Second Quantization Model of Surface Plasmon Polariton at Metal Planar Surface

Dao Thi Thuy Nga¹, Nguyen Thi Phuong Lan² and Nguyen Ai Viet³

¹Han Thuyen high school, Bac Ninh City, Bac Ninh Province, Vietnam
²Hanoi Pedagogical University No.2, Nguyen Van Linh Street, Phuc Yen Town, Vinh Phuc Province, Vietnam
³Institute of Physics, Vietnam Academy of Science and Technology, 10 Dao Tan, Thu Le, Ba Dinh, Ha Noi, Vietnam

E-mail: daothuyngaht@gmail.com

Abstract. We study on surface plasmon polariton modes at a metal planar surface. A model effective Hamiltonian with two interaction parameters is proposed in the second quantized representation for system of surface plasmons and photon. Using the Bogoliubov transformation technique, the dispersion relations of surface plasmon polariton was calculated. The surface plasmon photon vertexes also are found. A simple second quantized Hamiltonian of surface polaritons was obtained and could be useful for further investigations more complex systems.

1. Introduction

The plasmon is a quasiparticle resulting from the quantization of plasma oscillations. Plasmons are collective oscillations of the free electron gas density. Plasmons can couple with a photon to create another quasiparticle called a plasmon-polariton. Surface plasmons are those plasmons that are confined to surfaces and that interact strongly with light resulting in a polariton. They occur at the interface of a vacuum and material with a small positive imaginary and large negative real dielectric constant (usually a metal or doped dielectric). They play an important role in Surface Enhanced Raman Spectroscopy (SERS), Surface Plasmon Energy Transfer (SET) and Forster Resonance Energy Transfer (FRET), and have numerous applications in plasmonics, nanotechnology and modern medical treatments [1-3]. In this work we investigate quantum theory of surface plasmons and plasmon-polariton.

2. Drude model for bulk plasmon polariton

Consider metal as consisting of plasma (free electrons as a gas of free charge) in an ionic background (atoms).Existing the plasma will lead to waves in electron density which can be quantized by introducing the quasiparticle plasmon. Plasmons will again interact with surrounding electromagnetic field (photons) and found a new type of quasiparticle plasmon-polariton. The concept of plasmon-polariton is again useful as it was for exciton-polariton and phonon-polariton in condensed mater physics. In the frame work of phenomenological Drude model for metal, the metals dielectric constant is

\[ \epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 - \omega_p^2 + i\gamma\omega}, \]
where $\gamma$ is the collision rate, $\omega_0$ is the frequency of restoring force, $\omega_p$ is the bulk plasma frequency, $\omega_p = \sqrt{\frac{ne^2}{\varepsilon_0 m}}$ in which $n$ is the density, $\varepsilon_0$ is the vacuum permittivity and $m$ is effective electron mass.

For simplicity we take the case of $\omega_0 = 0$ (no restoring force), and $\gamma \approx 0$ small collision rate, now the dielectric constant of a metal equals to

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}. \quad (2)$$

Bulk plasmon polariton is related to the bulk oscillations of plasma-like medium. The propagation of light through a bulk medium is governed by Maxwell’s equations. In the case of plane wave with the wave vector $\vec{k}$, and a source-free isotropic medium, the equation $\text{div}\vec{D} = 0$ gives $\epsilon(\omega).(\vec{k}.\vec{E}) = 0$, which has the two solutions:

i) the first solution $\epsilon(\omega) = 0$ is associated to longitudinal modes $\omega = \omega_p$ where the gas of electrons oscillates as a collective whole;

ii) the second solution $(\vec{k}.\vec{E}) = 0$ is the transversality condition which yields, with the help of the Maxwell’s equations $\text{rot}\vec{H} = \partial\vec{D}/\partial t$ and $\text{rot}\vec{E} = -\partial\vec{B}/\partial t$.

$$\epsilon(\omega)\omega^2 = c^2 k^2. \quad (3)$$

where $c$ is the speed of light in vacuum. Replacing equation (2) into equation (3) we found the dispersion relation for the transverse bulk plasmon polariton

$$\omega = \sqrt{\omega_p^2 + c^2 k^2}. \quad (4)$$

Using plasmon energy $\omega_p$ as the energy unit and $\omega_p/c$ as the momentum unit, the dispersion relation of bulk plasmon polaritons in metals is presented in the figure 1.

![Figure 1. The dispersion relation of bulk plasmon polariton.](image-url)

For $\omega > \omega_p$ bulk plasmon polaritons can propagate. In the large $k$ limit, $\omega_p \rightarrow ck$ the photon in vacuum dispersion line. Frequency interval below plasma frequency $0 < \omega < \omega_p$ is the highly damped range, in which no propagation.
3. Drude model for surface plasmon polariton

Surface plasmon polariton (SPP) often referred simply as surface plasmons that are electromagnetic surface waves (photons) bound to the metal/dielectric interfaces. Physically, surface plasmon polaritons may be thought of as a collective oscillation of charge carriers in the conducting layer, with the result that the energy is transferred parallel to the interface. The SPP is by definition the solution of Maxwell’s equations describing an electromagnetic surface wave with lateral extensions evanescently decaying on either side of the interface. A plane wave with TE polarization (s-polarization) with its electric field parallel to the interface merely results in a motion of the electric charges parallel to the interface involving no restoring forces of the charges, and consequently no wave can propagate along the interface. For a TM-polarized wave (p-polarization) with its magnetic field vector parallel to the interface, the electric field has a non-null perpendicular component which results in the accumulation of electric charges at the interface. In this case, a restoring force is created because the charges are trapped inside the solid resulting in the formation of a propagating surface wave with the charges moving along the interface in the direction of propagation. The wave equation leads to a dispersion relation for plasmon polariton which depends on the dielectric constant. Solving the Maxwell’s equations at the metal/dielectric planar interface (for simplicity we take the case of metal/vacuum interface), the dispersion relation for surface plasmons propagating on the interface when coupled to transverse magnetic (TM) illumination (photon) is

\[ c_k = \omega \sqrt{\epsilon(\omega) / (1 + \epsilon(\omega))}, \]  

(5)

With Drude model, this dispersion relation can be rewritten in an explicit form

\[ \omega_D(k) = \sqrt{c^2 k^2 + \omega_p^2 / 2} - \sqrt{c^4 k^4 + \left(\omega_p^2 / 2\right)^2}. \]  

(6)

The dispersion relation of surface plasmon polariton \( \omega_D(k) \) in the Drude model is presented in the figure 2.

For small \( k \) surface plasmon polariton is photon like, for large \( k \) it is surface plasmon like with strong coupling of mechanical and electromagnetic wave. In the large \( k \) limit, \( \omega_p \rightarrow \omega_p / \sqrt{2} \) surface plasmon like dispersion relation. Frequency gap between the bulk and surface plasmon \( \omega_p / \sqrt{2} < \omega < \omega_p \) is highly damped range, in which no propagation.

4. Second quantized Hamiltonian Model for surface plasmon polariton

In analogy the cases of exciton plariton and phonon polariton, we consider a Hamiltonian model for surface plasmon polariton in second quantization form

\[ H = \sum_k \mathcal{H}_k = \sum_k \omega_n k a_k^+ a_k + E_{pk} c_k^+ c_k + g_k (a_k^+ c_k + c_k^+ a_k), \]  

(7)

where \( a \) and \( a^+ \), \( c \) and \( c^+ \) are annihilation-creation photon and surface plasmon operators corresponding to momentum \( k \), respectively; \( \omega_n k = c \) is the photon energy, \( E_{pk} = \omega_p / \sqrt{2} \) is the surface plasmon energy.

We denote \( g_k \) is the plasmon-photon transition vertex (or coupling constant). This vertex is absence in traditional plasmon theory because plasmon is longitudinal excitation, while photon is transversal excitation. For surface plasmon, we consider plasmon-photon transition vertex is not equal zero, and being a main parameter of our theory. Using the Feynman diagram technique, we can express the plasmon polariton in the random phase approximation (RPA) as the sum in the figure 3.
5. Bogoliubov Transformations
We use the Bogoliubov transformation technique taken from superconductivity theory to diagonalization plasmon polariton Hamiltonian

$$H_k = \sum_k \omega_{ik} \gamma_{ik}^+ \gamma_{ik},$$  \hspace{1cm} (8)

where $\gamma_{ik}$ and $\gamma_{ik}^+$ are the annihilation and creation plasmon polariton operators with momentum $k$ and $i$ is branch number: $i = 1$ for lower and $i = 2$ for upper branch.

The transformations with condition $u_k^2 + \nu_k^2 = 1$ are

$$\gamma_{1k} = u_k a_k + \nu_k c_k, \quad \gamma_{2k} = -\nu_k a_k + u_k c_k.$$  \hspace{1cm} (9)
Using the commutation relations for annihilation and creation operators
\[ [a_k, a^+_k] = 1, [c_k, c^+_k] = 1, [\gamma_k, \gamma^+_k] = 1, \text{ and zero for others}, \]
by standard calculation as in [4] we found the plasmon polariton energies
\[ \omega_{ik} = \frac{1}{2} \left[ (\omega_{\gamma k} + E_{pk}) + (-1)^i \sqrt{(\omega_{\gamma k} - E_{pk})^2 + 4g^2_k} \right]. \tag{10} \]
The upper branch is lying in the energy gap where damping is high. We take the lower branch for surface plasmon polariton dispersion relation
\[ \omega_{SP}(k) = \omega_{1k} = \frac{1}{2} \left[ (ck + \frac{\omega_p}{\sqrt{2}}) - \sqrt{(ck - \frac{\omega_p}{\sqrt{2}})^2 + 4g^2_k} \right]. \tag{11} \]
The surface plasmon polariton dispersion relation \( \omega_{SP} \) depends on wave vector \( k \) and coupling constant \( g \) is presented in the figure 4.

![Figure 4](image)

**Figure 4.** The surface plasmon polariton dispersion relation \( \omega_{SP} \) depends on wave vector \( k \) and coupling constant \( g \).

The surface plasmon polariton dispersion relation \( \omega_{SP} \) depends on wave vector \( k \) and coupling constant \( g = 0, 0.1, 0.2, 0.3 \) is presented in the figure 5.

The full picture of bulk and surface plasmon polariton dispersion relation \( \omega_{SP} \) depends on wave vector \( k \) and coupling constant \( g = 0, 0.1, 0.2, 0.3 \) with photon and surface plasmon guide lines is presented in the figure 6.

The figure 6 shows that the simple two bands model of surface plasmon polariton might be good in the most important bottom neck region but may be fare in the long wave limit \( k = 0 \).

6. **Comparison with experiment**
We compare our simple two-bands plasmon polariton model with reflection experiment in InSb [5] and Ag [6]. The comparison between the theoretical dispersion relation of surface plasmon
Figure 5. The surface plasmon polariton dispersion relation \( \omega_{SP} \) depends on wave vector \( k \) and coupling constant \( g = 0, 0.1, 0.2, 0.3 \).

Figure 6. The full picture of bulk and surface plasmon polariton dispersion relation \( \omega_{SP} \) depends on wave vector \( k \) and coupling constant \( g = 0, 0.1, 0.2, 0.3 \) with photon and surface plasmon guide lines.
polariton with the fitting value of plasmon-photon coupling constant $g_k = 0.1 \omega_p$, and experiment data of a) InSb (dotted line), and b) Ag (dashed line, lower line is Drude and $g$ with $k$-dependence) are presented in the figure 7.

![Graph](image)

**Figure 7.** The comparison between the theoretical dispersion relation of surface plasmon polariton with the fitting value of plasmon-photon coupling constant $g_k = 0.1 \omega_p$, and experiment data of a) InSb (dotted line), and b) Ag (dashed line, lower line is Drude and $g$ with $k$-dependence).

We note here our theoretical obtained results from two bands quantum model with $g_k = 0.1 \omega_p$ have quite good agreement with the experimental data in neck region but fare in the long wave limit. The Drude model and two bands quantum model with $k$-dependence of coupling constant give the same results and are good at low $k$ limit but fare at bottom neck region.
7. Coupling constant with $k$-dependence
As mentioned above, the simple two bands model of surface plasmon polariton might be good in the most important neck region but may be fare in the long wave limit $k = 0$. In this part, we propose to overcome this problem by investigation the $k$-dependence of the plasmon-photon coupling constant.

Assuming the two dispersion relations of Drude $\omega_D(k)$ and our model $\omega_{SP}(k)$ are equal $\omega_D(k) = \omega_{SP}(k)$, we have an equation for finding the plasmon-photon coupling constant $g_k$

$$\sqrt{c^2 k^2 + \frac{\omega_p^2}{2}} - \sqrt{c^4 k^4 + \left(\frac{\omega_p}{\sqrt{2}}\right)^2} = \frac{1}{2} \left[ (ck + \omega_p) - \sqrt{ck - \omega_p} \right] + \frac{4g_k^2}{\sqrt{2}}. \quad (12)$$

The value of the plasmon-photon coupling constant $g_k$ depends on wave vector $k$ is plotted in the figure 8.

Figure 8. The value of the plasmon-photon coupling constant $g_k$ depends on wave vector $k$.

At bottom neck point $g_k \approx 0.165 \omega_p$. In the low $k$ limit, $g_k \rightarrow 0$ when $k \rightarrow 0$, $g_k$ reaches its approximate maximum value $0.185 \omega_p$ in the bottom neck region, and decreases in the large $k$ limit.

The common picture of bulk and surface plasmon polariton dispersion relation $\omega_{SP}$ depends on wave vector $k$ with photon and surface plasmon guide lines is presented in the figure 9.

8. Conclusion and discussion
We proposed a simple two band model Hamiltonian of surface plasmon-polariton in second quantized representation. The main parameter of the model is surface plasmon-photon transition vertex (surface plasmon-photon coupling constant) $g_k$. We compare the lower surface plasmon polariton branch with experiment and have rather good agreement in the crossing region but not so well in the long wave limit. To overcome this problem we suggested a $k$-dependence of $g_k$ and for that an explicit formula was found and investigated.

Our theoretical obtained results from two bands quantum model with $g_k = 0.1 \omega_p$ have quite
Figure 9. The common picture of bulk and surface plasmon polariton dispersion relation $\omega_{SP}$ depends on wave vector $k$ with photon and surface plasmon guide lines.

good agreement with the experimental data in neck region but fare in the long wave limit. The Drude model and two bands quantum model with $k$-dependence of coupling constant $g_k$ give the same results and are good at low $k$ limit but fare at bottom neck region. Because surface plasmon polariton has a too large damping region from surface to bulk plasmon frequency in comparing with exciton and phonon polaritons, so the connection between the bulk and surface plasmon polariton dispersion relations still lacked. To investigate this problem we suggest constructing a new 3-band model for surface plasmon polariton, that will be investigated in the near future.

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