0 corresponding to the extreme value of the effective action functional are described by the fluctuation field ζ generating the plasmons. The dynamical equation for this fluctuation field was derived. The solution of the dynamical equation would determine the plasmon energy spectrum.

Keywords: plasmon, plasmonic, functional integral, collective oscillation, fluctuation Classification numbers: 3.00, 5.04

1. Introduction

During the last two decades, a new scientific discipline called plasmonics has emerged and has rapidly developed [1, 2]. At the present time it has extended into a large area of experimental and theoretical research works. In particular, significant scientific results were achieved in the study of plasmonic molecular resonance coupling [3–15], plasmonically enhanced fluorescence [16-22] and plasmonic nanoantennae [23-30]. To explain experimental data or to guide the experimental research works, different phenomenological quantum theories were proposed. Recently an attempt was performed to construct a unified quantum theory of plasmonic processes and phenomena-the theoretical quantum plasmonics, starting from general principles of electrodynamics and quantum theory [31-33]. In these theoretical works, for simplicity the authors have limited to the case of the homogeneous interacting electron gas in the whole three-dimensional physical space. However, in practice we always deal with the electron gas in metallic media with boundaries. The purpose of the present work and the subsequent ones is to generalize the calculations in previous works [31-33] to the case of the electron gas in a plane metallic slab with a finite thickness.

The formulation of the problem is presented in section 2, and a general form of the dynamical equation for the fluctuation quantum field ζ is proposed. In section 3 the effective action functional of the interacting electron gas in the metallic slab is established in the harmonic approximation, and the derivation of the proposed dynamical equation for the fluctuation field ζ is demonstrated. The Fourier transformation of this dynamical equation is performed in section 4. As the final result we obtain the system of homogeneous linear integral equations for the Fourier components of the fluctuation field ζ . The conclusion and discussions are presented in section 5.

2. Formulation of the problem

Consider a plane metallic slab with the small thickness d and choose the orthogonal coordinate system such that the axis Oz is perpendicular to the plane of this slab and the coordinate

(cc)





Figure 1. Plane metallic slab in the orthogonal coordinate system Oxyz.

plane xOy is located in its middle. As usual, in the quantization of the electron motion inside the slab, we consider a rectangular box with the vertical side d and two horizontal square bases of the side L, and impose on the electron wave functions the periodic boundary conditions along the directions of the Ox and Oy axes. Denote

$$R = (\mathbf{r}, z; t) = (x, y, z; t)$$
(1)

the four-dimensional coordinate vector of a point in the spacetime and choose the center of the box to be the origin O of the coordinate system, as this represented in following figures 1 and 2.

Suppose that the electron motion along the Oz axis and those along all directions in the coordinate plane xOy are independent, and consider electron wave functions of the form

$$u(\mathbf{r}, z; t) = u_{II}(\mathbf{r}; t)u_{\perp}(z; t) = u_{II}(x, y; t)u_{\perp}(z; t).$$
(2)

Wave functions of the horizontal motion must satisfy the following periodic boundary conditions

$$u_{II}(-L/2, y; t) = u_{II}(L/2, y; t),$$

$$u_{II}(x, -L/2; t) = u_{II}(x, L/2; t).$$
(3)

For simplicity, suppose that the metallic slab can be considered as a quantum well with the infinite depth: the potential energy of electron equals to zero inside the slab and becomes infinitely large outside the slab. Then the wave functions $u_{\perp}(z; t)$ must satisfy the vanishing boundary condition

$$u_{\perp}(-d/2; t) = u_{\perp}(d/2; t) = 0.$$
 (4)

Free election Hamiltonian has the following eigenvalues and eigenfunctions:

$$E_{II}(\mathbf{p}) = \frac{\mathbf{p}^2}{2m},$$

$$p_x = n_x \frac{2\pi}{L}, p_y = n_y \frac{2\pi}{L};$$
(5)



Figure 2. Projection of plane metallic slab with thickness d on a plane containing axis Oz.

$$\varepsilon_{v}^{(+)} = \frac{1}{2m} \left(v + \frac{1}{2} \right)^{2} \left(\frac{2\pi}{d} \right)^{2},$$

$$\varepsilon_{v}^{(-)} = \frac{1}{2m} v^{2} \left(\frac{2\pi}{d} \right)^{2};$$
 (6)

$$u_{\mathbf{p}}(\mathbf{r}) = \frac{1}{L}e^{i\mathbf{p}\mathbf{r}};\tag{7}$$

$$u_{\varepsilon_{\nu}^{(+)}} = \sqrt{\frac{2}{d}} \cos\left(\nu + \frac{1}{2}\right) \frac{2\pi}{d} z,$$

$$u_{\varepsilon_{\nu}^{(-)}} = \sqrt{\frac{2}{d}} \sin\nu \frac{2\pi}{d} z.$$
 (8)

The purpose of this work is to demonstrate that there exists a scalar hermitian quantum field $\zeta(R) = \zeta(\mathbf{r}, z;t)$ such that the energy spectrum of plasmons in the metallic slab is determined by a dynamical equation of the form

$$\int dR_2 A(R_1, R_2) \zeta(R_2) = 0, \qquad (9)$$

and to derive the explicit expression of the kernel $A(R_1, R_2)$.

3. Effective action functional in the harmonic approximation

Now we extend the method elaborated in the previous works [31–33], introduce the scalar field $\varphi(R)$ of collective oscillations of electrons and establish the effective action functional $I_0[\varphi]$ of the electron gas in the harmonic approximation. Denote

$$u(R_1 - R_2) = u(\mathbf{r}_1 - \mathbf{r}_2, z_1 - z_2)\delta(t_1 - t_2), \qquad (10)$$

where $u(\mathbf{r}_1-\mathbf{r}_2, z_1-z_2)$ is the potential energy of the Coulomb interaction between two electrons located at two points (\mathbf{r}_1 , z_1) and (\mathbf{r}_2 , z_2) in the metallic slab, and $S(R_1, R_2)$ the Green

function of non-interacting (i.e. without their mutual Coulomb repulsion) electrons. Then we have

$$A(R_1, R_2) = U(R_1 - R_2) + i \int dR_3 \int dR_4 U(R_1 - R_3) \times S(R_3, R_4) S(R_4, R_3) U(R_4 - R_2)$$
(11)

and

$$I_{0}[\phi] = -\int dR_{1} \int dR_{2} \phi(R_{1} - R_{2}) n(\mathbf{R}_{2}) + \frac{1}{2} \int dR_{1} \\ \times \int dR_{2} \phi(R_{1}) A(R_{1}, R_{2}) \phi(R_{2}),$$
(12)

where $n(\mathbf{R}_2)$ is the constant (time-independent) electron density. Functions $u(\mathbf{r}_1-\mathbf{r}_2, z_1-z_2)$ and $S(R_1, R_2)$ have following explicit expressions:

$$u(\mathbf{r}_{1} - \mathbf{r}_{2}, z_{1} - z_{2}) = \frac{e^{2}}{\varepsilon_{0} \Big[(\mathbf{r}_{1} - \mathbf{r}_{2})^{2} + (z_{1} - z_{2})^{2} \Big]^{1/2}}, \quad (13)$$

where e is the electron charge, ε_0 is the dielectric constant of the medium,

$$S(R_{1}, R_{2}) = S(\mathbf{R}_{1}, \mathbf{R}_{2}; t_{1} - t_{2}) = \frac{1}{2\pi} \int d\omega \ e^{-i\omega(t_{1} - t_{2})}$$

$$\times \sum_{\mathbf{p}, \varepsilon_{v}^{(\pm)}} u_{\mathbf{p}, \ \varepsilon_{v}^{(\pm)}}(\mathbf{R}_{1}) \ u_{\mathbf{p}, \ \varepsilon_{v}^{(\pm)}}(\mathbf{R}_{2})^{*}$$

$$\times \left[\frac{1 - n(\mathbf{p}, \ \varepsilon_{v}^{(\pm)})}{\omega - E(\mathbf{p}, \ \varepsilon_{v}^{(\pm)}) + io} + \frac{n(\mathbf{p}, \ \varepsilon_{v}^{(\pm)})}{\omega - E(\mathbf{p}, \ \varepsilon_{v}^{(\pm)}) - io} \right], \qquad (14)$$

$$u_{\mathbf{p}, \ \varepsilon_{\nu}^{(\pm)}}(\mathbf{R}) = u_{\mathbf{p}}(\mathbf{r})u_{\varepsilon_{\nu}^{(\pm)}}(z),$$

$$u_{\mathbf{p}}(\mathbf{r}) = \frac{1}{L}e^{i\mathbf{p}\mathbf{r}},$$

$$u_{\varepsilon_{\nu}^{(\pm)}}(z) = \sqrt{\frac{2}{d}}\cos\left(\sqrt{2m\varepsilon_{\nu}^{(\pm)}}z\right),$$

$$u_{\varepsilon_{\nu}^{(-)}}(z) = \sqrt{\frac{2}{d}}\sin\left(\sqrt{2m\varepsilon_{\nu}^{(-)}}z\right),$$
(15)

and $n(\mathbf{p}, \varepsilon_{\nu}^{(\pm)})$ is the occupation number at the corresponding quantum state of electron $0 \leq n(\mathbf{p}, \varepsilon_{\nu}^{(\pm)}) \leq 1$.

The expression in rhs of relation (11) contains the function

$$\Pi(R_1, R_2) = iS(R_1, R_2)S(R_2, R_1).$$
(16)

Using formula (14) of $S(R_1, R_2)$, after lengthy but standard analytical calculations we derive following formula

$$\Pi(R_{1}, R_{2}) = \Pi(\mathbf{r}_{1} - \mathbf{r}_{2}; z_{1}, z_{2}; t_{1} - t_{2})$$

$$= \sum_{\mathbf{k}} \sum_{\varepsilon_{v}^{(\pm)}} \sum_{\varepsilon_{v}^{(\pm)}} \frac{1}{2\pi} \int d\omega \ u_{\mathbf{k}}(\mathbf{r}_{1})$$

$$\times u_{\varepsilon_{v}^{(\pm)}}(z_{1}) \ u_{\varepsilon_{v}^{(\pm)}}(z_{1})^{*}e^{-i\omega t}$$

$$\times \widetilde{\Pi}(\mathbf{k}; \varepsilon_{v}^{(\pm)}, \varepsilon_{v'}^{(\pm)}; \omega) u_{\mathbf{k}}(\mathbf{r}_{2})^{*}$$

$$\times u_{\varepsilon_{v}^{(\pm)}}(z_{2})^{*} \ u_{\varepsilon_{v}^{(\pm)}}(z_{2})e^{i\omega t} , \qquad (17)$$

where

$$\tilde{\Pi}\left(\mathbf{k}; \, \varepsilon_{\nu}^{(\pm)}, \, \varepsilon_{\nu}^{(\pm)}; \, \omega\right) = \frac{1}{(2\pi)^2} \\ \times \int d\mathbf{p} \frac{1}{\omega - E\left(\mathbf{p} + \frac{\mathbf{k}}{2}\right) - \varepsilon_{\nu}^{(\pm)} + E\left(\mathbf{p} - \frac{\mathbf{k}}{2}\right) - \varepsilon_{\nu}^{(\pm)}} \\ \times \left\{ \left[1 - n\left(\mathbf{p} - \frac{\mathbf{k}}{2}, \, \varepsilon_{\nu}^{(\pm)}\right)\right] n\left(\mathbf{p} + \frac{\mathbf{k}}{2}, \, \varepsilon_{\nu}^{(\pm)}\right) - \left[1 - n\left(\mathbf{p} + \frac{\mathbf{k}}{2}, \, \varepsilon_{\nu}^{(\pm)}\right)\right] n\left(\mathbf{p} - \frac{\mathbf{k}}{2}, \, \varepsilon_{\nu}^{(\pm)}\right) \right\}.$$
(18)

4. Fourier transformation of dynamical equation

Formula (17) represents the Fourier transformation of the kernel $\Pi(R_1, R_2)$ of an integral operator. For the functions $U(R_1-R_2)$ and $A(R_1, R_2)$ we have similar formulae

$$U(R_{1} - R_{2}) = u(\mathbf{r}_{1} - \mathbf{r}_{2}, z_{1} - z_{2}) \,\,\delta(t_{1} - t_{2})$$

$$= \sum_{\mathbf{k}} \sum_{\varepsilon_{v}^{(\pm)}} \sum_{\varepsilon_{v}^{(\pm)}} \frac{1}{2\pi} \int d\omega \,\,u_{\mathbf{k}}(\mathbf{r}_{1}) u_{\varepsilon_{v}^{(\pm)}}(z_{1})$$

$$\times u_{\varepsilon_{v}^{(\pm)}}(z_{1})^{*} e^{-i\omega t}$$

$$\times \tilde{U}(\mathbf{k}; \,\varepsilon_{v}^{(\pm)}, \,\varepsilon_{v}^{(\pm)}) \,\,u_{\mathbf{k}}(\mathbf{r}_{2})^{*}$$

$$\times u_{\varepsilon_{v}^{(\pm)}}(z_{2})^{*} u_{\varepsilon_{v}^{(\pm)}}(z_{2}) e^{i\omega t} , \qquad (19)$$

where

$$\tilde{U}(\mathbf{k}; \varepsilon_{\nu}^{(\pm)}, \varepsilon_{\nu}^{(\pm)}) = \int d\mathbf{r}_{1} \int d\mathbf{r}_{2} \int dz_{1} \int dz_{2} \ u_{\mathbf{k}}(\mathbf{r}_{1})^{*} u_{\varepsilon_{\nu}^{(\pm)}}(z_{1})^{*} \\ \times u_{\varepsilon_{\nu}^{(\pm)}}(z_{1}) u(\mathbf{r}_{1} - \mathbf{r}_{2}, z_{1} - z_{2}) \\ \times u_{\mathbf{k}}(\mathbf{r}_{2}) u_{\varepsilon_{\nu}^{(\pm)}}(z_{2}) u_{\varepsilon_{\nu}^{(\pm)}}(z_{2})^{*},$$
(20)

and

$$A(R_1, R_2) = \sum_{\mathbf{k}} \sum_{\varepsilon_{\nu}^{(\pm)}} \sum_{\varepsilon_{\nu}^{(\pm)}} \frac{1}{2\pi} \int d\omega \ u_{\mathbf{k}}(\mathbf{r}_1) \ u_{\varepsilon_{\nu}^{(\pm)}}(z_1)$$
$$\times u_{\varepsilon_{\nu}^{(\pm)}}(z_1)^* e^{-i\omega t} \times \tilde{A}(\mathbf{k}; \varepsilon_{\nu}^{(\pm)}, \varepsilon_{\nu'}^{(\pm)}; \omega)$$
$$\times u_{\mathbf{k}}(\mathbf{r}_2)^* u_{\varepsilon_{\nu}^{(\pm)}}(z_2)^* \ u_{\varepsilon_{\nu}^{(\pm)}}(z_2) e^{i\omega t} \ . \tag{21}$$

Then the integral formula (11) is reduced to following algebraic relation

$$\tilde{A}\left(\mathbf{k}; \, \varepsilon_{\nu}^{(\pm)}, \, \varepsilon_{\nu}^{(\pm)}; \, \omega\right) = \tilde{U}\left(\mathbf{k}; \, \varepsilon_{\nu}^{(\pm)}, \, \varepsilon_{\nu'}^{(\pm)}\right) + \tilde{U}\left(\mathbf{k}; \, \varepsilon_{\nu}^{(\pm)}, \, \varepsilon_{\nu'}^{(\pm)}\right) \\
\times \tilde{\Pi}\left(\mathbf{k}; \, \varepsilon_{\nu}^{(\pm)}, \, \varepsilon_{\nu'}^{(\pm)}; \, \omega\right) \\
\times \tilde{U}\left(\mathbf{k}; \, \varepsilon_{\nu}^{(\pm)}, \, \varepsilon_{\nu'}^{(\pm)}\right).$$
(22)

Let us now perform the corresponding Fourier transformation of the quantum field $\zeta(R)$ in the dynamical equation (9):

$$\begin{aligned} \zeta(R) &= \sum_{\mathbf{k}} \sum_{\varepsilon_{v}^{(\pm)}} \sum_{\varepsilon_{v}^{(\pm)}} \frac{1}{2\pi} \int d\omega \ u_{\mathbf{k}}(\mathbf{r}) \ u_{\varepsilon_{v}^{(\pm)}}(z) \ u_{\varepsilon_{v}^{(\pm)}}(z)^{*} e^{-i\omega t} \\ &\times \tilde{\zeta}\Big(\mathbf{k}; \ \varepsilon_{v}^{(\pm)}, \ \varepsilon_{v'}^{(\pm)}; \ \omega\Big). \end{aligned}$$

$$(23)$$

Then the dynamical equation becomes

$$\sum_{\mathbf{k}} \sum_{\varepsilon_{v}^{(\pm)}} \sum_{\varepsilon_{v}^{(\pm)}} \frac{1}{2\pi} \int d\omega \ \tilde{A} \left(\mathbf{k}; \, \varepsilon_{v}^{(\pm)}, \, \varepsilon_{v'}^{(\pm)}; \, \omega \right) \\ \times \tilde{\zeta} \left(\mathbf{k}; \, \varepsilon_{v}^{(\pm)}, \, \varepsilon_{v'}^{(\pm)}; \, \omega \right) = 0.$$
(24)

By solving this system of linear homogeneous integral equations, we can calculate the plasmon frequency ω as a function of the quantum numbers **k**, *v* and *v'* of plasmons in the metallic slab with a finite thickness d.

5. Conclusion and discussions

In this work we have presented the general formulation of the quantum field theory of plasmons in a plane metallic slab with a finite thickness. Starting from the expression of the effective action functional of the electron collective oscillation field φ (*R*) we have derived the dynamical equation for the fluctuation quantum field ζ (*R*) in the form of a homogeneous linear integral equation. Then we performed the Fourier transformation and rewrote this equation in the form of a system of homogeneous linear integral equation for the fluctuation quantum field ζ . The comparison with experimental data requires the approximate numerical solution of this system of equations.

For the experimental study of physical processes and phenomena with the participation of plasmons, the most popular and powerful method is to investigate the electromagnetic processes with the presence of plasmons. In all these processes the photon–plasmon interaction plays a significant role. In solids there always exists the electron–phonon interaction leading to the plasmon–phonon coupling. The quantum theory of interacting plasmon–photon–phonon system in a metallic slab will be elaborated in subsequent works. Moreover, beside of conventional metallic conductors, there exists a particular two-dimensional conductor with excellent conduction properties: graphene [34–36]. The elaboration of quantum theory of plasmons in graphene would be a very interesting work.

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