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Simplified theory of the acoustic surface plasmons at the two-dimentional electron gas

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ABSTRACT

In the two-dimensional electron gas (2DEG), the system can be polarized by metal ions on the 2D surface, resulting in screening of Coulomb interaction between electrons. We calculate the 2D screened Coulomb interaction in Thomas–Fermi approximation and find that both electron–hole (e–h) and collective excitations occurring in the 2DEG can be described with the use of effective dielectric function, in the random-phase approximation (RPA). In this paper we show that the mode proportional to in-plane momentum, called acoustic surface plasmon (ASP), can appear in long-wavelength limit. We calculate ASP dispersion and determine the critical wave number and frequency for the ASP decay into e–h pair, and the velocity of ASP. Our result agrees qualitatively with previous ones in tendency.

1. Introduction

Low energy surface plasmon by collective motion of the surface of noble metals, such as Ag, Au and Cu, has been attracted long before because of its potential application in sensing, imaging, surface enhanced spectroscopy and catalysis [1].

In the two-dimensional electron gas (2DEG) the plasmon frequency ω is proportional to $\sqrt{q_\parallel}$ for small in-plane momentum $q_\parallel$ [2]. The $\sim\sqrt{q_\parallel}$ dispersion makes a distortionless propagation of nonmonochromatic signals inherently impossible, since the different frequencies components propagate at different velocities. This drawback can be overcome using a plasmon energy with a linear rather than a square root dispersion [3]. Such a mode, called an acoustic surface plasmon (ASP), was observed for a variety of noble and simple metal surface [4–8], and also for graphene grown on a metallic substrate [9,10]. The detail of ASP has been studied theoretically [3,11–16].

The ASP energy ω_{ASP} varies as [11]

$$\omega_{ASP} = \alpha\, v_F^{2D}\, q_\parallel, \tag{1}$$

for small in-plane momentum $q_\parallel$ with $\omega_{ASP} \to 0$ as $q_\parallel \to 0$, where v_F^{2D} is the 2D Fermi velocity and the coefficient α is only slightly larger than unity.

In this paper, we have shown that the appearance of ASP can be explained by taking into account the static Coulomb screening between the electrons on the bare metal surface. We have also calculated the critical frequency and the velocity of ASP comparing them with previous results.

2. Model

We consider a simplified model in which electrons comprise 2 DEG. The electrons of the 2 DEG move in a rather complicated potential. The periodic potential of the metal is represented in the effective-mass approximation in order to smooth out the microscopic structure of the metal. We use the simplest version of the effective-mass approximation where the electrons are assumed to have the mass which is characteristic of the conduction band minimum at the Brillouin zone center (Γ) neglecting nonparabolicity and coupling band extreme. On this potential the relatively slowly varying potential is superimposed. According to symmetry of the problem the electron motion is quasi-free in the x–y plane with the wave vector component $\mathbf{k}_\parallel$ and the energy $\hbar^2\mathbf{k}_\parallel^2/2m_{2D}$, where m_{2D} is the effective mass of the conduction electron.

This system can be considered to form a 2D state band with a 2D Fermi energy ε_F^{2D}. Within this model, one finds that both electron–hole (e–h) and collective excitations occurring within the

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2 DEG can be described with the use of a 2D dielectric function, which in the random-phase approximation (RPA) takes the form [11]:

$$\varepsilon_{eff}^{2D}(q_{\|}, \omega) = 1 - \bar{U}(q_{\|})\chi_{2D}^{0}(q_{\|}, \omega), \tag{2}$$

where $\bar{U}(q_{\|})$ is the 2D Fourier transform of the screened Coulomb interaction and $\chi_{2D}^{0}(q_{\|}, \omega)$ is the polarization function of a homogeneous 2 DEG [2]. For the discussion of the collective excitations it is necessary to consider the screened Coulomb interaction $\bar{U}(q_{\|})$ and the polarization function $\chi_{2D}^{0}(q_{\|}, \omega)$ in detail.

3. The screened potential

At the 2 DEG electrons can be scattered by electron–electron interaction (bare Coulomb interaction). Since the 2 DEG is polarizable, this bare interaction is screened.

We calculate this screened potential in Thomas–Fermi approximation. When we consider an electron in 2D system(x–y plane) 3D potential by induced charge resulting from the electron and the system polarization obeys the following Poisson equation:

$$\nabla^2\phi_{eff}^{3D}(\mathbf{r}) = -4\pi e\delta(\mathbf{r}) - 4\pi e n_{2D}(r_{\|})\delta(z), \tag{3}$$

where $r_{\|}$ is the 2D position coordinate in the x–y plane. The application of Thomas–Fermi approximation yields:

$$\frac{\hbar^2 k_F^2(r_{\|})}{2m_{2D}} = \varepsilon_F^{2D} - e\phi_{eff}^{2D}(r_{\|}),$$

and since sheet electron concentration is $n_{2D} = k_F^2/2\pi = m_{2D}\varepsilon_F^{2D}/\pi\hbar^2$, we obtain:

$$n_{2D}(r_{\|}) = -\frac{em_{2D}}{\pi\hbar^2}\phi_{eff}^{2D}(r_{\|}).$$

After substituting the above expression into Eq. (3), performing Fourier transformation lead to:

$$\left(q_{\|}^2 + q_z^2\right)\phi_{eff}^{3D}\left(q_{\|}, q_z\right) = 4\pi e - 2q_D\phi_{eff}^{2D}(q_{\|}), \tag{4}$$

with

$$q_D = 2m_{2D}e^2/\hbar^2.$$

The 2D effective potential is calculated from Eq. (4) using the following iterative method: In 0th approximation, neglecting the attribution from induced charge, we have

$$\phi_{eff}^{3D(0)}(q_{\|}, q_z) = \frac{4\pi e}{q_{\|}^2 + q_z^2}.$$

The Fourier transformation of q_z into coordinate representation gives:

$$\phi_{eff}^{3D(0)}(q_{\|}, z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dq_z e^{iq_z z}\phi_{eff}^{3D(0)}(q_{\|}, q_z) = \frac{2\pi e}{q_{\|}}e^{-q_{\|}|z|}.$$

Putting $z = 0$ in the above expression we obtain the following bare Coulomb potential:

$$\phi_{eff}^{2D(0)}(q_{\|}) = \phi_{eff}^{3D(0)}(q_{\|}, 0) = \frac{2\pi e}{q_{\|}}. \tag{5}$$

In next approximation substituting Eq. (5) into Eq. (4), and calculating in the same way, we have

$$\phi_{eff}^{2D(1)}(q_{\|}) = \frac{2\pi e}{q_{\|}}\left(1 - \frac{q_D}{q_{\|}}\right).$$

Repeating this, the resulting 2D screened Coulomb potential is obtained:

$$\phi_{eff}^{2D}(q_{\|}) = \frac{2\pi e}{q_{\|}}\left(1 - \frac{q_D}{q_{\|}} + \left(\frac{q_D}{q_{\|}}\right)^2 - \left(\frac{q_D}{q_{\|}}\right)^3 + \cdots\right) = \frac{2\pi e}{q_{\|} + q_D}.$$

From the above expression screened Coulomb interaction has the type

$$\bar{U}(q_{\|}) = \frac{2\pi e^2}{q_{\|} + q_D}. \tag{6}$$

4. The polarization function and 2D dielectric function

In the RPA the polarization function takes the form [2]:

$$\chi_{2D}^{0}(q_{\|}, \omega) = \frac{2}{A}\sum_{\mathbf{k}_{\|}}\frac{f_{\mathbf{k}_{\|}} - f_{\mathbf{k}_{\|}+\mathbf{q}_{\|}}}{\hbar\omega - \varepsilon_{\mathbf{k}_{\|}} + \varepsilon_{\mathbf{k}_{\|}+\mathbf{q}_{\|}} + i0^{+}}, \tag{7}$$

where the factor 2 is the sum versus spin variable of the electrons and A the area of x–y plane. $\varepsilon_{\mathbf{k}_{\|}} = \hbar^2\mathbf{k}_{\|}^2/2m_{2D}$ is energy of a electron with 2D effective mass m_{2D}, $\varepsilon_F = \hbar^2k_F^2/2m_{2D}$ is the Fermi energy (chemical potential) and $f_{\mathbf{k}_{\|}}$ denotes the Fermi distribution function

$$f_{\mathbf{k}_{\|}} = \frac{1}{\exp\left(\frac{\varepsilon_{\mathbf{k}_{\|}} - \varepsilon_F^{2D}}{kT}\right) + 1}.$$

For simplicity we want to discuss the polarization function in the zero-temperature limit. In this case the Fermi distribution function has simple form $f_{\mathbf{k}_{\|}} = \theta(k_F - |\mathbf{k}_{\|}|)$ with the Fermi wave vector $k_F = (2\pi n_{2D})^{1/2}$ and the unit step function $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x < 0$. From the polarization function given by Eq. (7) one derives for the real and imaginary parts of the $\chi_{2D}^{0}(q_{\|}, \omega)$

$$\begin{aligned}\mathrm{Re}\,\chi_{2D}^{0}(q_{\|}, \omega) &= \frac{m_{2D}k_F}{\pi\hbar^2 q_{\|}}\left\{-\frac{q_{\|}}{k_F} + \theta\left(\eta_+^2 - 1\right)\sqrt{\eta_+^2 - 1} - \mathrm{sgn}(\eta_-)\theta\left(\eta_-^2 - 1\right)\right.\\ &\left.\sqrt{\eta_-^2 - 1}\right\}\end{aligned} \tag{8}$$

and

$$\begin{aligned}\mathrm{Im}\chi_{2D}^{0}(q_{\|}, \omega) &= \frac{m_{2D}k_F}{\pi\hbar^2 q_{\|}}\left\{\theta\left(1 - \eta_+^2\right)\sqrt{1 - \eta_+^2} - \theta\left(1 - \eta_-^2\right)\sqrt{1 - \eta_-^2}\right\},\end{aligned} \tag{9}$$

with

$$\eta_{\pm} = \frac{\omega}{q_{\|}v_F^{2D}} \pm \frac{q_{\|}}{2k_F}. \tag{10}$$

Herein $v_F = \hbar k_F/m_{2D}$ denotes the Fermi velocity and $\mathrm{sgn}(x) = +1$ for $x > 0$ and -1 for $x < 0$.

Metal surface, such as Au(111), Ag(111) and Cu(111), can be considered to form a 2DEG with a 2D Fermi energy ε_F^{2D}(see Table 1 [14]).

Fig. 1 exhibit 2D dielectric function determined by Eqs. (2), (6), (8) and (9) corresponding to the (111) surfaces of Au, Ag and Cu. The real and imaginary parts of $\varepsilon_{eff}^{2D}(q_{\|}, \omega)$ are represented by dash-dotted and dashed line, respectively. The solid lines represent the effective 2D energy-loss function $-1/\pi\mathrm{Im}[1/\varepsilon_{eff}^{2D}(q_{\|}, \omega)]$. Here, we used the parameters of Table 1. In Fig. 1, (a), (b), (c) correspond to $q_{\|} = 0.02a_0^{-1}$, $q_{\|} = 0.04a_0^{-1}$, $q_{\|} = q_C = 0.058a_0^{-1}$ on Au(111) surface, (d), (e), (f) to $q_{\|} = 0.01a_0^{-1}$, $q_{\|} = 0.02a_0^{-1}$, $q_{\|} = q_C = 0.029a_0^{-1}$ on Ag