Analytical solutions to zeroth-order dispersion relations of a cylindrical metallic nanowire

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I. INTRODUCTION

Surface Plasmon-polaritons (SPPs) induced by the coupling between the free-electron plasma and electromagnetic field at the metal-dielectric interfaces are known for the wide application in nano optics. Due to the spatial localization at the metal-dielectric interfaces, the SPPs can be guided to manipulate light in nanoscaled photonics. It has also been found that other effects of SPPs, including field enhancement, and influence on lifetime of emitters close to the SPPs. In various plasmonic structures, cylindrical metallic nanowire as a symmetric plasmonic structure has been widely studied for the applications of the optical waveguide and the scanning near-field optical microscopy (SNOM). In order to understand the physical properties of SPPs in those structures, it is important to get the dispersion relations of the frequency and wave vector of the SPPs, which determine the basic properties of the SPPs. Principally, the dispersion relations can be obtained by solving the Maxwell equations with the boundary conditions of the plasmonic structures imposed. For the cylindrical nanowire, the SPPs dispersion relations can be numerically calculated from the dispersion equation. The SPPs dispersion relations of plasmonic structures are complex when the metal Ohmic losses are introduced. There exist two types of solutions to the complex dispersion relations. One solution specifies a complex frequency as a function of a real wave vector, noted as $\text{complex} - \omega$ for convenience. The other one specifies a complex wave vector as a function of a real frequency, noted as $\text{complex} - k$. Even though the two types of solutions are obtained from one same structure, they are rather different. For the sections of the dispersion relations with frequencies close to the surface Plasmon frequency, the $\text{complex} - k$ solution has a back bending, which is absent in the $\text{complex} - \omega$ solution. The latter is an asymptotic curve.

The back bending of the dispersion relation has some unique properties. For example, it has been calculated that the minimum energy velocity is exactly at the back bending. Furthermore, the local density of states (LDOS) of SPPs is a key parameter influencing the lifetime of an emitter close to the SPPs. According to the definition of the LDOS that is proportional to $1/|\nabla \omega(k)|$, the LDOS close to the back bending point in the $\text{complex} - k$ dispersion has a small and broad peak, while the LDOS in $\text{complex} - \omega$ dispersion has a large and narrow peak due to the asymptotic curve. Thus, in order to compare the physical results between the two types of solutions, it is necessary to understand the behaviors of the asymptotic curve and the back bending of the SPPs.

It has been suggested that the $\text{complex} - k$ solution describes the SPPs mode decaying spatially while the $\text{complex} - \omega$ solution is for the SPPs decaying in time rather than in space. The discrepancy of the two solutions has been considered to be originated from the metal Ohmic loss. Such conclusion is originally drawn from the study of SPPs on planar metallic-dielectric surfaces. When a perfect metal without damping is considered in this planar case, the two types of solutions of the SPPs dispersion relations overlap with the same asymptotic behavior. When the metal Ohmic loss is introduced into the dielectric response of the metal, the two types of solutions are then different. Before such conclusion is extended to the case of the cylindrical metallic nanowire, it is necessary to exhibit how the metal Ohmic loss leads to the back bending of the dispersion relations of the metallic nanowire. In this paper, we derive approximate analytical solutions to the complex dispersion relations of a cylindrical metal nanowire for the description of the back bending as well as the asymptotic behavior of the SPPs. Based on the analytical expressions, the role of metal Ohmic loss in the determination of the back bending is discussed. The utility of the back bending for the measurement of the metal Ohmic loss has also been suggested.

II. DISPERSION EQUATION

The metal nanowire is modeled to have the shape of a circular cylinder with the radius $r$ and the infinite length in a medium. The electromagnetic field in this model can be expanded with cylindrical harmonics. By imposing the electromagnetic boundary conditions at the metal-dielectric interface, we obtain the following transcendental equation:

$$
\begin{bmatrix}
H_{0}^{\text{in}}(k_{0}r) & 0 & -J_{0}(k_{0}r) & 0 \\
-k_{0}H_{1}^{\text{in}}(k_{0}r)k_{0} & k_{0}H_{1}^{\text{in}}(k_{0}r) & k_{0}J_{1}(k_{0}r) & -k_{0}J_{1}(k_{0}r) \\
-k_{0}H_{1}^{\text{in}}(k_{0}r) & k_{0}H_{1}^{\text{in}}(k_{0}r) & -k_{0}J_{1}(k_{0}r) & k_{0}J_{1}(k_{0}r) \\
-k_{0}H_{1}^{\text{in}}(k_{0}r)k_{0} & -k_{0}H_{1}^{\text{in}}(k_{0}r) & k_{0}J_{1}(k_{0}r) & -k_{0}J_{1}(k_{0}r)
\end{bmatrix} = 0.
$$

(1)
which repeats the reported results. Here, $H_n^{(1)}$ is the first kind of Hankel function with the order of integer $n$ and $J_n$ is the Bessel function of $n$th order. The Hankel and Bessel functions with denote represent the first order differentiation. $k_{j(0,1)}$ is the wave vector with the value of $k_j = \sqrt{\varepsilon} \omega/c$, where $\varepsilon$ is the dielectric function and the subscript $j$ labels the quantities outside the nanowire ($j = 0$) or inside it ($j = 1$). $c$ is the speed of light in vacuum. The dielectric function of the metal can be expressed as

$$\varepsilon_1(\omega) = \varepsilon_{\infty}[1 - \frac{\omega_p^2}{\omega(\omega + i\tau)}],$$  \hspace{1cm} (2)$$

where $\omega_p$ is the bulk-plasmon frequency and $\tau$ is the bulk electron relaxation rate which reflects the metal Ohmic loss. $\varepsilon_{\infty}$ in equation (2) is a constant for the general description of the dielectric function of the metal. $k_z$ is the component of the SPPs wave vector along the cylinder axial and the radial components of the wave vectors are defined as $k_{r,j} = k_{j} - k_{z}^2$. We note that the value of $k_{r,j}$ should be chosen to guarantee the imaginary part of $k_{r,j}$ to be positive since the light intensity should be decaying away from the metal cylinder. The dispersion relation between $k_z$ and $\omega$ then can be obtained from the equation (1). However, it is impossible to get an analytical solution to the equation for the whole dispersion relation. We show in the following that the sections of the dispersion relations whose frequencies are close to the Surface Plasmon frequency can be solved out from equation (1) analytically with approximate methods. For clarity in the following derivation, we renormalize the $\omega$ and $\tau$ by $\omega_p$. Wave vector components of $k_{r(j=0,1)} - k_z$ and $k_{r(j=0,1)}$ are renormalized by $\omega_p/c$ and $\tau$ is renormalized by $c/\omega_p$.

III. ANALYTICAL SOLUTIONS

For the sections of the dispersion relations with frequencies close to the Surface Plasmon frequency $\omega_{sp} = \sqrt{\varepsilon_{\infty} \varepsilon_{0} + \varepsilon_{\infty}}$, the SPPs modes of the metal nanowires are nonradiative and the real parts of $k_z$ noted as $Re[k_z]$ at those sections have larger values than the imaginary parts $Im[k_z]$. The values of $Re[k_z]$ play more important role in the Bessel and Hankel functions than the values of $Im[k_z]$, which makes the Bessel functions and Hankel functions in the equation (1) behave as modified Bessel functions. In order to verify this point, we have conducted numerical calculations on the Bessel functions and Hankel functions with the frequency close to the Surface Plasmon frequency, and found that the Bessel function approaches to infinity while the Hankel function goes to be zero. Thus, it is reasonable to replace the Bessel and Hankel functions in equation (1) by the following approximate expressions:

$$J_n(it) \approx \sqrt{\frac{2}{\pi t}} e^{-t - \frac{\pi}{4}},$$ \hspace{1cm} (3a)$$

$$H_n^{(1)}(it) \approx -i \sqrt{\frac{2}{\pi t}} e^{-t - \frac{\pi}{4}}.$$ \hspace{1cm} (3b)$$

with $t$ replaced by $-ik_{r,j} \tau$ in the derivation. In order to get the analytical solutions to equation (1), $k_{r(j=0,1)}$ should be expanded by $k_z$ as

$$k_{r,j} = \sqrt{k_{r,j}^2 - k_z^2} \approx \frac{2k_z^2 - k_{r,j}^2}{2k_z^2}. \hspace{1cm} (3c)$$

In this paper we only discuss the zeroth-order analytical solutions with $n = 0$. Substituting equation (3) into the equation (1), we obtain the following equation

$$k_z^4 - k_z^2 (k_z^2 - k_0^2) - 2 \frac{k_z^2(1 + k_z^2) + k_0^2 k_z^2}{2} \frac{k_z^2 + k_0^2}{2} = 0. \hspace{1cm} (4)$$

There exist four solutions to the equation (4). However, only one solution is correct. Especially for the case of $r \to \infty$, the equation (4) is then solved out to be $k_z^2 = \frac{k_0^2}{k_z^2}$, which is the right dispersion relation of SPPs on a planar metal surface.

A. Solutions for $\varepsilon_0 = 1$ and $\varepsilon_{\infty} = 1$

For clarity to show our derivation, we set the dielectric constants as $\varepsilon_0 = \varepsilon_{\infty} = 1$. Then, the Surface Plasmon frequency is $\omega_{sp} = 1/\sqrt{2}$. Firstly, we consider the complex $-k$ solution. We rewrite the equation (4) expressed by $k_z$, $\omega$, and $\tau$ as

$$[(4 \omega^2 - 2) + (\tau)(\frac{8 \omega^2 - 2}{\omega}) + 4(\tau)^2]k_z^4 + [1 + \frac{\tau}{\omega}]k_z^3 + \frac{6 \omega^2 (1 - \omega^2) - 1 + 6 \omega^2 (1 - \omega^2) - 6 \omega^2 (\tau)^2]k_z^2 + (2 \omega^2 - 1)(\omega^2 - 1)\omega^2 + (\tau)(4 \omega^2 - 3)\omega^3 + 2(\tau)^2 \omega^4 = 0.$$ \hspace{1cm} (5)$$

In the complex $-k$ solution, there exists a back bending of the SPPs where the frequency $\omega$ is close to the Surface Plasmon frequency $\omega_{sp} = 1/\sqrt{2}$. Comparing to the terms with the same order of $\tau$, we find that the last three terms without $k_z$ can be neglected since the $Re[k_z]$ is large enough at the back bending point. Thus, equation (5) can be further simplified as

$$[(4 \omega^2 - 2) + (\tau)(\frac{8 \omega^2 - 2}{\omega}) + 4(\tau)^2]k_z^4 + [1 + \frac{\tau}{\omega}]k_z^3 + \frac{6 \omega^2 (1 - \omega^2) - 1 + 6 \omega^2 (1 - \omega^2) - 6 \omega^2 (\tau)^2]k_z^2 + (2 \omega^2 - 1)(\omega^2 - 1)\omega^2 + (\tau)(4 \omega^2 - 3)\omega^3 + 2(\tau)^2 \omega^4 = 0.$$ \hspace{1cm} (6)$$

Then, the complex $k_z$ can be solved out from the equation (6). The approximate methods in above derivation are valid for larger $Re[k_z]$ than $Im[k_z]$, which has been confirmed at the sections of the dispersion relations by our numerical calculations. And in the derivation, the approximate methods are conducted regardless of $Im[k_z]$. Thus, the correct solution to the equation (6) for the $Re[k_z]$ is

$$Re[k_z] = Re\left[-\frac{\left[1 + \left(\frac{\tau}{\omega}\right)^2\right]^{1/2} - \sqrt{\left[1 + \left(\frac{\tau}{\omega}\right)^2\right]^{1/2}}}{2k_A}\right].$$ \hspace{1cm} (7)$$
with
\[ k_A = 4\omega^2 - 2 + (ir)(\frac{8\omega^2 - 2}{\omega}) + 4(ir)^2, \]
\[ k_C = 6\omega^2(1 - \omega^2) - 1 + 6\omega(ir)(1 - 2\omega^2) - 6\omega^2(ir)^2. \]
Especially for the case of \( \tau = 0 \), \( Re[k_c] \) is then equal to
\[ Re[k_c] = \frac{-1}{2} - \frac{\sqrt{\omega^2 - 4(4\omega^2 - 2)(6\omega^2(1 - \omega^2) - 1)}}{2(4\omega^2 - 2)}. \] (8)

Now we consider the complex - \( \omega \) solution. We rewrite the equation (5) expanded with the frequency \( \omega \) as the following equation:
\[ 2\omega^3 + 4(i\tau)\omega^2 - 6k_c^2 - 2(2i\tau)^2 + 3\omega^3 - [12(ir)k_c^3 + 3(i\tau)k_c^2 + [4k_c^2 - 6(2i\tau)^2]k_c^2 + 6k_c^2 + 1]\omega^3 - [8(ir)k_c^2 + 6(i\tau)k_c^2]\omega^2 - [-4(i\tau)^2k_c^4 + 2k_c^2 + k_c^2 - r]\omega + (ir)k_c^2/r - 2(ir)^2k_c^2 = 0. \] (9)

Similarly, comparing to the terms with the same order of \( i\tau \), we simplify equation (9) by neglecting the terms with small values to get
\[ \omega^3 + 2(i\tau)\omega^2 + [1/(4rk_c) - 1/2]\omega + (ir)[1/(4rk_c) - 1/2] = 0. \] (10)

The imaginary part of \( \omega \) has been calculated to be small [15]. Thus, the correct approximate solution to equation (10) is
\[ Re[\omega] = Re[\sqrt{-\frac{q}{2} - \sqrt{\frac{q^2}{4} + \frac{P}{3}} + \sqrt{-\frac{q}{2} + \sqrt{\frac{q^2}{4} + \frac{P}{3}}}], \] with
\[ p = \frac{1}{4rk_c} - 1, q = \frac{16i\tau^3}{27} + \frac{ir(1 - 2rk_c)}{12rk_c}. \] (11)

B. General solutions

For the general case with the dielectric constants \( \varepsilon_0 \) and \( \varepsilon_\infty \) introduced into the wave vectors, analytical solutions to Equation (4) can be obtained similarly by neglecting the terms with small values. The approximate methods are still valid for the sections of the dispersion relations with frequencies close to the Surface Plasmon frequency \( \omega_{sp} = \frac{\varepsilon_\infty}{\varepsilon_0 + \varepsilon_\infty} \). Here, we only show the results. For the complex - \( k \) solution, the \( Re[k_c] \) is
\[ Re[k_c] = Re[\frac{-B - \sqrt{B^2 - 4A X C}}{2A}], \] (12)
with
\[ A = \omega^3 - P\omega + ir(2\omega^2 - P) - \omega^2 r^2, B = \frac{Q\omega^3 + \omega P}{2r}, \]
\[ C = -R\omega^3 + S\omega^3 - \varepsilon_\infty P\omega/2 + ir\omega^2(S - 2R\omega^2) + \omega^3 R^2 r^2, \]
\[ P = \frac{\varepsilon_{msf}}{\varepsilon_0 + \varepsilon_\infty}, Q = \frac{\varepsilon_0 - \varepsilon_\infty}{\varepsilon_0 + \varepsilon_\infty}, R = \frac{\varepsilon_0 + \varepsilon_\infty}{2}, \]
\[ S = \varepsilon_\infty + \frac{\varepsilon_{msf}}{\varepsilon_0 + \varepsilon_\infty}. \]

For the complex - \( \omega \) solution, the \( Re[\omega] \) has the same formation to the equation (11) as
\[ Re[\omega] = Re[\sqrt{-\frac{v}{2} - \sqrt{\frac{v^2}{4} + \frac{\mu}{3}} + \sqrt{-\frac{v}{2} + \sqrt{\frac{v^2}{4} + \frac{\mu}{3}}}, \] (13)

with
\[ u = b - \frac{a^2}{3}, v = \frac{2a^3}{27}, \]
\[ a = \frac{ir(2k_c^2 + Qk_c^2/r + S k_c^2)}{k_c^2 + Qk_c^2/(2r) + S k_c^2 + EP + R r^2 k_c^2}, \]
\[ b = \frac{-[Pk_c^2 + \varepsilon_\infty P k_c^2 - P k_c^2/(2r) + \tau^2(k_c^2 + Qk_c^2/(2r))] k_c^2 + Qk_c^2/(2r) + S k_c^2 + EP + R r^2 k_c^2}{ir(P k_c^2 - P k_c^2)} \]
\[ c = \frac{k_c^2 + Qk_c^2/(2r) + S k_c^2 + EP + R r^2 k_c^2}. \]

IV. DISCUSSION

The solutions of equation (7), (11), (12) and (13) are the main results of this paper. In order to verify these results, we perform direct numerical calculations to solve the equation (1) for the comparison (Figure (1)). The comparison is conducted on an Aluminum nanowire with the radius of 100nm, which is corresponding to the renormalized parameter \( r = 1.90415 \).

The renormalized \( r \) takes the value of \( r = 0.039062 \) and dielectric constants of \( \varepsilon_0 = \varepsilon_\infty = 1 \) are for the comparison.

Figure 1(a) is for the comparison of the complex - \( k \) solution while figure 1(b) is for the complex - \( \omega \) solution. The scattered data in the figure are the exact solutions to the equation (1) by the direct numerical calculations, while the solid line in figure 1(a) (figure 1(b)) is obtained from equation (7) (equation (11)). It shows that the \( Re[k_c] \) at the section of the complex - \( k \) dispersion relation close to the back bending point in figure 1(a) can be well fitted by the equation (7) and the asymptotic curve of \( Re[\omega] \) in figure 1(b) can be described by the equation (11) accurately. We have also conducted the comparisons with various \( r \) and \( \tau \) for the Aluminum nanowires and get the same result of figure 1. To show the result, we only summarize the comparisons of complex - \( k \) solutions in figure 2 since the comparisons of complex - \( \omega \) solutions are tedious with the same asymptotic curve. We plot \( k_{c0} \), the value of \( Re[k_c] \) at the back bending point indicated in figure 1(a), as functions of the \( r \) and \( \tau \) in figure 2. The scattered data are the exact solutions to the equation (1) by direct numerical calculations while the solid lines are the analytical results from the equation (7). In figure 2(a), the \( \tau \) is fixed to be \( \tau = 0.039062 \), while in figure 2(b) the \( r \) is fixed to be \( r = 0.2 \). The coincidence between the scattered data and the solid lines in figure 2 confirms that our analytical solution of equation (7) can be used to accurately describe the section of SPPs dispersion close to the back bending point.

Figure 2 also shows that \( k_{c0} \) is sensitive to the radius and the metal loss of the nanowire, especially for the nanowire with radius less than 50nm. For the SPPs application, the metallic
nanowires are fabricated normally with the radius having the order of few nanometers. The size of such nanowires can be identified by the Atomic Force Microscopy (AFM) and Transmission Electron Microscopy (TEM) techniques. Thus, we suggest that equation (7) can be used to fit the metal loss of the nanowire with the radius given by AFM or TEM, if the back bending of the dispersion relation can be experimentally obtained. In this way, the difference of the metal loss between the bulk material and the nanowire can be distinguished. It has been reported that the attenuated-total-reflection techniques can be used to measure the SPPs back bending of metal films experimentally. However, the discussion of the extension of the experimental techniques from metal films to metal nanowires is out of the scope of this paper. For the suggested parameter fitting, equation (1) can not be used directly due to the lack of $\text{Im}[k_z]$, which can not be measured experimentally. Equation (7) is suitable for the fitting because equation (7) is just only valid for $\text{Re}[k_z]$ regardless of $\text{Im}[k_z]$. This is the advantage of our result for the parameter fitting.

The SPPs back bending at the complex $- k$ dispersion relation is considered to be induced by the metal Ohmic loss. Such conclusion has been drawn in the case of planar metal films, but never confirmed in the case of metallic nanowires. We show in the following how the metal Ohmic loss induces the back bending by using the equation (8) for clarity. For a nanowire fabricated with a perfect metal $\tau = 0$, the denominator of equation (8) has only one term of $2(4\omega^2 - 2)$. The denominator is real since the frequency is real in the complex $- k$ solution. When the frequency $\omega$ approaches the Surface Plasmon frequency $\omega_{sp} = 1/\sqrt{2}$, the $\text{Re}[k_z]$ behaves as an asymptotic curve to infinity with the denominator going to be zero. However, when the metal loss $\tau$ is introduced, the denominator in the equation (8) will no longer be a real value, but a complex, which can be found in equation (7). The absolute value of the complex denominator will never be zero no matter what value the real frequency $\omega$ is. Thus, the $\text{Re}[k_z]$ will be finite instead of infinite at the Surface Plasmon frequency of $\omega_{sp}$. This is the key point to understand how the metal loss changes the asymptotic curve of the SPPs to a back bending.

Last, we consider the general case with $\varepsilon_0$ and $\varepsilon_\infty$ introduced. Equation (12) shows that for a perfect metal with $\tau = 0$ used in nanowires, the dispersion relation is an asymptotic curve with $\text{Re}[k_z]$ approaching infinity when the frequency $\omega$ is close to $\omega_{sp} = \sqrt{\frac{\varepsilon_0}{\varepsilon_\infty}}$. When the metal loss is introduced, the dispersion relation then has a back bending near $\omega_{sp}$. The
dependence of the back bending on the dielectric constants $\varepsilon_0$ and $\varepsilon_\infty$ is shown in figure 3. The comparison between the analytical solution of equation (12) and the numerical solution of equation (1) has been performed, confirming that equation (12) can be used to describe the back bending accurately. However, for clarity, we only show the analytical results by solid lines in the figure. Figure 3(a) shows the dependence of the back bending position on $\varepsilon_0$ with the fixed value $\varepsilon_\infty = 9$, indicating that $k_{z0}$ changes to be large with the increase of $\varepsilon_0$. Figure 3(b) is for the dependence on $\varepsilon_\infty$ with the fixed value $\varepsilon_0 = 1$, which exhibits that $k_{z0}$ changes to be small with the increase of $\varepsilon_\infty$. The dependence of the back bending position on dielectrics shown in figure (3) indicates that equation (12) can also be used for the parameter fitting of the dielectric constants of the medium and the metal. The dependence of the complex – $\omega$ solutions on the dielectric constants is not shown due to the tedious reason, which has an asymptotic curve with $\text{Re}[k_z]$ approaching infinity when the frequency $\omega$ is close to $\omega_\text{SP} = \frac{\varepsilon_\infty}{\varepsilon_0 + \varepsilon_\infty}$.

V. SUMMARY

We have derived approximate analytical solutions to the SPPs dispersion relations with $n = 0$ of cylindrical metal nanowires for the relation sections whose frequencies are close to the Surface Plasmon frequency in this paper. The back bending of the complex – $k$ dispersion relation has been confirmed to be originated from the metal loss, which introduces an imaginary value into the denominator of the expression of $\text{Re}[k_z]$ and moves the value of $\text{Re}[k_z]$ from infinity to finiteness at the Surface Plasmon frequency, resulting in the back bending of the dispersion relation. The analytical solutions are suggested to be used for the parameter fitting of the physical parameters of the nanowires by taking the advantage that $\text{Im}[k_z]$ can be unknown in the fitting.

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FIG. 3: back bending position of the $\text{Re}[k_z]$ dependent on $\varepsilon_0$ and $\varepsilon_\infty$ for the metallic nanowire with $r = 0.2$ and $\tau = 0.039062$. Figure 3 (a) shows the dependence of the back bending position on $\varepsilon_0$ with $\varepsilon_\infty = 9$. Figure 3 (b) shows the dependence of the back bending position on $\varepsilon_\infty$ with $\varepsilon_0 = 1$. 

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