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Second quantization model for surface plasmon polariton in metallic nano wires

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Abstract. A model of effective Hamiltonian is proposed in second quantization representation for system of surface plasmons and photon (polariton) in metallic nano wires. The dispersion relation curves of surface plasmon polariton was calculated by mean of the Bogoliubov diagonalization method. The surface plasmon photon vertexes are considered. The conditions for excitation surface plasmon, existence plasmon radiate modes, and a possible application of metallic nano wires were also discussed.

1. Introduction

In the last tens years, the new field of plasmon has been developed, which discussed the interesting features of metals with nano structure, exciting with an electromagnetic radiation: the plasmon resonance.

The plasmon is a quasiparticle resulting from the quantization of plasma oscillations. Plasmons are collective oscillations of the free electron gas density. A Plasmon can couple with a photon to create another quasiparticle called a plasmon polariton. Surface plasmons are plasmons which are restricted in surfaces and interact strongly with light resulting in a polariton. They occur in the interface of a vacuum and material with a small positive imaginary and large negative real dielectric constant. It is usually a metal or doped dielectric.

The result of this combination is the interesting optical properties of absorption and scatter in the Vis - IR region and can be exploited for many applications in modern technology. They also play an important role in new interesting physics phenomena such as Surface Enhanced Raman Spectroscopy (SERS), Surface Plasmon Energy Transfer (SET), and Forster Resonance Energy Transfer (FRET) and have numerous other applications in plasmonics and nanotechnology and medical treatments [1-16].

Since for all these surface plasmon polariton (SPP) systems the downscaling of the cross section is not limited by the light wavelength, they represent a promising alternative to dielectric optical waveguides. Thus, there is a substantial interest in the fundamental properties of SPP propagation in nanoscale structured matter, which is determined by the respective dispersion relations.

Nowadays, the experimental determination of the dispersion relation in the confined metallic films with nanoscopic cross sections nanowires is a challenging task, as the methods such as total internal reflective attenuated spectroscopy cannot be applied easily because of the small size



of the nanowires. An alternate experimental technique, conventional spectroscopic extinction, was proposed in [5], allowing the measurement of plasmon resonances in metallic nanowires with finite length. Absorption and scattering in a nanowire give rise to an extinction band, the maximum of which is used to define the frequency of the resonance of the SPP mode.

In the article [17], the experimental determination of the dispersion relation for Ag and Au nanowires was reported. Interestingly, it was shown at the multipolar plasmon resonances of metal nanowires can be described in terms of standing plasmon waves, allowing one to deduce the dispersion relation from optical extinction measurements. The proposed model is supported by additional investigations with a modified experimental setup.

The focus was taken into the metallic nanowire systems which have already great interests in the SPP waveguides, and could produce a strong evanescence field near their surface. It is also known as an intrinsic problem restricting the applications of surface plasmons, which is the energy loss. To overcome this obstacle, hybrid surface plasmon modes supported by a composite waveguide of metal, spacer and dielectric, have been introduced.

In the previous work [19], a simple second quantization Hamiltonian for SPP with planar geometry was proposed.

In this research, we studied the quantum theory of surface plasmons, and plasmon polaritons with metallic nanowires. The Drude model was reviewed first and then applied for the metallic nanowires with cylindrical symmetry. Using the Mie theory for small radius metallic nanowires, the dispersion relation of surface plasmon polaritons was found. Based on that results, a simple two branch surface plasmon polariton model was considered for metallic nanowires with a definition of plasmon-photon effectiveness correlation constant. The dispersion relation SPP was found by applying the Bogoliubov diagonalization technique to the the second quantization model Hamiltonian for system of surface plasmon and photon in metallic nano wires. The comparison of the theoretical results obtained from our model and experimental data give good agreement.

2. Drude model for single mode surface plasmon polaritons

In this part we presented a simple semi-classical model, like Dude model for single mode surface plasmon polariton in metallic nano particle.

In the semi-classical theory, the dielectric response of surface palsmon is characterized by the Drude formula, which is the generalized Lorentz model for metals

$$\epsilon_m(\omega) = \epsilon_\infty - \frac{\omega_{SP}^2}{[\omega(\omega + i\gamma_P)]}, \quad (1)$$

where γ_P is the damping constant, $\omega_P = \eta\omega_{SP}$ is the surface plasmon frequency with the parameter η defined by the dimension and geometry properties of metallic nano particles, $\omega_P = \sqrt{ne^2/\epsilon_0 m^*}$ is the bulk plasmon frequency, ϵ_∞ and ϵ_0 are the high frequency and static dielectric constants, n is the density and m^* is the effective mass of electrons in the metal.

Considering $\gamma_P \ll \omega_{SP}$ - the damping constant is much smaller than surface plamon frequency, the standard Drude model is

$$\epsilon_m = \epsilon_\infty - \frac{\omega_P^2}{\omega^2}. \quad (2)$$

Like in the case of Lorentz model, we can separate the real and imaginary parts of the dielectric constant by analyzing the function around the value of $\omega \simeq \omega_P$

$$\epsilon_m(\omega) \simeq \epsilon_\infty - \frac{\omega_{SP}^2}{(\omega - \omega_{SP})^2 + \gamma_P^2} + i \frac{\omega_{SP}^2 \gamma_P}{\omega [(\omega - \omega_{SP})^2 + \gamma_P^2]}. \quad (3)$$

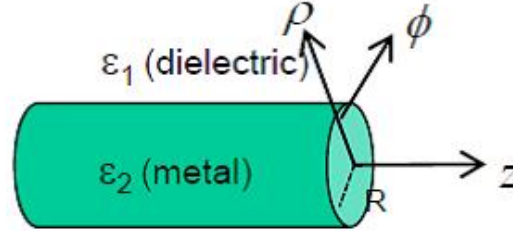


Figure 1. Model metallic nano wire

The real part Re and imaginary part Im of plasmon dielectric constant $\epsilon_m(\omega)$ now have the Lorentz-like forms, i.e. have a dispersive

$$\epsilon_{1m}(\omega) = Re \epsilon_m(\omega) = \epsilon_\infty - \frac{\omega_{SP}^2}{(\omega - \omega_{SP})^2 + \gamma_P^2} = A_{dis}, \quad (4)$$

and for absorption part

$$\epsilon_{2m}(\omega) = Im \epsilon_m(\omega) = \frac{\omega_{SP}^2 \gamma_P}{\omega [(\omega - \omega_{SP})^2 + \gamma_P^2]} = A_{abs}. \quad (5)$$

It is noted here that the asymmetric absorption peak around ω_{SP} is the common behavior of plasmon absorption. For the case of metallic half space with planar geometry, we have $\eta_{planar} = 1/\sqrt{1 + \epsilon_d}$ or $\eta_{planar} = 1/\sqrt{2}$ in the vacuum $\epsilon_d = \epsilon_0 = 1$.

The dispersion laws of surface plasmon polariton $\Omega(k)$ are defined from the boundary conditions.

3. Drude like model for surface plasmon polariton in nano wires

To calculate the group velocity $d\omega = dk$ as a function of a metallic nano wire radius R , a model consisting of a metallic cylinder with a dielectric constant ϵ_m surrounded by a dielectric medium of dielectric constant ϵ_d was used (see the figure 1).

For the special case with TM mode ($H_z = 0$) and fundamental mode with no winding $m = 0$, continuity of the remaining tangential components E_z and H_ϕ at the boundary lead to the equation for SPP dispersion relations. In this case the surface plasmon propagation is governed by the dispersion relation for the fundamental transverse magnetic modes, which is given by [16]

$$\frac{k_2^2}{k_{2\perp}} \frac{J'_0(k_{2\perp}R)}{J_0(k_{2\perp}R)} - \frac{k_1^2}{k_{1\perp}} \frac{H'_0(k_{1\perp}R)}{H_0(k_{1\perp}R)} = 0, \quad (6)$$

where $k_i = \sqrt{\epsilon_i \omega / c} = \sqrt{k_{i\perp}^2 + k_{i\parallel}^2}$ and J_m, H_m are Bessel and Hankel functions of the first kind, respectively. By numerically solving the above equation (6), we can calculate the group velocity as a function of R with frequency ω and given ϵ_d and ϵ_m . In the limit of $k_{i\perp} = \sqrt{k_i^2 - k_{i\parallel}^2} \simeq ik_{i\parallel}$ we have

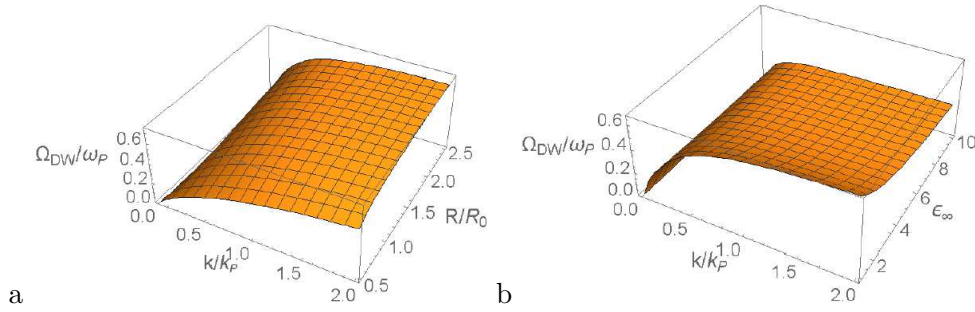


Figure 2. SPP dispersion relation for metallic nano wire in the Drude like model

$$\frac{\epsilon_m}{\epsilon_d} = \frac{K'_0(k_{\parallel}R) I_0(k_{\parallel}R)}{K_0(k_{\parallel}R) I'_0(k_{\parallel}R)}, \quad (7)$$

where K_m, I_m are modified Bessel and Hankel functions, respectively.

Taking the case of metal/vacuum interface $\epsilon_d = 1$, from the Drude model the frequency ω_k equals

$$\omega^2 = \omega_P^2 (\epsilon_{\infty} - \epsilon_m) \quad (8)$$

In the Drude like model, the SPP dispersion relation for metallic nano wires is

$$\omega_{DW}(k_{\parallel}, R) = \omega_P \left\{ \epsilon_{\infty} - \frac{K'_0(k_{\parallel}R) I_0(k_{\parallel}R)}{K_0(k_{\parallel}R) I'_0(k_{\parallel}R)} \right\}^{-1/2}, \quad (9)$$

or using the properties of modified Bessel and Hankel functions, it can be rewritten as follow

$$\omega_{DW}(k_{\parallel}, R) = \omega_P \left\{ \epsilon_{\infty} - \frac{K_1(k_{\parallel}R) I_0(k_{\parallel}R)}{K_0(k_{\parallel}R) I_1(k_{\parallel}R)} \right\}^{-1/2}, \quad (10)$$

and is plotted in the figure for the cases $\epsilon_{\infty} = 1$, and $\epsilon_{\infty} = 3.7$ (Ag).

For almost metals $[\epsilon_m/\epsilon_d] \gg 1$ that $[k_{\parallel}R] \ll 1$

$$\frac{\epsilon_m}{\epsilon_d} \simeq \frac{2}{[a + \ln(k_{\parallel}R)] (k_{\parallel}R)^2}, \quad (11)$$

where $a = \gamma_E - \ln 2$, $\gamma_E = 0.577$ is the Euler's constant. Denote $k_{\parallel} = nk_0$ we got

$$n(R) \simeq \frac{C(\epsilon_d, \epsilon_m)}{k_0 R}, \quad (12)$$

where the function C is

$$C(\epsilon_d, \epsilon_m) = \frac{\sqrt{-2\epsilon_d/\epsilon_m}}{\ln \sqrt{-4\epsilon_m/\epsilon_d} - \gamma_E}. \quad (13)$$

For $k_0 R \rightarrow 0$, the phase velocity $v_{ph} = c/n \rightarrow 0$, and the group velocity $v_{gr} = c/[d(n\omega)/d\omega] \rightarrow 0$.

In the case of small radius nanowires $k_{\parallel}R \leq 1$, we obtain the dispersion relation for SPP

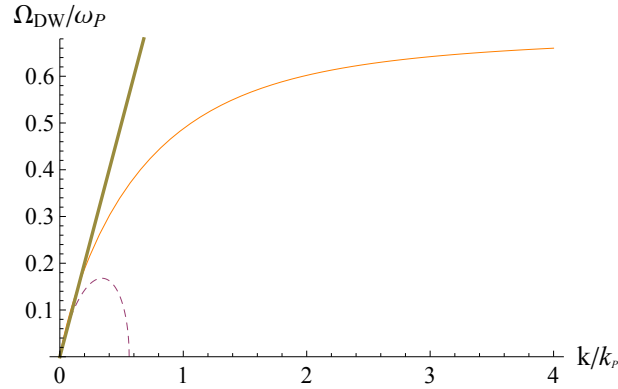


Figure 3. The dispersion relations for SPP obtained by equation (10) curve, and (14) dashed line

$$\omega_{DW}(k_{\parallel}, R) \simeq \omega_P \left\{ \epsilon_{\infty} - \frac{2\epsilon_d}{[a + \ln(k_{\parallel}R)](k_{\parallel}R)^2} \right\}^{-1/2}. \quad (14)$$

In the figure 3, we plot the dispersion relations for SPP obtained by equation (10) curve, and (14) dashed line. For guiding, the photon line (thick) also is plotted. The dispersion relation from (14) valid only for small nanowires.

4. Second quantization quantum Hamiltonian model for surface plasmon polaritons in metallic nano wires

In the similar cases of exciton polariton and phonon polariton, we consider a model Hamiltonian in 2nd quantization form for surface plasmon polariton in metallic nano wires with single mode

$$H = \sum_k H_k = \sum_k \left\{ \omega_{\gamma k} a_k^+ a_k + \omega_{P1} b_k^+ b_k + g_k (a_k^+ b_k + b_k^+ a_k) \right\}, \quad (15)$$

where $a_k(a_k^+)$ and $b_k(b_k^+)$ are the annihilation (and creation) photon and plasmon operators correspondingly with momentum k , ω_{P1} is the surface surface plasmon energy with $m = 1$, and $\omega_{\gamma k} = ck/\sqrt{\epsilon_d}$ is the photon dispersion law. We denote g_k the plasmon-photon transition vertex (or coupling constant), this vertex is absence in traditional plasmon theory $g_{Bk} = 0$ because the bulk plasmon is longitudinal excitation, while photon is transverse excitation. For the case of surface plasmons due to the existence of the boundary conditions that electromagnetic waves must be satisfied at the interface, the plasmon-photon transition vertex might not be zero, and being the main parameter of our theory.

5. Bogoliubov transformation and dispersion relation

We use the Bogoliubov transformation technique taken from the theory of superconductivity for the plasmon polariton diagonalized Hamiltonian

$$H_k = \sum_k \left\{ \Omega_{Uk} \gamma_{Uk}^+ \gamma_{Uk} + \Omega_{Lk} \gamma_{Lk}^+ \gamma_{Lk} \right\}, \quad (16)$$

where γ_{ik} (and γ_{ik}^+) are the annihilation (and creation) operators of the surface plasmon polariton SPP with momentum k , and i is the branch number $i = L = 1$ for lower and $i = U = 2$ for upper branch.

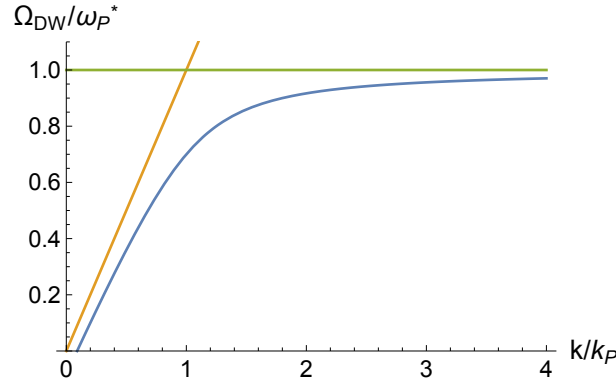


Figure 4. Simple two bands SPP model with the effective $g_k = const$

The transformations with unity condition $u_k^2 + v_k^2 = 1$ are

$$\gamma_{1k} = u_k a_k + v_k b_k, \quad \gamma_{2k} = -v_k a_k + u_k b_k. \quad (17)$$

Using the commutative relations for annihilation and creation operators $[a_k, a_k^+] = 1$, $[b_k, b_k^+] = 1$, $[\gamma_{ik}, \gamma_{ik}^+] = 1$, and equalling to zero in other cases, by standard calculation as in [4] we obtain the surface plasmon polariton SPP dispersion relations for lower branch

$$\Omega_{Lk}(R) = \frac{1}{2} \left\{ [\omega_{\gamma k} + \omega_{P1}(R)] - \sqrt{[\omega_{\gamma k} - \omega_{P1}(R)]^2 + 4g_k^2} \right\}, \quad (18)$$

and for upper branch

$$\Omega_{Uk}(R) = \frac{1}{2} \left\{ [\omega_{\gamma k} + \omega_{P1}(R)] + \sqrt{[\omega_{\gamma k} - \omega_{P1}(R)]^2 + 4g_k^2} \right\}. \quad (19)$$

Note that in the case of planar boundary geometry, the upper branch is lying in the energy gap where damping is too high so only the lower branch exist, while in the case of metallic nano spherical geometry, both branches could be exist. The surface plasmon polariton dispersion relation Ω_k depends on wave vector k and coupling constant $g_k = 0.3\omega_P^*$ is presented in the figure 4.

Note that the simple two bands model with the effective $g_k = const$ of surface plasmon polariton might be best in the most important bottom region but may be fare in the long wave limit $k = 0$.

6. Coupling constant g_k with k -dependence

As mentioned above, the simple two bands model of surface plasmon polariton might be best in the most important neck region but may be failed 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 and lower SPP branch with $\omega_{\gamma k} \leq \omega_{P1}$ of our quantum model are equal $\omega_{DW} = \Omega_{Lk}$, and putting $k = k_{||}$ we got the equation for finding the plasmon-photon coupling constant g_{Wk}

$$\omega_{DW}(k, R) = \frac{1}{2} \left\{ (\omega_{\gamma k} + \omega_{P1}) - \sqrt{(\omega_{\gamma k} - \omega_{P1})^2 + 4g_{Wk}^2} \right\}. \quad (20)$$

The solution of this equation is

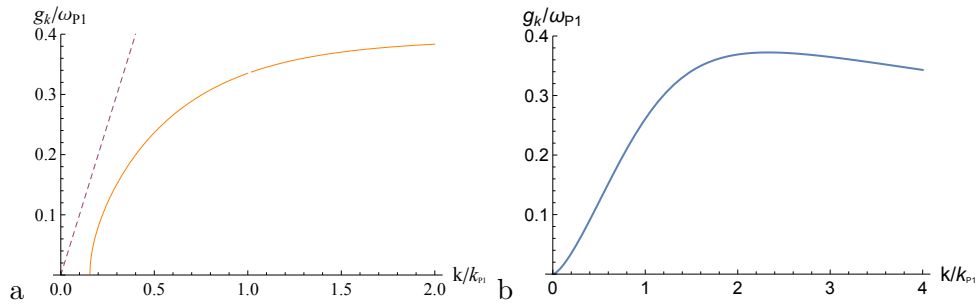


Figure 5. The value of the plasmon-photon coupling constant g_k depends on wave vector k , a) calculated from equation (10) (curve), and from optical model [15] (dashed line), b) from comparison with Drude mode

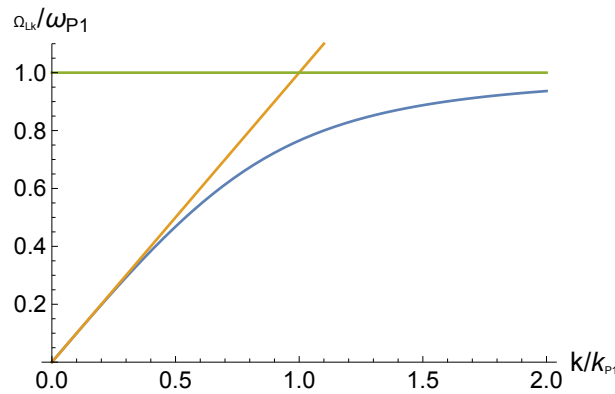


Figure 6. The dispersion relation obtained by our model

$$g_{Wk}^2(R) = [\omega_{k+} - \omega_{DW}(k, R)]^2 - \omega_{k-}^2, \tag{21}$$

where

$$\omega_{k\pm} = \frac{1}{2}(\omega_{p1} \pm \omega_{\gamma k}), \tag{22}$$

for the SPP lower branch $k = k$ if $k < k_{p1}$, and $k = k_{p1}$ if $k \geq k_{p1}$.

The value of the plasmon-photon coupling constant g_k depends on wave vector k at the metal/vacuum interface ($\epsilon_d = 1$) is plotted in the figure 5, here, and will be taken as parameter of our model.

With this plasmon-photon coupling constant, the dispersion relation obtained by our model is presented in the figure 6.

Two branches of surface plasmon polariton of metallic nano wires (curve and Dashing [Large]) is plotted in the figure 7 with the proposed coupling constant g_k (DotDashed).

Note that the existence of upper branch. This branch might play an important role in some physics phenomena.

Discussion

In this work, we reviewed and studied several semiclassical and quantum models of surface plasmons and surface plasmon polariton in the cylindrical symmetry. We proposed a simple two branch model Hamiltonian for surface plasmon polarization in second quantification

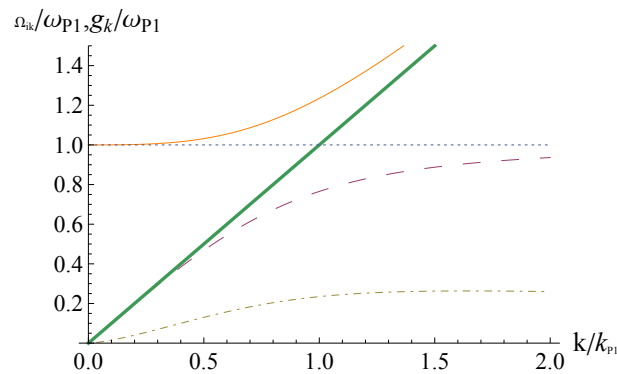


Figure 7. Two branch model for surface plasmon polariton of metallic nano wires (Up-curve and Low-Dashing [Large]) with the proposed coupling constant g_k (DotDashed)

representation for metallic nanowires. The main parameter of the model is surface plasmon photon transition vertex (surface plasmon photon effective coupling constant) was obtained. We compared the two cases planar and cylindrical geometries. For the case of planar geometry, the conditions for excitation are needed, while that do not need for the case of cylindrical geometry. The existence of upper surface plasmon polariton branch with the photon-like behavior at high frequency will play an important role in explanation the some experimental results.

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