

# Hermitian two-band model for one-dimensional plasmonic crystals

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We propose an analytical two-band model for surface plasmon polaritons on corrugated metal surfaces. The generalized eigenvalue equation is derived from Maxwell's equation and matching conditions for electromagnetic fields at the metal surface. Our basic equation is Hermitian for the bands outside of the light cone and perturbation theory is therefore justified. We solve the equation and show the dispersion of the one-dimensional plasmonic crystal, and compare the behaviors of eigenfrequencies with previous works for analytic plasmonic crystals and the band theory for electrons in solids.

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## I. INTRODUCTION

When the electric permittivity in a metal becomes negative due to the plasma frequency, electromagnetic modes propagating along the metal surface exist. Those electromagnetic modes, called surface plasmon polaritons (SPPs), have attracted interest because of their applications such as sensing devices<sup>1–3</sup> and optical waveguides.<sup>4–6</sup> Similar to photonic crystals, SPPs form a band structure when the metal surface is periodically corrugated. Such a microscopic structure of the metal surface is called a plasmonic crystal. Plasmonic crystals are widely investigated by experiments<sup>7–9</sup> and numerical calculations.<sup>10,11</sup>

One of the standard numerical approaches to plasmonic crystals is the rigorous coupled-wave analysis (RCWA),<sup>10</sup> in which the metal surface is divided into layers. The distributions of electromagnetic fields are exactly solved in each layer and they are connected by matching conditions at the interfaces. The slow convergence for transverse-magnetic (TM) modes in RCWA was suggested earlier, and it was solved by Granet and Guizal.<sup>11</sup> However, this method is not convenient for analytical investigations.

Analytical theories for one-dimensional plasmonic crystals have been developed in Refs. 12–16, and the frequencies of the SPPs were derived by various approaches. In particular, in Refs. 12 and 13, in their theory, an eigenvalue equation is derived from the matching conditions of electromagnetic fields at the interface between the vacuum and the metal. Nevertheless, since the matrix involved in the eigenvalue equation<sup>12,13</sup> is non-Hermitian and the eigenvalues are generally complex, the perturbation theory cannot be applied in a controlled manner. In addition, the eigenfrequency of the SPP was calculated only on the Brillouin zone boundary. More importantly, in order to study the geometrical and topological properties of the SPP band structure, similarly to electrons and photons, it is essential to have a Hermitian effective theory.

The purpose of the present paper is to develop such a Hermitian effective theory for one-dimensional (1D) SPPs. To this end, we begin with the plane-wave solution of Maxwell's equation, and there we perform a coordinate transformation to incorporate surface corrugation. Subsequently, we impose the matching condition on the linear combination of plane-wave solutions. Finally, within the two-band approximation, we derive the eigenfrequency of the SPP by the perturbation theory in a controlled manner, both on the Brillouin zone boundary

and away from it. Thus our theory gives analytical results for the eigenfrequencies and eigenmodes for small corrugations and it clarifies how the plasmonic band gap is formed.

We note that in the present paper we neglect the imaginary part of the permittivity of the metal, which causes a decay of the SPPs with propagation. The importance of our formalism is to derive Hermitian eigenvalue equations for the SPPs, which is convenient for studying the geometric structure of the wave functions. The imaginary part will make the otherwise Hermitian eigenvalue equations non-Hermitian, which is beyond the scope of the paper.

## II. EIGENVALUE EQUATION FOR THE 1D PLASMONIC CRYSTAL

### A. Free SPP solution of the Maxwell's equation

Before an analysis of the 1D plasmonic crystal, we review the SPP for a flat metal surface. On the metal surface, the transverse-electric (TE) and TM modes are decoupled due to the plasma oscillation of the electrons, and the SPP corresponds to the TM mode. We put the  $xy$  plane to be the metal surface, and consider a wave propagating along the  $x$  axis. Maxwell's equation for the TM mode [ $\mathbf{H} = (0, H_y, 0)$ ] is

$$\begin{aligned} -i\omega\epsilon E_x &= -\partial_z H_y, \\ -i\omega\epsilon E_y &= 0, \\ -i\omega\epsilon E_z &= \partial_x H_y, \\ i\omega\mu H_y &= \partial_z E_x - \partial_x E_z, \end{aligned} \quad (1)$$

where  $\mu$  is the magnetic permeability,  $\epsilon$  is the electric permittivity, and  $\omega$  is the eigenfrequency. This equation can be rewritten in the matrix form

$$\begin{pmatrix} 0 & 0 & -i\partial_z \\ 0 & 0 & i\partial_x \\ -i\partial_z & i\partial_x & 0 \end{pmatrix} \phi(x, z) = \omega B^{-1} \phi(x, z), \quad (2)$$

where

$$\phi(x, z) = \begin{pmatrix} E_x(x, z) \\ E_z(x, z) \\ H_y(x, z) \end{pmatrix}, \quad B^{-1} = \begin{pmatrix} \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \mu \end{pmatrix}.$$

Equation (2) is a generalized eigenvalue problem, which is different from the usual eigenvalue equations by the matrix  $B^{-1}$  multiplied to its right-hand side. If we rewrite the equation

by putting  $\psi = B^{-1/2}\phi$ , the equation becomes the usual eigenvalue equation for  $\psi$ :

$$\frac{1}{\sqrt{\varepsilon\mu}} \begin{pmatrix} 0 & 0 & -i\partial_z \\ 0 & 0 & i\partial_x \\ -i\partial_z & i\partial_x & 0 \end{pmatrix} \psi = \omega\psi. \quad (3)$$

The plane-wave solution of this equation is

$$\psi(x, z) = \frac{c}{\sqrt{2}\omega} \begin{pmatrix} -\lambda \\ k \\ \omega/c \end{pmatrix} e^{-i(kx + \lambda z)}, \quad (4)$$

where  $c = (\varepsilon\mu)^{-1/2}$  is the speed of light in the material.  $\lambda$  and  $k$  represent the  $z$  and  $x$  components of the wave vector. The eigenfrequency of this equation is  $\omega = c\sqrt{k^2 + \lambda^2}$ .

We refer to the vacuum region ( $z > 0$ ) with positive permittivity  $\varepsilon_a$  ( $=\varepsilon_0$ ) as region  $a$  and the metal region ( $z < 0$ ) with negative permittivity  $\varepsilon_b$  as region  $b$ . For simplicity, we neglect the frequency dependence and imaginary part of the permittivity  $\varepsilon_b$ , and assume the permeability in the metal is the same as that in the vacuum  $\mu_0$ . On the interface, the tangential components of the electric and magnetic fields in region  $a$  must be equal to those in region  $b$ . Furthermore, the eigenvalues in the two regions must be equal. These conditions give the wave number along the  $z$  direction,

$$\lambda^a = -ik\sqrt{\left|\frac{\varepsilon_a}{\varepsilon_b}\right|}, \quad \lambda^b = ik\sqrt{\left|\frac{\varepsilon_b}{\varepsilon_a}\right|}, \quad (5)$$

in regions  $a$  and  $b$ , respectively. Because they are imaginary, it is clear that the electromagnetic fields decay with distance from the metal surface (Fig. 1). Straightforwardly, the eigenvalue can be determined as

$$\omega_{\text{SPP}}^2 = \frac{k^2}{\mu_0} \left( \frac{1}{\varepsilon_a} + \frac{1}{\varepsilon_b} \right). \quad (6)$$

In reality, the permittivity  $\varepsilon_b$  of the metal depends on the frequency because of the plasmonic resonance and both sides of Eq. (6) depend on the frequency. The dispersion of the SPP is determined by solving Eq. (6) in terms of the frequency  $\omega$ .

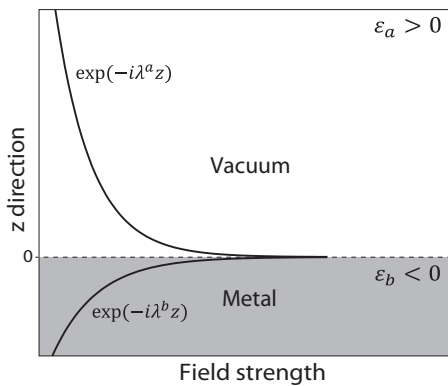


FIG. 1. A schematic picture of the field strength distribution along the  $z$  direction. Electromagnetic fields decay with the distance from the metal surface  $z = 0$ .

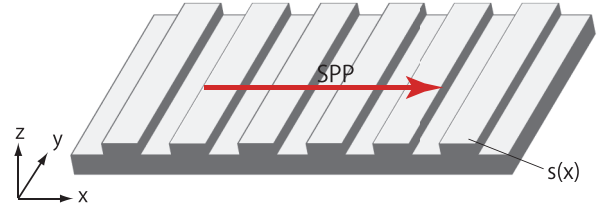


FIG. 2. (Color online) A schematic picture of a one-dimensional plasmonic crystal. The  $x$  axis is the propagation direction of the SPP, and  $z$  is a direction normal to the metal surface when  $s(x) = 0$ . The crystal is uniform along the  $y$  direction.

For example, within the free-electron approximation,  $\varepsilon_b$  is

$$\varepsilon_b = \varepsilon_0 \left( 1 - \frac{\omega_p^2}{\omega^2} \right).$$

When the metal is in the vacuum ( $\varepsilon_a = \varepsilon_0$ ), the frequency (6) becomes

$$\omega_{\text{SPP}}^2 = \frac{\omega_p^2 + 2(c_0 k)^2 - \sqrt{\omega_p^4 + 4(c_0 k)^4}}{2}, \quad (7)$$

where  $c_0$  is the speed of light in the vacuum. This equation reproduces the dispersion of the free surface plasmons.

### B. Perturbation theory

Next, we introduce corrugation to the interface. In 1D plasmonic crystals, periodicity is unidirectional, and we define this direction as  $x$ . For simplicity we assume the corrugation to consist of a single Fourier component with wave number  $2K$ . Then the surface profile is represented by a periodic function  $s(x)$  (Fig. 2), which can be represented as

$$\begin{aligned} s'(x) &= 2g \cos(2Kx + \phi), \\ s(x) &= -\frac{g}{2iK} (e^{-2iKx - i\phi} - e^{2iKx + i\phi}). \end{aligned} \quad (8)$$

Here  $g$  and  $\phi$  are dimensionless real constants.

It is not possible to analytically solve the eigenvalue problem for SPP for finite  $s(x)$ . Therefore, for our purpose of understanding the mechanism of the gap opening, we assume  $s(x)$  to be sufficiently small and treat  $s(x)$  as the perturbation. Nevertheless, it is not still straightforward. Even if  $s(x)$  is small, the local change of the permittivity at some points will not be small; some points in the vacuum may turn into the metal after the perturbation is introduced, and the change of the permittivity ( $\varepsilon_a \rightarrow \varepsilon_b$ ) is not small there. To avoid this problem, we use Chandezon's technique.<sup>17</sup> In this technique, different coordinates ( $v, w, u$ ) are employed instead of ( $x, y, z$ ),

$$\begin{aligned} v &= x, \\ w &= y, \\ u &= z - s(v). \end{aligned} \quad (9)$$

In this coordinate system, the metal surface is given by the  $u = 0$  plane. After the eigenvalue equations are transformed into coordinates ( $v, w, u$ ), we treat  $s(v)$  as a perturbation within the transformed eigenvalue equation.

In the present case, it is even easier to perform the coordinate transformation to the plane-wave solution (4) than

to do it to the eigenvalue equation and to solve the transformed equation. By performing the coordinate transformation in Eq. (4), we can derive the exact plane-wave solution in the alternate coordinates:

$$\begin{aligned}\psi(v, u) &= \frac{c}{\sqrt{2\omega}} \begin{pmatrix} -\lambda \\ k \\ \omega/c \end{pmatrix} e^{-i(kv+\lambda u) + (\xi/2)(\tau-1/\tau)} \\ &= \frac{c}{\sqrt{2\omega}} \begin{pmatrix} -\lambda \\ k \\ \omega/c \end{pmatrix} \sum_{n=-\infty}^{\infty} J_n(\xi) e^{-i(kv+\lambda u+2nKv+n\phi)},\end{aligned}\quad (10)$$

where  $\xi = \lambda g/K$ ,  $\tau = \exp(-2iKv - i\phi)$ , and  $J_n(\xi)$  is the Bessel function. The frequency  $\omega$  is given by  $\omega = c\sqrt{k^2 + \lambda^2}$  from the eigenequation (3) and it is not varied by the perturbation. More generally, a linear combination of the eigenstates with the same eigenfrequency is also an eigenstate. With coefficients  $C_m$  a general eigenstate is given by the Bloch form as

$$\begin{aligned}\psi(v, u) &= \sum_{n,m} C_m \frac{c}{\sqrt{2\omega}} \begin{pmatrix} -\lambda_m \\ k + 2mK \\ \omega/c \end{pmatrix} J_n(\xi_m) \\ &\quad \times e^{-i[kv+\lambda_m u + 2(n+m)Kv+n\phi]}.\end{aligned}\quad (11)$$

Here we limited the Bloch wave number  $k$  in the Brillouin zone from  $-K$  to  $K$ .  $\lambda_m$  is determined by the condition that  $\omega = c\sqrt{(k+2mK)^2 + \lambda_m^2}$  is identical for all  $m$ .

We now consider the interface between the metal (region  $b$ ) and the vacuum (region  $a$ ). In each region, the wave function

is given by (11). The permittivity  $\varepsilon$  and the speed of light  $c$  is different between the two regions, while the frequency  $\omega$  and the Bloch wave number  $k$  are common. Similar to the previous section, we impose matching conditions on the wave function given by Eq. (11).

Because of the spatial periodicity, the wave number  $k$  is considered modulo  $2K$ . When we draw the band structure of the free SPP in Eq. (6) in the repeated zone scheme known in electronic band theory in crystals, the dispersion is degenerated at the zone boundary  $k = K$ . Therefore, it is expected that if we introduce corrugation, the bands with  $m = 0$  and  $m = -1$  in Eq. (11) are strongly mixed near the zone boundary  $k = K$ . Therefore, here we employ a two-band approximation retaining the two bands with  $m = 0$  and  $m = -1$ , which is valid when  $k$  is close to  $K$ ;  $|k - K| \ll K$ . The boundary condition for the magnetic field leads to

$$\begin{pmatrix} J_0(\xi_0^a) & J_1(\xi_{-1}^a)e^{-i\phi} \\ J_{-1}(\xi_0^a)e^{i\phi} & J_0(\xi_{-1}^a) \end{pmatrix} \begin{pmatrix} C_0^a \\ C_{-1}^a \end{pmatrix} = (a \rightarrow b), \quad (12)$$

where superscripts such as  $\xi_m^{a,b}$  and  $C_m^{a,b}$  represent those quantities in regions  $a$  ( $u > 0$ ) or  $b$  ( $u < 0$ ).

Similarly, the boundary condition for the electric field is

$$\begin{aligned}E_{\parallel}^a &= \frac{1}{\sqrt{1 + [s'(v)]^2}} [E_x^a + s'(v)E_z^a] \\ &= \frac{1}{\sqrt{1 + [s'(v)]^2}} [E_x^b + s'(v)E_z^b] = E_{\parallel}^b.\end{aligned}\quad (13)$$

Within the two-band approximation, this condition can be represented as

$$\frac{1}{\varepsilon_a} \begin{pmatrix} -\lambda_0^a J_0(\xi_0^a) & -\lambda_{-1}^a J_1(\xi_{-1}^a)e^{-i\phi} + (k - 2K)J_0(\xi_{-1}^a)g \\ -\lambda_0^a J_{-1}(\xi_0^a)e^{i\phi} + kJ_0(\xi_0^a)g & -\lambda_{-1}^a J_0(\xi_{-1}^a) \end{pmatrix} \begin{pmatrix} C_0^a \\ C_{-1}^a \end{pmatrix} = (a \rightarrow b). \quad (14)$$

From these equations, we can determine the wave number  $\lambda^{a,b}$  along the  $z$  direction and the frequency. To solve these equations, we first rewrite them in a simpler form. If we define  $\varphi$  as the value of Eq. (12),  $C_0$  and  $C_{-1}$  are represented as

$$\begin{pmatrix} C_0^\alpha \\ C_{-1}^\alpha \end{pmatrix} = \frac{1}{J_0(\xi_0^\alpha)J_0(\xi_{-1}^\alpha) + J_1(\xi_0^\alpha)J_1(\xi_{-1}^\alpha)} \times \begin{pmatrix} J_0(\xi_{-1}^\alpha) & -J_1(\xi_{-1}^\alpha)e^{-i\phi} \\ J_1(\xi_0^\alpha)e^{i\phi} & J_0(\xi_0^\alpha) \end{pmatrix} \varphi, \quad (15)$$

where  $\alpha = a, b$ . Since  $g$  is assumed to be small,  $\xi_m^\alpha \equiv \frac{\lambda_m^\alpha g}{K}$  is also small. Therefore we retain up to the first order in  $\xi_m^\alpha$ , and combine Eqs. (12) and (14). Then we have

$$\begin{pmatrix} i\left(\frac{\lambda_0^a}{\varepsilon_a} - \frac{\lambda_0^b}{\varepsilon_b}\right) & -iu(k)g \\ iu(k)g & i\left(\frac{\lambda_{-1}^a}{\varepsilon_a} - \frac{\lambda_{-1}^b}{\varepsilon_b}\right) \end{pmatrix} \varphi = 0, \quad (16)$$

where

$$\begin{aligned}u(k) &= \frac{1}{2K} \left( \frac{\lambda_0^a \lambda_{-1}^a}{\varepsilon_a} - \frac{\lambda_0^b \lambda_{-1}^b}{\varepsilon_b} \right) \Big|_{g=0} \\ &\quad - k \left( 1 - \frac{k}{2K} \right) \left( \frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b} \right)\end{aligned}\quad (17)$$

is evaluated for zero order in  $g$ . This equation is our basic equation for the two-band model for 1D plasmonic crystals. Notice that when  $\lambda$ 's are pure imaginary numbers and  $u(k)$  is a real function, Eq. (16) is a Hermitian problem with a zero eigenvalue.

### C. Eigenfrequency of the SPP on the zone boundary

Subsequently, we solve the basic equation (16) and derive the frequency of the SPP at the zone boundary  $k = K$ . First we see that, for  $g = 0$ , Eq. (16) reproduces the result of the free SPP in the previous section. When  $g = 0$ , the free SPPs are degenerate on the zone boundary  $k = K$ , and we have

$\lambda_0^\alpha = \lambda_{-1}^\alpha = \lambda^\alpha$ . We can then derive the result

$$\lambda^a = -iK\sqrt{\left|\frac{\varepsilon_a}{\varepsilon_b}\right|}, \quad \lambda^b = iK\sqrt{\left|\frac{\varepsilon_b}{\varepsilon_a}\right|}, \quad (18)$$

which agrees with Eq. (5).

Next we consider the case  $g \neq 0$ . At the zone boundary, because of  $\lambda_0^\alpha = \lambda_{-1}^\alpha = \lambda^\alpha$ , the nontrivial solution for Eq. (16) exists when

$$\frac{\lambda^a}{\varepsilon_a} - \frac{\lambda^b}{\varepsilon_b} = \pm i g u(K). \quad (19)$$

From Eq. (17),  $u(k)$  can be calculated in the zeroth order in  $g$  as

$$u(K) = -K \left( \frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b} \right). \quad (20)$$

As previously mentioned, the frequency  $\omega$  is given by  $c\sqrt{k^2 + \lambda^2}$ , and  $\omega$  in region  $a$  ( $u < 0$ ) is equal to that in region  $b$  ( $u > 0$ ). Therefore we have

$$\omega = \sqrt{\frac{k^2 + (\lambda^a)^2}{\varepsilon_a \mu_0}} = \sqrt{\frac{k^2 + (\lambda^b)^2}{\varepsilon_b \mu_0}}. \quad (21)$$

The wave number  $\lambda^{a,b}$  along the  $z$  direction and the frequency can be determined by this relation and Eq. (19). Up to first order in  $g$ , we get

$$\omega_\pm^2 = \frac{K^2}{\mu_0} \left( \frac{1}{\varepsilon_a} + \frac{1}{\varepsilon_b} \pm 2g\sqrt{\frac{1}{|\varepsilon_a \varepsilon_b|}} \right). \quad (22)$$

The result shows that the dispersion of the SPP in a 1D plasmonic crystal is gapped and the gap width is approximately proportional to the perturbation  $g$ . This picture coincides with the two-band theory of electrons in a crystal.<sup>18</sup> (See Fig. 3.)

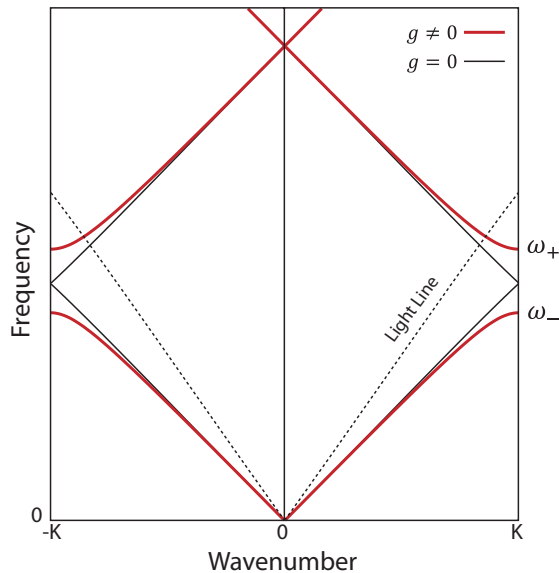


FIG. 3. (Color online) A schematic picture of the SPP dispersion on the flat surface (black line), SPP dispersion on the corrugated surface (red line), and light dispersion in the vacuum (dashed line).  $\omega_\pm$  is the eigenfrequency of the SPP on the zone boundary.

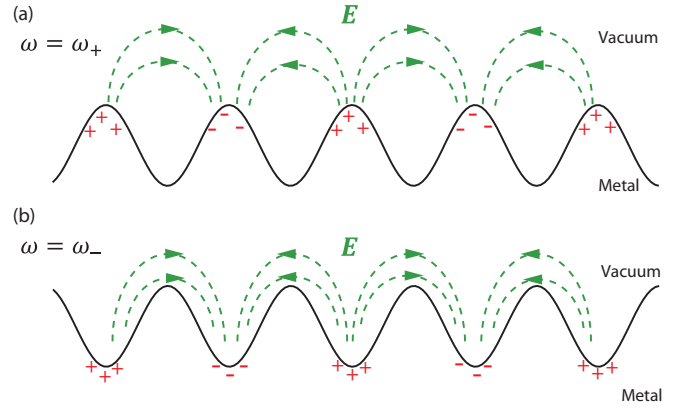


FIG. 4. (Color online) A schematic picture of the electric field and charge distribution when the wave number is on the zone boundary. “+” and “-” signs denote charge distribution and the arrows represent the electric field. (a) When  $\omega = \omega_+$ , the electric field has its nodes on the peaks of the metal surface. (b) When  $\omega = \omega_-$ , the electric field has its nodes on the valleys of the metal surface.

The wave function can also be determined from Eq. (16) as

$$\varphi = \begin{pmatrix} 1 \\ \pm i e^{i\phi} \end{pmatrix} \approx \begin{pmatrix} C_0^\alpha \\ C_{-1}^\alpha \end{pmatrix}. \quad (23)$$

The upper sign corresponds to  $\omega_+$  while the lower sign corresponds to  $\omega_-$ . The distribution of electromagnetic fields is given by substituting  $C_0^\alpha$  and  $C_{-1}^\alpha$  into Eq. (11),

$$\begin{aligned} E_x &\propto \sqrt{\frac{1 \mp \sin(2Kx + \phi)}{2}} \cos(Kx + \omega t - \phi/2) e^{-i\lambda_\alpha z}, \\ E_z &\propto \sqrt{\frac{1 \pm \sin(2Kx + \phi)}{2}} \cos(Kx + \omega t - \phi/2) e^{-i\lambda_\alpha z}, \\ H_y &\propto \sqrt{\frac{1 \mp \sin(2Kx + \phi)}{2}} \cos(Kx + \omega t - \phi/2) e^{-i\lambda_\alpha z}. \end{aligned} \quad (24)$$

A sketch of the electric field distribution is shown in Fig. 4. Because  $s(x) = (g/K)\sin(2Kx + \phi)$ , this result implies the charge distribution near the metal surface. When the eigenfrequency on the zone boundary is  $\omega_+$ , charges concentrate on the peaks of the metal surface. In contrast, when the eigenfrequency is  $\omega_-$ , charges concentrate on the valleys of the metal surface.

In the previous work by Barnes *et al.*,<sup>12,13</sup> the eigenfrequency on the zone boundary is

$$\omega^2 = \frac{K^2}{\mu_0} \left( \frac{1}{\varepsilon_a} + \frac{1}{\varepsilon_b} \right) (1 - 2g^2) \pm 2g \frac{K^2}{\mu_0 \sqrt{|\varepsilon_a \varepsilon_b|}} (1 - 3g^2). \quad (25)$$

Our result coincides with theirs in the first order in  $g$ .

#### D. Eigenfrequency away from the zone boundary

Next, we solve the problem for  $0 < k < K$ . When a wave number is apart from the zone boundary, the upper and lower bands are not degenerated any more even when  $g = 0$ . If we focus on the lower band, the zeroth order of  $\lambda_0^{a,b}$  is equal to that in Eq. (5). Since the eigenfrequency can be represented

using  $\lambda_{0,-1}^{a,b}$  as

$$\omega = \sqrt{\frac{k^2 + \lambda_0^{a,b}}{\varepsilon_{a,b}\mu_0}} = \sqrt{\frac{(k-2K)^2 + \lambda_{-1}^{a,b}}{\varepsilon_{a,b}\mu_0}}, \quad (26)$$

$\lambda_{-1}^{a,b}$  can be expressed in terms of  $\lambda_0^{a,b}$  as

$$\begin{aligned} \lambda_{-1}^a &= -i\sqrt{-(\lambda_0^a)^2 - 4K(k-K)}, \\ \lambda_{-1}^b &= i\sqrt{-(\lambda_0^b)^2 - 4K(k-K)}, \end{aligned} \quad (27)$$

and the first term of  $u(k)$  in Eq. (17) becomes

$$\begin{aligned} &\frac{1}{2K} \left( \frac{\lambda_0^a \lambda_{-1}^a}{\varepsilon_a} - \frac{\lambda_0^b \lambda_{-1}^b}{\varepsilon_b} \right) \Big|_{g=0} \\ &= -\frac{k}{2K} \left( \sqrt{\frac{k^2}{\varepsilon_a^2} + \frac{4K(k-K)}{\varepsilon_a \varepsilon_b}} + \sqrt{\frac{k^2}{\varepsilon_b^2} + \frac{4K(k-K)}{\varepsilon_a \varepsilon_b}} \right). \end{aligned} \quad (28)$$

We now solve the basic equation (16) up to the lowest order in  $g$ . In contrast to the previous section, the solution depends on the second order in  $g$ . From Eq. (16), the relation between  $\lambda_0^a$  and  $\lambda_0^b$  is

$$\frac{\lambda_0^a}{\varepsilon_a} - \frac{\lambda_0^b}{\varepsilon_b} = -i \frac{u(k)^2}{D(k)} g^2, \quad (29)$$

where  $D(k)$  is represented by the zeroth order of  $(\lambda_{-1}^a/\varepsilon_a) - (\lambda_{-1}^b/\varepsilon_b)$ ,

$$\begin{aligned} -iD(k) &= \frac{\lambda_{-1}^a}{\varepsilon_a} - \frac{\lambda_{-1}^b}{\varepsilon_b} \Big|_{g=0} \\ &= \sqrt{\frac{4K(k-K)}{\varepsilon_a^2} + \frac{k^2}{\varepsilon_a \varepsilon_b}} - \sqrt{\frac{4K(k-K)}{\varepsilon_b^2} + \frac{k^2}{\varepsilon_a \varepsilon_b}}. \end{aligned} \quad (30)$$

Finally, we have the frequency  $\omega_I$  away from the zone boundary as

$$\omega_I(k)^2 = \frac{k^2}{\mu_0} \left( \frac{1}{\varepsilon_a} + \frac{1}{\varepsilon_b} \right) + \frac{2k}{\mu_0} \frac{\varepsilon_a \varepsilon_b}{\varepsilon_a - \varepsilon_b} \sqrt{\frac{1}{|\varepsilon_a \varepsilon_b|} \frac{u(k)^2}{D(k)}} g^2, \quad (31)$$

and the eigenfunction is

$$\varphi = \begin{pmatrix} i e^{-i\phi} D(k) \\ u(k)g \end{pmatrix}. \quad (32)$$

The frequency now depends on the second order in  $g$ . This dependence also coincides with the band theory of electrons in crystals. Notice that  $D(k)$  vanishes when the wave number is on the zone boundary, and the present approximation breaks down. In such a case the correction term to the frequency is linear in  $g$ , as in Eq. (22).

So far we have seen how the gap behaves at the zone boundary [Eq. (22)] and away from the zone boundary [Eq. (31)]. In the following we calculate the frequency which describes a crossover between the two cases near the zone

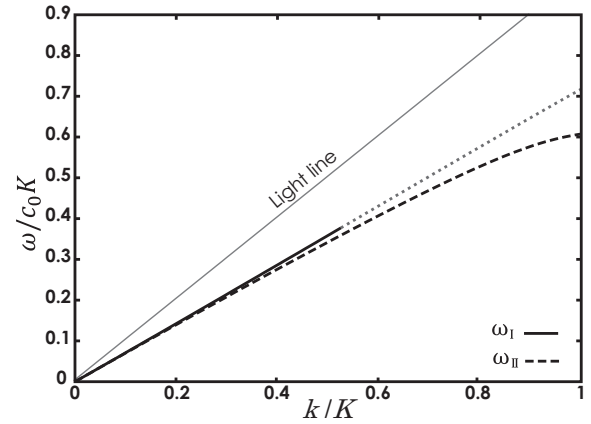


FIG. 5. The SPP dispersions of the lower band.  $\omega_I$  (solid line) represents the expression (31) for the eigenfrequency away from zone boundary, and  $\omega_{II}$  (dashed line) is the expression (33) for the eigenfrequency describing the crossover.  $c_0$  is the speed of light in the vacuum. We put  $g = 0.01$ , and the permittivity  $\varepsilon_a = \varepsilon_0$  and  $\varepsilon_b = -2\varepsilon_0$ , where  $\varepsilon_0$  is the vacuum permittivity.

boundary. We expand the frequency and wave number near the zone boundary:

$$\begin{aligned} \omega_{II} &= \omega_0 + \delta\omega, \quad k = K + \delta k, \\ \omega_0^2 &= \frac{K^2}{\mu_0} \left( \frac{1}{\varepsilon_a} + \frac{1}{\varepsilon_b} \right). \end{aligned}$$

Then  $\lambda_{0,-1}$  and  $u(k)$  in the basic equation (16) can be expanded in terms of  $\delta\omega$  and  $\delta k$ , and a straightforward calculation gives

$$\delta\omega^2 = \frac{\delta k^2}{\mu_0} \left( \frac{1}{\varepsilon_a} + \frac{1}{\varepsilon_b} \right) - \frac{\varepsilon_a^2 \varepsilon_b^2}{\mu_0 (\varepsilon_a + \varepsilon_b) (\varepsilon_a - \varepsilon_b)^2} u(k)^2 g^2. \quad (33)$$

It can be verified that  $\omega_{II}$  coincides with Eq. (22) when  $\delta k = 0$ , and coincides with Eq. (31) when  $g \ll \delta k/K$ , as shown in our numerical calculation in Fig. 5.

### III. DISCUSSION

Our basic equation (16) becomes Hermitian when the wave numbers along the  $z$  direction,  $\lambda_{0,-1}$ , are purely imaginary. This hermiticity means that the eigenmode does not decay in time. It coincides with the fact that the eigenfrequency of the SPP is smaller than the frequency of light and it is outside of the light line. This condition is automatically satisfied in metals with a flat surface and in the lowest band of 1D plasmonic crystals. In contrast to the previous work of 1D plasmonic crystals done by Barnes *et al.*,<sup>12,13</sup> our eigenvalue equation is Hermitian, and the perturbation theory is developed in a controlled manner, thereby we can derive the frequency away from the zone boundary. The perturbation expansion in this paper is exact up to the calculated order. We note that to reproduce the realistic SPP dispersion, the frequency dependence of the permittivity  $\varepsilon_b$  of the metal is crucial. Within our theory it can be incorporated into (16), and we can determine the dispersion of the SPP, as has been done, e.g., in Ref. 15.



On the other hand, for the upper band,  $\lambda_0^a$  in the Eq. (16) can be expressed by the zeroth order of  $\lambda_{-1}^a$  in  $g$  as

$$\begin{aligned} (\lambda_0^a)^2 &= (k - 2K)^2 - k^2 + (\lambda_{-1}^a)^2 \Big|_{g=0} \\ &= (k - 2K)^2 \left( 1 - \left| \frac{\varepsilon_a}{\varepsilon_b} \right| \right) - k^2 \\ &= (\omega_{\text{SPP}}/c_0)^2 - k^2, \end{aligned}$$

where  $\omega_{\text{SPP}}$  is the frequency of the SPP on a flat surface [Eq. (6)]. When the eigenfrequency is inside the light cone, i.e., when  $\omega_{\text{SPP}}$  is larger than the frequency of light in vacuum  $c_0 k$ ,  $\lambda_0^a$  becomes real and the matrix in Eq. (16) becomes non-Hermitian. This corresponds to the fact that SPPs in the light cone usually couple with the electromagnetic wave in the vacuum and are radiated, except for special cases.<sup>19</sup> The radiation of SPPs inhibits the realization of plasmonic devices. Nevertheless, the experimental solution for this radiation problem is proposed, and it might still be useful for applications.<sup>20</sup>

Equation (31) shows that the dependence of the eigenfrequency on the surface corrugation  $g$  is from the second order in  $g^2$  away from the zone boundary. The approximation applied in Eq. (31) is broken near the zone boundary. In contrast, the eigenfrequency and the band gap at the zone boundary depends linearly in  $g$ , as shown in Eq. (22). The upper and lower bands of the free SPPs are degenerated only at the zone boundary and the singularity due to this degeneracy causes the difference between the zone boundary and away from it. As mentioned above, such a behavior of SPPs coincides with the usual two-band model for electrons in crystals. However, it is important to keep in mind that the Hamiltonian of our system is the same as the flat surface. The band structure of the SPPs is not caused by any perturbation Hamiltonian but the boundary condition of the eigenvalue problem.

We explain here how the present work is different from the previous works on SPP dispersion in 1D plasmonic crystals. In Refs. 12, 13, and 16 the SPP dispersion is calculated from the matching conditions of the electromagnetic fields at the interface. On the other hand, Refs. 14 and 15 are based on the

theory of the scattering problem of electromagnetic waves at the interface. Our method is similar to the former one, but the important difference from the previous papers is that we derived an eigenvalue equation for a Hermitian matrix. Because of this hermiticity, we can apply the perturbation theory systematically by using the eigenvalue equation, and the validity of the approximation is guaranteed, as is the case for the electronic band theory in solids. Such Hermitian eigenvalue equations are also useful for describing phenomena caused by Berry's phase, as have been applied in magnons in ferromagnets<sup>21,22</sup> and photons.<sup>23,24</sup>

In the present paper, we have assumed that the plasmonic crystal is made from a single metal. We note that our method is expected to apply for general metallic or dielectric structures with spatial periodicity, such as metal nanostructures and photonic crystals. In these cases, the eigenfrequency of the SPPs is determined from multiboundary conditions, thereby wave functions and band structures near and far from the Brillouin zone boundary can be studied in a similar way.

#### IV. CONCLUSION

We have theoretically investigated the plasmonic band structure in 1D plasmonic crystals. The effective two-band model is introduced and the basic equation is derived from matching conditions of electromagnetic fields at the metal surface. Our eigenvalue equation is Hermitian. When the wave number is on the zone boundary, our solution indicates the plasmonic band gap and its physical picture coincides with the previous work. Even if the wave number is away from the zone boundary, the wave number and corrugation dependences of the SPP modes coincide with the usual two-band theory of electrons in solids.

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