Additional-boundary-condition-free theory of an exciton polariton in a slab

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The electric field associated with an exciton polariton in a slab of spatially dispersive medium has been calculated "from first principles" according to the general framework by Cho in which the argument of additional boundary condition (ABC) is completely avoided. As the exciton wave function, we have considered, in addition to the bulk component, the distortion of the type $\exp(-PZ)$ near the surfaces according to the analytic model of D'Andrea and Del Sole, and the slab thickness d has been assumed to satisfy $\exp(-Pd) \ll 1$. The result has been shown to be equivalent to that obtained from the explicit use of ABC on the same model. In this way, it is demonstrated that the ABC-free formalism is not only of conceptual, but also of practical, use.

I. INTRODUCTION

For spatially dispersive media specified by explicit wave-vector (k) dependence of bulk dielectric function $\epsilon(k,\omega)$, the dispersion relation of transverse-mode polariton in the bulk is given by the solution of the equation

$$\epsilon(k,\omega)=c^2k^2/\omega^2 \; . \tag{1.1}$$

This provides the solution $k(\omega)$ as a multivalued function because of the k dependence of the dielectric function. Namely, when an external light with frequency ω is incident on this medium, there arise several modes of polaritons in the medium. Therefore, additional boundary conditions (ABC's) are usually required, in addition to Maxwell boundary conditions (MBC's), to uniquely determine the relative amplitudes of the polariton modes. This is well known as the ABC problem,[1] and has been studied from various viewpoints for about 30 years since the first treatment by Pekar.[2]

After careful consideration, it has become clear that the solution of this problem is obtained solely from the Maxwell equation of the (finite or semi-infinite) medium in consideration,

$$\text{rot rot}\, \mathcal{E}(\mathbf{R})-(\omega^2/c^2)\mathcal{E}(\mathbf{R}) -(4\pi\omega^2/c^2)\int d\mathbf{R}'\,\chi(\mathbf{R},\mathbf{R}')\mathcal{E}(\mathbf{R}')=0 \; , \tag{1.2}$$

where the electric field $\mathcal{E}$ and polarizability χ refer to frequency ω, and the integration is done over the medium. As a first-principles theory, χ must be calculated from the eigenvalues and the eigenfunctions of the system through the linear response theory. Thereby, the quantum-mechanical boundary condition must be properly considered. Historically, there have been two types of description of the solutions of Eq. (1.2); the traditional one, which explicitly deals with the form of the ABC (ABC theory),[3-6] and a new one, which never refers to the ABC (ABC-free theory).[7]

In the ABC theory, bulk polaritons are found to be the possible solutions of (1.2). At the same time, one finds the condition(s) to be satisfied among the coefficients of bulk polaritons, which play the role of the ABC. In order to carry out the whole program, one must (i) calculate the energies and wave functions of the system, with explicit consideration of the boundary condition, (ii) calculate $\chi(\mathbf{R},\mathbf{R}';\omega)$ in a closed form, and (iii) solve Eq. (1.2). Before the full step [(i)–(iii)] calculations[3-6] were presented, it had been demonstrated in terms of (macroscopic) model susceptibilities, i.e., those without the step (i), that Eq. (1.2) contains all the necessary information including the ABC.[8-10]

In the ABC-free theory, one makes use of the characteristic form of $\chi(\mathbf{R},\mathbf{R}')$ to solve Eq. (1.2). Quite generally from linear-response theory, one may write

$$\chi(\mathbf{R},\mathbf{R}')=\sum_{\lambda}\bar{\chi}_{\lambda}(\omega)\rho_{\lambda}^{*}(\mathbf{R})\rho_{\lambda}(\mathbf{R}') \; , \tag{1.3}$$

where λ refers to the quantum number of excited states. This form of integral kernel allows us to solve Eq. (1.2) without referring to the ABC. According to this formalism, one need not calculate χ in a closed form; that is, step (ii) can be omitted. The summation over λ appears in the final expression of $\mathcal{E}(\mathbf{R})$, and, after the summation, bulk polariton modes emerge in the case of the semi-infinite medium. Since the ABC-free theory is based on the general form of $\chi(\mathbf{R},\mathbf{R}')$, it can be applied also to such systems as very thin films and quantum wells (QW's), where no bulk polaritons are expected.

Although the ABC and ABC-free theories give physically equivalent results, their feasibility may not be always the same with respect to the model systems to be considered. Therefore, it is of theoretical interest to see the range of applicability of the ABC-free method. In Ref. 7, one considers a very simple example, i.e., the case of no-escape boundary conditions without distortion of wave functions at the surfaces of a slab, and derives a result equivalent to Pekar's ABC. In this paper, we take a more realistic model for excitons, i.e., the analytic model of D'Andrea and Del Sole (DA-DS) (Ref. 4) applied to a slab. In this model, exciton wave functions are allowed to be distorted near the surfaces according to a single evanescent wave of the form $\exp(-PZ)$. The same model has been treated by Cho and Kawata[5] and Cho and Ishihara,[6] at progressive levels of approximation, from the viewpoint of the ABC theory. The later work, with which we want to compare the present result in a later section, is based on a single approximation,

$\exp(-Pd) \ll 1$, where d is the thickness of the slab. It would be useful to show the ability of the ABC-free theory by demonstrating an equivalent result to that of the ABC theory. With this result, the ABC-free theory proves itself to be not only a useful concept, but also a practical method.

Before we show the details of our calculation, a brief explanation of the ABC-free theory is given in Sec. II. In Sec. III, a detailed calculation, based on the DA-DS model applied to a slab, is carried out according to the ABC-free formalism, and it is shown that the final result is physically equivalent to our previous one obtained from the ABC theory.[6] Section IV is allotted for discussion.

A brief summary of the ABC and ABC-free theories for a slab of DA-DS–type model is reported in Ref. 11.

II. OUTLINE OF THE ABC-FREE THEORY

As we mentioned in Sec. I, the starting point of the ABC-free theory is the same Maxwell equation, (1.2), as in the ABC theory. The essential point of this formulation is based on the general form of polarizability $\chi(\mathbf{R},\mathbf{R}';\omega)$ in site representation which is to be used as the kernel in this integro-differential equation, (1.2). Generally $\chi(\mathbf{R},\mathbf{R}';\omega)$ can be written in the form of (1.3), i.e., a sum of the products of functions of $\mathbf{R}$ and $\mathbf{R}'$ respectively. This is clear from linear response theory, according to which the polarizability (at 0 K, for simplicity) is expressed as

$$\chi(\mathbf{R},\mathbf{R}';\omega)=(1/\hbar V_0^2)\sum_\lambda \left\{ \frac{\langle 0|\mathbf{P}(\mathbf{R})|\lambda\rangle\langle\lambda|\mathbf{P}(\mathbf{R}')|0\rangle}{\omega_\lambda-\omega-i\Gamma} + \frac{\langle 0|\mathbf{P}(\mathbf{R}')|\lambda\rangle\langle\lambda|\mathbf{P}(\mathbf{R})|0\rangle}{\omega_\lambda+\omega+i\Gamma} \right\} , \tag{2.1}$$

where λ stands for the quantum number of the system with excitation energy $\hbar\omega_\lambda$, V_0 is the volume of one of the small cells into which the whole medium is divided, $\mathbf{P}(\mathbf{R})$ is the polarization density operator for electrons integrated over the cell at $\mathbf{R}$, and Γ is a phenomenologically introduced damping constant. [In Eq. (2.3) of Ref. 7, V_0 must be replaced with V_0^2.] All the information about the bulk and surface are included in $\{\hbar\omega_\lambda, |\lambda\rangle\}$. Putting aside the nonresonant terms as a background constant, we can rewrite $\chi(\mathbf{R},\mathbf{R}';\omega)$ in the form of (1.3) with the following definitions:

$$\bar{\chi}_\lambda(\omega)=(\mu^2/\hbar V_0)/(\omega_\lambda-\omega-i\Gamma) , \tag{2.2}$$

$$\rho_\lambda(\mathbf{R})=\langle\lambda|\mathbf{P}(\mathbf{R})|0\rangle/\mu V_0^{1/2} , \tag{2.3}$$

where μ is a constant with the dimension of dipole moment. All the information of the bulk and surface wave functions is included in $\rho_\lambda(\mathbf{R})$.

Considering the case of the normal incidence of external light to a slab of thickness d, we have only to deal with the surface-normal (Z) components of $\mathbf{R}$ and $\mathbf{R}'$, so that (1.3) can be replaced by

$$\chi(Z,Z')=\sum_\lambda \bar{\chi}_\lambda(\omega)\rho_\lambda^*(Z)\rho_\lambda(Z') . \tag{1.3'}$$

Substituting (1.3') in Eq. (1.2) [where $(\mathbf{R},\mathbf{R}')$ are replaced with (Z,Z')], we can reduce this integro-differential equation to the following second-order differential equation:

$$d^2\mathcal{E}(Z)/dZ^2+q^2\mathcal{E}(Z)+Q^2\sum_\lambda \bar{\chi}_\lambda(\omega)\rho_\lambda^*(Z)F_\lambda=0 , \tag{2.4}$$

where

$$F_\lambda=\int_0^d \rho_\lambda(Z)\mathcal{E}(Z)dZ , \tag{2.5}$$

$$q^2=\varepsilon_0\omega^2/c^2, \quad Q^2=4\pi\omega^2/c^2 , \tag{2.6}$$

where ε_0 is the background constant to which the nonresonant terms of polarizability contributes. In this one-dimensional formulation, $\rho_\lambda(Z)$ should be redefined as (2.3) multiplied by a certain length. Thus, the problem is just to solve the second-order differential equation (2.4) in a consistent way with (2.5). Since we may regard $\{F_\lambda\}$ as given constants, the general solution of (2.4) can be written as

$$\mathcal{E}(Z)=\mathcal{E}_1 e^{iqZ}+\mathcal{E}_2 e^{iq\bar{Z}}-\sum_\lambda G_\lambda(Z)F_\lambda , \tag{2.7}$$

where

$$G_\lambda(Z)=(Q^2\bar{\chi}_\lambda(\omega)/2iq)\int_0^d e^{iq|Z-Z'|}\rho_\lambda^*(Z')dZ' , \tag{2.8}$$

$$\bar{Z}=d-Z , \tag{2.9}$$

$\mathcal{E}_1$ and $\mathcal{E}_2$ are arbitrary constants, and we have used the identity

$$(d^2/dZ^2+q^2)e^{iq|Z-Z'|}=2iq\delta(Z-Z') . \tag{2.10}$$

Substituting (2.7)–(2.9) in (2.5), we obtain the linear simultaneous equations to determine the expansion coefficients $\{F_\lambda\}$ of the electric field as

$$F_\lambda=\mathcal{E}_1\int \rho_\lambda(Z)e^{iqZ}dZ+\mathcal{E}_2\int \rho_\lambda(Z)e^{iq\bar{Z}}dZ - \sum_{\lambda'} F_{\lambda'}\int G_{\lambda'}(Z)\rho_\lambda(Z)dZ . \tag{2.11}$$

Evidently, the solution of this equation has the form

$$F_\lambda=a_\lambda\mathcal{E}_1+b_\lambda\mathcal{E}_2 . \tag{2.12}$$

From (2.7) and (2.12), it is clear that the final expression of $\mathcal{E}(Z)$ contains only two arbitrary constants, $\mathcal{E}_1$ and $\mathcal{E}_2$.

Thus, according to the ABC-free theory, the electric field $\mathcal{E}(Z)$ in the slab can be directly calculated in the form which contains the minimum number of arbitrary constants. Therefore, just a set of MBC is enough for the unique connection of the external and internal fields across the surfaces; that is, no discussion of ABC is necessary in this theory. In the limit of the semi-infinite slab ($d\to\infty$), the summation over λ yields bulk polariton waves in (2.7) as shown in Ref. 7, and in that way, we can compare the result of this theory with that of the ABC theory. However, for finite d, the summation in (2.7) leads, not to bulk polaritons, but to the eigenmodes of the finite d slab. In this way, this approach can be used for any thickness of the slab, including QW's. Moreover, the fact that the closed form of $\chi(Z,Z';\omega)$ is not necessary in this formalism could, in some cases, be more advantageous than the ABC theory.

A problem to be encountered in practice is how to solve the equations for $\{F_\lambda\}$, (2.11), especially when the number of $\{F_\lambda\}$ is infinite. In general, we can simply say that we should take a method suitable for each specific model. In the case of the DA-DS–type model for a slab, it is shown that Eq. (2.11) can be rewritten into two simultaneous linear equations for two different linear combinations of $\{F_\lambda\}$, with which the field expression (2.7) is given completely. This allows us to evaluate the field in the slab, which turns out to be equivalent to that of our previous work[6] according to the ABC theory.

III. CALCULATION OF ELECTRIC FIELD IN THE SLAB

The model of DA-DS for the first-principles calculation of ABC in the case of a semi-infinite medium is as follows: (i) Both conduction and valence bands are nondegenerate and parabolic. (ii) The crystal surface acts as a hard wall to both electrons and holes. (iii) The image potential for an exciton near the surface is neglected. (iv) Only the 1s exciton is explicitly treated as a resonant term of $\chi(\mathbf{R},\mathbf{R}';\omega)$. The contribution from other excited states of the exciton is considered as a constant background polarizability. (v) The distortion of the exciton wave function near the surface is explicitly taken into account. For the analytic treatment, its translational part is approximated by a single evanescent wave of the form e^{-PZ}. For a slab, a similar distortion is supposed to occur on both surfaces.

In the application of the ABC-free theory outlined in Sec. II to the above model, we take for the quantum number λ the translational wave vector K of the exciton. In the following, we confine ourselves to the case of normal incidence of light. It is easy to extend the treatment to the oblique incidence (s polarization). Then, the quantities $\bar{\chi}_K(\omega)$, $\rho_K(Z)$ to define the polarizability (1.3) are given as

$$\bar{\chi}_K(\omega)=B/[Q^2(K^2-q_0^2)] , \tag{3.1}$$

$$\rho_K(Z)=N(K)[e^{-iKZ}+A_K e^{iKZ}-(1+A_K)e^{-PZ} -(e^{-iKd}+A_K e^{iKd})e^{-P\bar{Z}}] , \tag{3.2}$$

where

$$N(K)=\left[2d-\frac{4}{P}\frac{P^2-K^2}{P^2+K^2}\right]^{-1/2} , \tag{3.3}$$

is the normalization factor of the wave function,

$$q_0=[2M(\hbar\omega-E_{1s}+i\hbar\Gamma)]^{1/2}/\hbar \quad [\mathrm{Im}(q_0)>0] , \tag{3.4}$$

the wave number of the exciton with total energy $\hbar\omega$, M the translational mass of the exciton, and

$$B=4\pi\omega^2\alpha_0\omega_0 M/c^2\hbar , \tag{3.5}$$

$$\alpha_0=4e^2|P_{vc}|^2|\varphi_{1s}(0)|^2/m_e^2\omega^2\hbar\omega_0 , \tag{3.6}$$

$$\hbar\omega_0=E_{1s} . \tag{3.7}$$

In the above expressions (3.4)–(3.7), $\hbar\Gamma$ is the damping constant of the exciton, P_{vc} the matrix element of the momentum operator between the Bloch states of conduction- and valence-band extrema, and $\varphi_{1s}(0)$ the ground-state wave function of the relative motion with $\mathbf{r}=0$.

The no-escape boundary condition (ii) for electron and hole on both surfaces leads to[5]

$$A_K=\frac{-P+iK}{P+iK} , \tag{3.8}$$

and to the quantization condition of K,

$$Kd-2\tan^{-1}(K/P)=\pi\times(\text{integer}) \text{ or } A_K^2=e^{-2iKd} , \tag{3.9}$$

as long as the following condition holds:

$$e^{-Pd}\ll 1 . \tag{3.9'}$$

Solving the second-order differential equation after the substitution of (3.1)–(3.8) in (2.4), we obtain a similar form of solution as (2.7), where $G_\lambda(Z)$ has the form ($\lambda\to K$):

$$G_K(Z)=-Q^2\bar{\chi}_K(\omega)N(K)\{(e^{iKZ}+A_K^* e^{-iKZ})/(K^2-q^2)-[(1+A_K^*)e^{-PZ}+(e^{ikd}+A_K^* e^{-iKd})e^{-P\bar{Z}}]/(P^2+q^2)\} . \tag{3.10}$$

Substituting this solution in the definition of F_K, (2.5), we obtain

$$F_K=C_K N(K)\left[D_K-\frac{(1+A_K)B_1+(e^{-iKd}+A_K e^{iKd})B_2}{(P^2+q^2)2P}\right] , \tag{3.11}$$

where

$$C_K=\{1-[N(K)]^2Q^2\bar{\chi}_K(\omega) \times[2d-4P/(P^2+K^2)]/(K^2-q^2)\}^{-1} , \tag{3.12}$$

$$D_K=\int_0^d[N(K)]^{-1}\rho_K(Z)(\mathcal{E}_1 e^{iqZ}+\mathcal{E}_2 e^{iq\bar{Z}})dZ , \tag{3.13}$$

$$B_1=\sum_K Q^2N(K)\bar{\chi}_K(\omega)(1+A_K^*)F_K , \tag{3.14a}$$

$$B_2=\sum_K Q^2N(K)\bar{\chi}_K(\omega)(e^{iKd}+A_K^* e^{-iKd})F_K . \tag{3.14b}$$

In deriving (3.11)–(3.14), we have taken advantage of the following relation which is characteristic of this model:

$$\int_0^d(e^{-iKZ}+A_K e^{iKZ})(e^{iK'Z}+A_{K'}^* e^{-iK'Z})dZ =\delta_{K,K'}[2d-4P/(P^2+K^2)] . \tag{3.15}$$

The simplicity of the present model is that Eqs. (3.14a) and (3.14b), together with (3.11), provide a closed set of linear simultaneous equations of B_1 and B_2. These equations can be solved as

$$B_1=(\alpha\gamma_1-\beta\gamma_2)/(\alpha^2-\beta^2)\ , \quad (3.16a)$$

$$B_2=(\alpha\gamma_2-\beta\gamma_1)/(\alpha^2-\beta^2)\ , \quad (3.16b)$$

where

$$\alpha=1+\left[\frac{1}{(P^2+q^2)2P}\right]\sum_K C_K[N(K)]^2Q^2\bar{\chi}_K(\omega)\times(2+A_K+A_K^*)\ , \quad (3.17a)$$

$$\beta=\left[\frac{1}{(P^2+q^2)2P}\right]\times\sum_K C_K[N(K)]^2Q^2\bar{\chi}_K(\omega)\times(e^{iKd}+e^{-iKd}+A_Ke^{iKd}+A_K^*e^{-iKd})\ , \quad (3.17b)$$

$$\gamma_1=\sum_K C_KN(K)Q^2\bar{\chi}_K(\omega)(1+A_K^*)D_K\ , \quad (3.17c)$$

$$\gamma_2=\sum_K C_KN(K)Q^2\bar{\chi}_K(\omega)(e^{iKd}+A_K^*e^{-iKd})D_K\ . \quad (3.17d)$$

From (3.10), (3.11), and (3.16), we see that the field $\mathcal{E}(Z)$, (2.7), is expressed only in terms of the known quantities. Now, if we note the definitions of $\bar{\chi}_K(\omega)$, (3.1), and $N(K)$, (3.3), the factor C_K, (3.12), which is contained in F_K, can be rewritten as

$$C_K=\frac{(K^2+\bar{P}^2)(K^2-q^2)(K^2-q_0^2)}{(K^2+\bar{P}^2)(K^2-q_0^2)(K^2-q^2)-B\left[\dfrac{K^2}{1+\tau}+\bar{P}^2\right]}\ , \quad (3.12')$$

where

$$\bar{P}^2=\frac{1-\tau}{1+\tau}P^2\ , \quad (3.18)$$

$$\tau=2/(Pd)\ . \quad (3.19)$$

It is remarkable that the equation to determine the poles of C_K,

$$(K^2+\bar{P}^2)(K^2-q_0^2)(K^2-q^2)=B\left[\frac{K^2}{1+\tau}+\bar{P}^2\right]\ , \quad (3.20)$$

is the equation to fix the dispersion relation of the polaritons in the slab.[6] Since F_K also has the same poles, we see that these eigenmodes of the slab certainly appear in the final expression of the electric field after the summation over K in (2.7). Beside these poles, the product $F_KG_K(Z)$ has another set of poles $K=\pm q$ through D_K. These poles lead to the modes with wave number $\pm q$ after the summation over K, and they just cancel the background field, $\mathcal{E}_1\exp(iqZ)+\mathcal{E}_2\exp(iq\bar{Z})$, in (2.7); that is, the extinction theorem holds true for this model. In terms of B_1 and B_2, the field $\mathcal{E}(Z)$ is expressed as

$$\mathcal{E}(Z)=\mathcal{E}_1e^{iqZ}+\mathcal{E}_2e^{iq\bar{Z}}+S(Z)-B_1T(Z)/[(P^2+q^2)2P]-B_2T(\bar{Z})/[(P^2+q^2)2P]+B_1e^{-PZ}/(P^2+q^2)+B_2e^{-P\bar{Z}}/(P^2+q^2)\ , \quad (3.21)$$

where

$$S(Z)=Q^2\sum_K C_K[N(K)]^2\bar{\chi}_K(\omega)\frac{e^{iKZ}+A_K^*e^{-iKZ}}{K^2-q^2}D_K\ , \quad (3.22a)$$

$$T(Z)=Q^2\sum_K C_K[N(K)]^2\bar{\chi}_K(\omega)\frac{e^{iKZ}+A_K^*e^{-iKZ}}{K^2-q^2}(1+A_K)\ . \quad (3.22b)$$

The summations over K in (3.17) and (3.22) can be converted to contour integrals in the complex K plane, where the contour picks up all the quantized values of K on the real axis. Then, by deforming the contour, each of the integrals is evaluated at the complex poles of the integrand. The evaluation of $\{S(Z),T(Z),\alpha,\beta,\gamma_1,\gamma_2\}$ is shown in Appendix A. Using the results of Appendix A, we obtain the final expression of $\mathcal{E}(Z)$, which contains just two arbitrary constants ($\bar{\mathcal{E}}$ and $\tilde{\mathcal{E}}$) as expected from (2.12), as

$$\mathcal{E}(Z)=\sum_{j=1}^{3}(\{\bar{\mathcal{E}}[I_j(P-iq_j)+J_j(P+iq_j)e^{-iq_jd}]-\tilde{\mathcal{E}}[I_j(P+iq_j)e^{-iq_jd}+J_j(P-iq_j)]\}e^{iq_jZ}-\{\bar{\mathcal{E}}[I_j(P+iq_j)e^{-iq_jd}+J_j(P-iq_j)]+\tilde{\mathcal{E}}[I_j(P-iq_j)+J_j(P+iq_j)e^{-iq_jd}]\}e^{iq_j\bar{Z}})+(\tilde{\mathcal{E}}U_1-\bar{\mathcal{E}}U_2)e^{-PZ}+(\bar{\mathcal{E}}U_1-\tilde{\mathcal{E}}U_2)e^{-P\bar{Z}}\ , \quad (3.23)$$

where

$$\bar{\mathcal{E}}=\frac{\mathcal{E}_1P}{P-iq}+\frac{\mathcal{E}_2P}{P+iq}e^{iqd},\quad \tilde{\mathcal{E}}=\frac{\mathcal{E}_1P}{P+iq}e^{iqd}+\frac{\mathcal{E}_2P}{P-iq}\ , \quad (3.24a)$$

$$I_j=S_j[2P(P^2+q^2)(P^2+q_j^2)(\alpha^2-\beta^2)+(q_j^2-q^2)(\alpha H_1+\beta H_2)]\ , \quad (3.24b)$$

$$J_j=S_j(q^2-q_j^2)(\alpha H_2+\beta H_1)\ , \quad (3.24c)$$

$$U_1=\frac{\alpha H_1+\beta H_2}{\alpha^2-\beta^2}\times\left[1+\frac{BP}{Pd+2}\frac{2P}{(P^2+q_1^2)(P^2+q_2^2)(P^2+q_3^2)}\right]\times\frac{1}{(P^2+q^2)P}\ , \quad (3.24d)$$

$$U_2=\frac{\alpha H_2+\beta H_1}{\alpha^2-\beta^2}\times\left[1+\frac{BP}{Pd+2}\frac{2P}{(P^2+q_1^2)(P^2+q_2^2)(P^2+q_3^2)}\right]\times\frac{1}{(P^2+q^2)P}, \quad (3.24e)$$

$$S_j=\tilde{A}_j/[4iP^2(P^2+q^2)(q_j^2+P^2)(q_j^2-q^2)(\alpha^2-\beta^2)], \quad (3.24f)$$

$$H_1=\sum_{j=1}^{3}\tilde{A}_jq_j\cos[q_jd-2\tan^{-1}(q_j/P)], \quad (3.24g)$$

$$H_2=\sum_{j=1}^{3}\tilde{A}_jq_j, \quad (3.24h)$$

$$\tilde{A}_1=\frac{BP}{Pd+2}\frac{d(P^2+q_1^2)-2P}{\sin[q_1d-2\tan^{-1}(q_1/P)]}\times\frac{1}{(q_1^2-q_2^2)(q_1^2-q_3^2)},$$

$$\tilde{A}_2=\tilde{A}_1|_{q_1\leftrightarrow q_2},$$

$$\tilde{A}_3=\tilde{A}_1|_{q_1\leftrightarrow q_3}. \quad (3.24i)$$

The polariton wave numbers (q_j) are the roots of Eq. (3.20), and their signs are defined by $\mathrm{Im}(q_j)>0$.

IV. DISCUSSION

A. Equivalence of ABC and ABC-free theory

We have treated the same microscopic (DA-DS) model for a slab by two different approaches: the ABC-free theory in this paper, and the ABC theory in Ref. 6. Since the solutions satisfy the same Maxwell integro-differential equation, (1.2), the two results should coincide. The solution of the ABC theory contains six parameters, and there are four ABC's relating the six parameters. If we eliminate four of them by using the ABC's, the resulting expression of $\mathcal{E}(Z)$ contains two free parameters. This should be compared with the present result, (3.21). Since the two parameters in each expression can be chosen arbitrarily, we need the following preparation to make the comparison. In Ref. 6, the electric field is given in the form

$$\mathcal{E}(Z)=\sum_{j=1}^{3}(\varepsilon_je^{iq_jZ}+\bar{\varepsilon}_je^{iq_j\bar{Z}})+ge^{-PZ}+\bar{g}e^{-P\bar{Z}}, \quad (4.1)$$

and the four ABC's and the relations between $\{g,\bar{g}\}$ and $\{\varepsilon_j,\bar{\varepsilon}_j\}$ can be written as

$$\begin{bmatrix} a_1 & a_2 & a_3 & b_1\tilde{h}_1 & b_2\tilde{h}_2 & b_3\tilde{h}_3\\ c_1 & c_2 & c_3 & d_1\tilde{h}_1 & d_2\tilde{h}_2 & d_3\tilde{h}_3\\ A_1 & A_2 & A_3 & A_1\tilde{h}_1 & A_2\tilde{h}_2 & A_3\tilde{h}_3\\ b_1\tilde{h}_1 & b_2\tilde{h}_2 & b_3\tilde{h}_3 & a_1 & a_2 & a_3\\ d_1\tilde{h}_1 & d_2\tilde{h}_2 & d_3\tilde{h}_3 & c_1 & c_2 & c_3\\ A_1\tilde{h}_1 & A_2\tilde{h}_2 & A_3\tilde{h}_3 & A_1 & A_2 & A_3 \end{bmatrix}\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \bar{\varepsilon}_1\\ \bar{\varepsilon}_2\\ \bar{\varepsilon}_3\end{bmatrix}=\begin{bmatrix}0\\0\\g\\0\\0\\ \bar{g}\end{bmatrix}, \quad (4.2a)$$

where

$$A_j=(q_j^2-q^2)/(P^2+q^2), \quad (4.2b)$$

$$\tilde{h}_j=e^{iq_jq}, \quad (4.2c)$$

$$a_j=1/(P-iq_j)+(\tilde{m}_1-iq_j)/(q_j^2-q_0^2)-\tilde{m}_2/(\bar{P}^2+q_j^2), \quad (4.2d)$$

$$b_j=a_j|_{q_j\to-q_j}, \quad (4.2e)$$

$$c_j=1/(P-iq_j)+(\tilde{n}_1-iq_j)/(\bar{P}^2+q_j^2)-\tilde{n}_2/(q_j^2-q_0^2), \quad (4.2f)$$

$$d_j=c_j|_{q_j\to-q_j}, \quad (4.2g)$$

$$\tilde{m}_1=-P+\tilde{U}[(1-\tau)P^2+q_0^2]/2P(1+\tau), \quad (4.2h)$$

$$\tilde{m}_2=\tau(1-\tau)P\tilde{U}/2(1+\tau)^2, \quad (4.2i)$$

$$\tilde{n}_1=\bar{P}\left[\frac{2\tau-\nu}{\tau-\nu}+\frac{\tilde{U}}{2}\left[\frac{1-\tau}{1+\tau}\right]^{1/2}\frac{1-\tau+\nu}{1+\tau}\right]\frac{\nu-2}{\nu}, \quad (4.2j)$$

$$\tilde{n}_2=\frac{\tilde{U}}{2P\tau}(P^2+q_0^2-\tau P^2)\frac{1-\tau+\nu}{1+\tau}\frac{\nu-2}{\nu}, \quad (4.2k)$$

$$\nu=(1-4\tau^2)^{1/2}, \quad (4.2l)$$

$$\tilde{U}=B/[(P^2+q^2)(\bar{P}^2+q_0^2)]. \quad (4.2m)$$

We regard (4.2a) as relations to define $\{\varepsilon_j,\bar{\varepsilon}_j\}$ in terms of two parameters g and $\bar{g}$. On the other hand, the electric field from the ABC-free theory, (3.21), can be rewritten as

$$\mathcal{E}(Z)=\sum_{j=1}^{3}(f_je^{iq_jZ}+\bar{f}_je^{iq_j\bar{Z}})+he^{-PZ}+\bar{h}e^{-P\bar{Z}}, \quad (3.21')$$

where

$$f_j=\bar{\mathcal{E}}F_j-\tilde{\mathcal{E}}\bar{F}_j,\quad \bar{f}_j=\tilde{\mathcal{E}}F_j-\bar{\mathcal{E}}\bar{F}_j, \quad (4.3a)$$

$$F_j=I_j(P-iq_j)+J_j(P+iq_j)e^{-iq_jd}, \quad (4.3b)$$

$$\bar{F}_j=I_j(P+iq_j)e^{-iq_jd}+J_j(P-iq_j), \quad (4.3c)$$

$$h=\tilde{\mathcal{E}}U_1-\bar{\mathcal{E}}U_2,\quad \bar{h}=\bar{\mathcal{E}}U_1-\tilde{\mathcal{E}}U_2. \quad (4.3d)$$

Originally, $\overline{\mathcal{E}}$ and $\tilde{\mathcal{E}}$ were introduced as free parameters and $\{f_j,\bar{f}_j\}$, h, and $\bar{h}$ were given in terms of them. However, we can rewrite (4.3) by eliminating $\overline{\mathcal{E}}$ and $\tilde{\mathcal{E}}$ as

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \bar{f}_1 \\ \bar{f}_2 \\ \bar{f}_3 \end{bmatrix} = \begin{bmatrix} -\bar{F}_1 & F_1 \\ -\bar{F}_2 & F_2 \\ -\bar{F}_3 & F_3 \\ F_1 & -\bar{F}_1 \\ F_2 & -\bar{F}_2 \\ F_3 & -\bar{F}_3 \end{bmatrix} \underline{H}^{-1} \begin{bmatrix} h \\ \bar{h} \end{bmatrix} , \tag{4.4}$$

where

$$\underline{H} = \begin{bmatrix} U_1 & -U_2 \\ -U_2 & U_1 \end{bmatrix} , \tag{4.5}$$

At this stage, we can regard $(h,\bar{h})$ as free parameters. In this way, the expressions of $\mathcal{E}(Z)$ from both ABC and ABC-free theories are given in a common form where the two coefficients of evanescent waves act as free parameters. In order for the two expressions to be equivalent, it is necessary and sufficient to have the relation

$$\underline{S} \begin{bmatrix} -\bar{F}_1 & F_1 \\ -\bar{F}_2 & F_2 \\ -\bar{F}_3 & F_3 \\ F_1 & -\bar{F}_1 \\ F_2 & -\bar{F}_2 \\ F_3 & -\bar{F}_3 \end{bmatrix} = \text{const} \times \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ U_1 & -U_2 \\ 0 & 0 \\ 0 & 0 \\ -U_2 & U_1 \end{bmatrix} , \tag{4.6}$$

where $\underline{S}$ is the (6×6) matrix on the left-hand side (lhs) of (4.2a). Due to the complex form of each term in (4.6), it is almost hopeless to check the validity of (4.6) analytically. Thus, we checked it numerically. As a numerical check of Eq. (4.6), we studied two sets of material parameters for CuCl and GaAs, which are the representatives of the "heavy-mass, large-oscillator-strength exciton" and the "light-mass, small-oscillator-strength exciton," respectively. For each material, we took several sets of "P, d, and $\hbar\omega$" values. All the sets of parameter values are summarized in Tables I and II. The matrix equation (4.6) consists of 12 equations, among which six are independent, as is easily seen from the symmetry. In each case we calculate the lhs, and see if it coincides with the corresponding element of the rhs, (0, U_1, or U_2)$\times$const. For the two equations having U_1 and U_2 on the rhs, we calculate the ratio of the expressions on the lhs, which should be equal to

$$U_2/U_1 = -(\alpha H_1+\beta H_2)/(\alpha H_2+\beta H_1) \tag{4.7}$$

from (3.24d) and (3.24e). This equality has been confirmed for more than 20 figures for all the cases studied. As for the equations with 0 on the rhs, we need a special criterion to check its validity numerically. Since the lhs of such equations consists of a sum of several terms, we compare the sum with the constitutent terms. If the sum is very much smaller than the largest term in the sum, we judge that the equation is valid. For all the cases studied, the sum is found to be smaller than the largest constituent term by at least a factor of 10^{-12}. In this way we have checked the equivalence of the ABC and ABC-free theories.

B. Limit of semi-infintie medium

Next we discuss the limit $d\to\infty$ of the result. In the limit, the form of the electric field (3.21) reduces to

$$\mathcal{E}(Z)=\tilde{\mathcal{E}}f(Z)+\overline{\mathcal{E}}f(\bar{Z}) , \tag{4.8}$$

where

$$f(X)=\frac{B}{P}\left[\frac{1}{k_1^2-k_2^2}\left[\frac{P-ik_1}{k_1^2-q^2}-\frac{R}{P+ik_1}\right]e^{ik_1X}+\frac{1}{k_2^2-k_1^2}\left[\frac{P-ik_2}{k_2^2-q^2}-\frac{R}{P+ik_2}\right]e^{ik_2X}\right]$$
$$-2R\left[\frac{B}{(P^2+k_1^2)(P^2+k_2^2)}+1\right]e^{-PX} , \tag{4.9}$$

$$R=\frac{1}{(P^2+q^2)2P}\left[1-\frac{B}{(P^2+q^2)2P}\left[\frac{k_1^2-q^2}{k_1^2-k_2^2}\frac{1}{P+ik_1}+\frac{k_2^2-q^2}{k_2^2-k_1^2}\frac{1}{P+ik_2}-\frac{2P(P^2+q^2)}{(P^2+k_1^2)(P^2+k_2^2)}\right]\right]^{-1}\frac{iB}{k_1+k_2} . \tag{4.10}$$

TABLE I. Material parameters for CuCl and GaAs.

Material	M	$\hbar\omega_0$ (eV)	ϵ_0	$4\pi\alpha_0$	Γ (meV)
CuCl	2.3	3.2022	5.7	2.029×10^{-2}	0.06
GaAs	0.298	1.515	12.6	0.22×10^{-2}	0.035

TABLE II. "P, d, and $\hbar\omega$" values for each material.

	P (Å^{-1})	d (Å)	$\hbar\omega$ (eV)
CuCl	0.3	15 000	1.500, 2.300, 3.100, 3.200, 3.2030, 3.2060, 3.2090, 3.2120, 3.2150, 3.900, 4.700, 5.500
	0.3	1500	1.500, 2.300, 3.100, 3.200, 3.2030, 3.2060, 3.2090, 3.2120, 3.2150, 3.900, 4.700, 5.500,
	0.3	10	1.500, 3.200, 3.300, 3.400, 3.500, 3.600, 3.700, 5.500,
	0.003	1500	1.500, 3.200, 3.2030, 3.2060, 3.2090, 3.2120, 3.2150, 3.500, 5.500
	20 000.0	1500	1.500, 3.200, 3.2030, 3.2060, 3.2090, 3.2120, 3.2150, 3.500, 5.500
GaAs	0.0154	20 000	0.500, 1.100, 1.5110, 1.5124, 1.5138, 1.5152, 1.5166, 1.5180, 1.700, 2.300, 2.900, 3.500
	0.0154	2000	0.500, 1.100, 1.5110, 1.5124, 1.5138, 1.5152, 1.5166, 1.5180, 1.700, 2.300, 2.900, 3.500
	0.0154	130	0.500, 1.100, 1.5140, 1.5164, 1.5188, 1.5212, 1.5236, 1.5260, 1.700, 2.300, 2.900, 3.500
	0.0011	2000	0.500, 1.5110, 1.5124, 1.5138, 1.5152, 1.5166, 1.5180, 2.000, 3.500
	1000.0	2000	0.500, 1.5110, 1.5124, 1.5138, 1.5152, 1.5166, 1.5180, 2.000, 3.500

The wave numbers of bulk polaritons, k_1 and k_2, satisfy the equation

$$(k_j^2-q^2)(k_j^2-q_0^2)-B=0\ , \tag{4.11}$$

where we take $\text{Im}(k_j)>0$. Since $f(X)\to 0$ for $X\to\infty$, $\overline{\mathcal{E}}f(Z)$ and $\tilde{\mathcal{E}}f(\overline{Z})$ describe the field in the regions $Z\sim 0$ and $Z\sim d$, respectively. As expected, $\overline{\mathcal{E}}f(Z)$ is equivalent to the result of DA-DS,

$$\overline{\mathcal{E}}f(Z)=[\mathcal{E}(Z)]_{\text{DA-DS}}\ . \tag{4.12}$$

Note that the two parameters $\mathcal{E}_1$ and $\mathcal{E}_2$ for a slab are combined to give $\overline{\mathcal{E}}$ and $\tilde{\mathcal{E}}$, each of which separately describes the field near front and back surfaces. Although the above argument is the proper way to see the situation for $d\to\infty$, there is another way to get the same result, for which we need much less calculation; we neglect several terms of $O(1/d)$ in the course of the ABC-free calculation. Since this procedure contains somewhat delicate points, we show the details in Appendix B. We hope that this simple version might be useful also for other semi-infinite media with different microscopic characteristics.

C. Remaining problems from previous model calculations

The first application of the ABC-free theory[7] has been made to simple models, i.e., a single QW and a slab with simple exciton wave function equivalent to Pekar ABC. Though the results were satisfactory within the models, the following questions have been left as to the generality of the results obtained from the simple models: (a) Do the poles which give the solutions of bulk polaritons appear in $F_K G_K$ in the case of less-simple slab models, too? In general, the solutions of polaritons in a slab deviate from those in the bulk, so it is of interest to see how the deviations of these poles appear in $F_K G_K$. (b) Does the extinction of background waves [$\sim\exp(\pm iqZ)$] occur also in the case of less-simple slab models? The result of this paper shows that (a′) the poles in F_K are the same as those which give the eigenmodes of a slab in the ABC treatment, two of which are bulk polaritonlike, and the third is evanescent, and (b') the extinction of background waves occurs also in this model. These conclusions are again limited within the framework of the present model, but we think that (a') would remain correct for more general cases, while (b') possibly changes, especially when the thickness of a slab becomes so small that the summation over k is cut off at a certain finite value.

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APPENDIX A: EVALUATION OF $\{S(Z), T(Z), \alpha, \beta, \gamma_1, \gamma_2\}$

These quantities, originally defined as summations over discrete K values, can be rewritten as the following contour integrals, and evaluated by the residues at complex poles. The function $S(Z)$ consists of the sum of the following form:

$$S(Z)=\mathcal{E}_1[e^{iqd}S'(Z,q)+S'(\bar{Z},-q)]+\mathcal{E}_2e^{iqd}[e^{-iqd}S'(Z,-q)+S'(\bar{Z},q)]-\tilde{\mathcal{E}}T(Z)-\bar{\mathcal{E}}T(\bar{Z}) . \tag{A1}$$

In (A1), $S'(Z,q)$ and $T(Z)$ are defined as

$$S'(Z,q)=\frac{BP}{2Pd+4}\left\{\frac{1}{2\pi i}\int_c \frac{[d(P^2+K^2)-2P]}{\sin[Kd-\delta(K)]}\frac{i(K+iP)e^{iKZ}}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)(q-K)(K-iP)}dK\right.$$
$$\left.+\frac{1}{2\pi i}\int_c \frac{[d(P^2+K^2)-2P]}{\sin[Kd-\delta(K)]}\frac{ie^{-iKZ}}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)(q-K)}dK\right\}$$
$$=\sum_{j=1}^{3}\tilde{A}_j\frac{P-iq}{(q_j^2-q^2)(q_j^2+P^2)}[P\sin(q_jZ)-q_j\cos(q_jZ)]+\tilde{A}\frac{1}{(q^2-q_1^2)(P+iq)}[P\sin(qZ)-q\cos(qZ)]$$
$$-\frac{BP}{Pd+2}\frac{4P^2e^{-P\bar{Z}}}{(P^2+q_1^2)(P^2+q_2^2)(P^2+q_3^2)(P+iq)} , \tag{A2}$$

$$\delta(K)=2\tan^{-1}(K/P), \quad \tilde{A}=\tilde{A}_1|_{q_1=q} , \tag{A3}$$

$$T(Z)=T_1(Z)+T_2(Z) , \tag{A4}$$

where

$$T_1(Z)=\frac{BP}{2Pd+4}\frac{1}{2\pi i}\int_c \frac{\cos[K\bar{Z}-\delta(K)]}{\sin[Kd-\delta(K)]}\frac{d(P^2+K^2)-2P}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)}dK$$
$$=-\tfrac{1}{2}\sum_{j=1}^{3}\tilde{A}_j\frac{1}{q_j}\cos[q_j\bar{Z}-\delta(q_j)] , \tag{A5}$$

$$T_2(Z)=-\frac{BP}{2Pd+4}\frac{1}{2\pi i}\int_c \frac{\cos(K\bar{Z})}{\sin[Kd-\delta(K)]}\frac{d(P^2+K^2)-2P}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)}dK$$
$$=-\tfrac{1}{2}\sum_{j=1}^{3}\tilde{A}_j\frac{1}{q_j}\cos(q_j\bar{Z})-\frac{BP}{Pd+2}\frac{4P^2e^{-P\bar{Z}}}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)} . \tag{A6}$$

The factors α, β, γ_1, and γ_2 are defined and evaluated as follows:

$$\alpha=\frac{BP}{Pd+2}\frac{1}{2\pi i}\int_c \frac{\cos[Kd-\delta(K)]}{\sin[Kd-\delta(K)]}\frac{(K^2-q^2)K\{d(P^2+K^2)-2P\}}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)(K-iP)}dK$$
$$=-\sum_{j=1}^{3}\tilde{A}_j\frac{q_j^2-q^2}{q_j^2+P^2}q_j\cos[q_jd-\delta(q_j)]+\frac{BP}{Pd+2}\frac{(P^2+q^2)2P^2}{(P^2+q_1^2)(P^2+q_2^2)(P^2+q_3^2)} , \tag{A7}$$

$$\beta=-\frac{BP}{Pd+2}\frac{1}{2\pi i}\int_c \frac{1}{\sin[Kd-\delta(K)]}\frac{(K^2-q^2)K[d(P^2+K^2)-2P]}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)(K-iP)}dK=\sum_{j=1}^{3}\tilde{A}_j\frac{q_j^2-q^2}{q_j^2+P^2}q_j \;, \tag{A8}$$

$$\gamma_1=\mathcal{E}_1\{e^{iqd}\gamma_a(q)+\gamma_b(q)\}+\mathcal{E}_2e^{iqd}[e^{-iqd}\gamma_a(-q)+\gamma_b(-q)]-\bar{\mathcal{E}}\alpha-\bar{\mathcal{E}}\beta \;, \tag{A9}$$

where

$$\gamma_a(q)=\frac{BP}{Pd+2}\frac{1}{2\pi i}\int_c \frac{1}{\sin[Kd-\delta(K)]}\frac{(K-q)iK[d(P^2+K^2)-2P]}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)(K+iP)}dK=-\sum_{j=1}^{3}\tilde{A}_j\frac{P-iq}{q_j^2+P^2}q_j \;, \tag{A10}$$

$$\begin{aligned}\gamma_b(q)&=\frac{BP}{Pd+2}\frac{1}{2\pi i}\int_c \frac{\cos[Kd-\delta(K)]}{\sin[Kd-\delta(K)]}\frac{(K-q)iK[d(P^2+K^2)-2P]}{(K^2-q_1^2)(K^2-q_2^2)(K^2-q_3^2)(K-iP)}dK\\&=\sum_{j=1}^{3}\tilde{A}_j\frac{P+iq}{q_j^2+P^2}q_j\cos[q_jd-\delta(q_j)]+\frac{BP}{Pd+2}\frac{2P^2(P+iq)}{(P^2+q_1^2)(P^2+q_2^2)(P^2+q_3^2)}dK \;,\end{aligned} \tag{A11}$$

$$\gamma_2=\mathcal{E}_1[e^{iqd}\gamma_b(-q)+\gamma_a(-q)]+\mathcal{E}_2e^{iqd}[e^{-iqd}\gamma_b(q)+\gamma_a(q)]-\bar{\mathcal{E}}\alpha-\bar{\mathcal{E}}\beta \;. \tag{A12}$$

APPENDIX B: CALCULATION IN THE CASE OF $d\to\infty$

When d is large enough, we can neglect $O(1/d)$, and so, $\rho_k(Z)$ is given as

$$\rho_k(Z)=(1/\sqrt{2d})[e^{-ikZ}+A_Ke^{ikZ}-(1+A_K)e^{-PZ}-(e^{-iKd}+A_Ke^{iKd})e^{-P\bar{Z}}] \;, \tag{B1}$$

As for $\bar{\chi}_K(\omega)$, we take the same one as (3.1). Hereafter, we follow the same procedure as in Sec. III, replacing $N(K)^2$ and (3.15) with $1/2d$ and

$$\int_0^d(e^{-iKZ}+A_Ke^{iKZ})(e^{iK'Z}+A_K^*e^{-iK'Z})dZ=\delta_{K,K'}2d \;, \tag{B2}$$

respectively. Then, C_K, (3.12), is replaced by

$$\tilde{C}_K=[1-Q^2\bar{\chi}_K(\omega)/(K^2-q^2)]^{-1} \;, \tag{B3}$$

which can be rewritten as

$$\tilde{C}_K=(K^2-q^2)(K^2-q_0^2)/[(K^2-q^2)(K^2-q_0^2)-B] \;. \tag{B4}$$

From the fact that the solutions of

$$(K^2-q^2)(K^2-q_0^2)-B=0 \tag{B5}$$

give the dispersion relation of the bulk polaritons, it is clear that F_K has poles at the wave numbers of bulk polaritons (k_1,k_2) [$\mathrm{Im}(k_j)>0$]. $\{F_K\}$ can be determined in the same way as in Sec. III with the replacement

$$\{B_1,B_2,\alpha,\beta,\gamma_1,\gamma_2\}\to\{\tilde{B}_1,\tilde{B}_2,\tilde{\alpha},\tilde{\beta},\tilde{\gamma}_1,\tilde{\gamma}_2\} \;,$$

where

$$\{\tilde{B}_1,\tilde{B}_2\}=\{B_1,B_2\}|_{(\alpha,\beta,\gamma_1,\gamma_2)\to(\tilde{\alpha},\tilde{\beta},\tilde{\gamma}_1,\tilde{\gamma}_2)} \;, \tag{B6}$$

$$\{\tilde{\alpha},\tilde{\beta},\tilde{\gamma}_1,\tilde{\gamma}_2\}=\{\alpha,\beta,\gamma_2,\gamma_2\}|_{C_K[N(K)]^2\to\tilde{C}_K/2d} \;. \tag{B7}$$

With this $\{F_K\}$ we can write the field $\mathcal{E}(Z)$ in the form which contains the summation over K. Before we show it, we make it clear that $\tilde{\beta}$ vanish as $d\to\infty$. With (3.1) and (3.8), $\tilde{\beta}$ can be written as

$$\tilde{\beta}=\{2/[(P^2+q^2)2P]\}\times\sum_K^{\text{all}}(B/2d)\times\{(K^2-q^2)iK/[(K^2-k_1^2)(K^2-k_2^2)\times(P+iK)]\}e^{iKd} \;, \tag{B8}$$

where the identity

$$(K^2-q^2)(K^2-q_0^2)-B=(K^2-k_1^2)(K^2-k_2^2) \tag{B9}$$

is utilized. The summation over K in (B8) can be performed again by the method of contour integral in the complex K plane. However, in this case, the quantization condition of K must be regarded as

$$\sin(Kd)=0 \tag{B10}$$

because the distance between two neighboring values of K should approach π/d as $d\to\infty$. Therefore the integral form of $\tilde{\beta}$ can be written as

$$\tilde{\beta}=\frac{1}{(P^2+q^2)2P}\frac{B}{2\pi i}\int_c\frac{1}{\sin(Kd)}\times\frac{K^2-q^2}{(K^2-k_1^2)(K^2-k_2^2)}\frac{iK}{P+iK}dK \;. \tag{B11}$$

The residues for the poles $K=\pm k_1$, $\pm k_2$, $-iP$ are easily seen to vanish for $d\to\infty$, if we note that $\mathrm{Im}(k_j)>0$. So, $\tilde{\beta}$ obviously vanishes as $d\to\infty$. In terms of the quantities with tildes, we can write $\mathcal{E}(Z)$ as

$$\begin{aligned}\mathcal{E}(Z)=&\mathcal{E}_1e^{iqZ}+\mathcal{E}_2e^{iq\bar{Z}}+\tilde{S}(Z)-(\tilde{\gamma}_1/\tilde{\alpha})\tilde{T}(Z)/[(P^2+q^2)2P]-(\tilde{\gamma}_2/\tilde{\alpha})\tilde{T}(\bar{Z})/[(P^2+q^2)2P]\\&+(\tilde{\gamma}_1/\tilde{\alpha})e^{-PZ}/(P^2+q^2)+(\tilde{\gamma}_2/\tilde{\alpha})e^{-P\bar{Z}}/(P^2+q^2) \;,\end{aligned} \tag{B12}$$

where

$$\{\tilde{S}(Z),\tilde{T}(Z)\}=\{S(Z),T(Z)\}|_{C_k[N(K)]^2\to\tilde{C}_K/2d}\ . \tag{B13}$$

The integral forms of $\{\tilde{S}(Z),\tilde{T}(Z),\tilde{\alpha},\tilde{\beta},\tilde{\gamma}_1,\tilde{\gamma}_2\}$ and their values are given as

$$\tilde{S}(Z)=\mathcal{E}_1\tilde{S}'(Z)+\mathcal{E}_2 e^{iqd}\tilde{S}''(Z)-\tilde{\mathcal{E}}\,\tilde{T}(Z)-\bar{\mathcal{E}}\tilde{T}(\bar{Z})\ , \tag{B14}$$

where

$$\begin{aligned}
\tilde{S}'(Z)=\frac{B}{2}&\Bigg[e^{iqd}\Bigg[\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{ie^{iKZ}}{(K^2-k_1^2)(K^2-k_2^2)(K-q)}dK\\
&\qquad+\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{(iK-P)e^{-iKZ}}{(K^2-k_1^2)(K^2-k_2^2)(K-q)(K-iP)}dK\Bigg]\\
&\quad-\Bigg[\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{ie^{-iK\bar{Z}}}{(K^2-k_1^2)(K^2-k_2^2)(K-q)}dK\\
&\qquad+\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{(iK+P)e^{iK\bar{Z}}}{(K^2-k_1^2)(K^2-k_2^2)(K-q)(K+iP)}dK\Bigg]\Bigg]\\
=B&\Bigg[e^{iqd}\Bigg[\frac{(P-iq)e^{ik_1\bar{Z}}}{(k_1^2-k_2^2)(k_1^2-q^2)(P+ik_1)}+\frac{(P-iq)e^{ik_2\bar{Z}}}{(k_2^2-k_1^2)(k_2^2-q^2)(P+ik_2)}\\
&\qquad+\frac{(P-iq)e^{iq\bar{Z}}}{(q^2-k_1^2)(q^2-k_2^2)(P+iq)}-\frac{2Pe^{-P\bar{Z}}}{(P^2+k_1^2)(P^2+k_2^2)(P+iq)}\Bigg]\\
&\quad+\frac{(P+iq)e^{ik_1Z}}{(k_1^2-k_2^2)(k_1^2-q^2)(P+ik_1)}+\frac{(P+iq)e^{ik_2Z}}{(k_2^2-k_1^2)(k_2^2-q^2)(P+ik_2)}\\
&\quad+\frac{e^{iqZ}}{(q^2-k_1^2)(q^2-k_2^2)}-\frac{2Pe^{-PZ}}{(P^2+k_1^2)(P^2+k_2^2)(P-iq)}\Bigg]\ ,
\end{aligned} \tag{B15}$$

$$\begin{aligned}
\tilde{S}''(Z)=\frac{B}{2}&\Bigg[e^{-iqd}\Bigg[\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{ie^{iKZ}}{(K^2-k_1^2)(K^2-k_2^2)(K+q)}dK\\
&\qquad+\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{(iK-P)e^{-iKZ}}{(K^2-k_1^2)(K^2-k_2^2)(K+q)(K-iP)}dK\Bigg]\\
&\quad-\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{ie^{-iK\bar{Z}}}{(K^2-k_1^2)(K^2-k_2^2)(K+q)}dK-\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{(ik+P)e^{iK\bar{Z}}}{(K-k_1^2)(K^2-k_2^2)(K+q)(K+iP)}dK\Bigg]\\
=B&\Bigg[e^{-iqd}\Bigg[\frac{(P+iq)e^{ik_1\bar{Z}}}{(k_1^2-k_2^2)(k_1^2-q^2)(P+ik_1)}+\frac{(P+iq)e^{ik_2\bar{Z}}}{(k_2^2-k_1^2)(k_2^2-q^2)(P+ik_2)}\\
&\qquad+\frac{e^{iq\bar{Z}}}{(q^2-k_1^2)(q^2-k_2^2)}-\frac{(P+iq)e^{iq(d+Z)}}{(q^2-k_1^2)(q^2-k_2^2)(P-iq)}-\frac{2Pe^{-P\bar{Z}}}{(P^2+k_1^2)(P^2+k_2^2)(P-iq)}\Bigg]\\
&\quad+\frac{(P-iq)e^{ik_1Z}}{(k_1^2-k_2^2)(k_1^2-q^2)(P+ik_1)}+\frac{(P-iq)e^{ik_2Z}}{(k_2^2-k_1^2)(k_2^2-q^2)(P+ik_2)}\\
&\quad+\frac{(P-iq)e^{iqZ}}{(q^2-k_1^2)(q^2-k_2^2)(P+iq)}-\frac{2Pe^{-PZ}}{(P^2+k_1^2)(P^2+k_2^2)(P+iq)}\Bigg]\ ,
\end{aligned} \tag{B16}$$

$$\begin{aligned}
\tilde{T}(Z)&=B\frac{1}{2\pi i}\int_c\frac{1}{\sin(Kd)}\frac{Ke^{-iK\bar{Z}}}{(K^2-k_1^2)(K^2-k_2^2)(K-iP)}dK\\
&=-B\left[\frac{e^{ik_1Z}}{(k_1^2-k_2^2)(P+ik_1)}+\frac{e^{ik_2Z}}{(k_2^2-k_1^2)(P+ik_2)}+\frac{2Pe^{-PZ}}{(P^2+k_1^2)(P^2+k_2^2)}\right]\ ,
\end{aligned} \tag{B17}$$

$$\tilde{\alpha}=1+\frac{1}{(P^2+q^2)2P}B\frac{1}{2\pi i}\int_c \frac{1}{\sin(Kd)}\frac{(K^2-q^2)Ke^{-iKd}}{(K^2-k_1^2)(K^2-k_2^2)(K-iP)}dK$$

$$=1+\frac{1}{(P^2+q^2)2P}B\left[-\frac{k_1^2-q^2}{k_1^2-k_2^2}\frac{1}{P+ik_1}-\frac{k_1^2-q^2}{k_2^2-k_1^2}\frac{1}{P+ik_2}+\frac{2P(P^2+q^2)}{(P^2+k_1^2)(P^2+k_2^2)}\right], \quad \text{(B18)}$$

$$\tilde{\beta}=\frac{1}{(P^2+q^2)2P}B\frac{1}{2\pi i}\int_c \frac{1}{\sin(Kd)}\frac{(K^2-q^2)K}{(K^2-k_1^2)(K^2-k_2^2)(K-iP)}dK=0, \quad \text{(B19)}$$

$$\tilde{\gamma}_1=\mathcal{E}_1\gamma_1'(q)+\mathcal{E}_2e^{iqd}\gamma_1'(-q)-\tilde{\mathcal{E}}\tilde{\alpha}-\bar{\mathcal{E}}\tilde{\beta}, \quad \text{(B20)}$$

where

$$\gamma_1'(q)=B\frac{1}{2\pi i}\int_c \frac{1}{\sin(Kd)}\frac{(K-q)iK}{(K^2-k_1^2)(K^2-k_2^2)(K-iP)}(e^{-iKd}-e^{iqd})dK$$

$$=B\left[-\frac{i(k_1-q)}{(k_1^2-k_2^2)(P+ik_1)}-\frac{i(k_2-q)}{(k_2^2-k_1^2)(P+ik_2)}+\frac{2P(P+iq)}{(P^2+k_1^2)(P^2+k_2^2)}\right], \quad \text{(B21)}$$

and

$$\tilde{\gamma}_2=\mathcal{E}_1\gamma_2'(q)+\mathcal{E}_2e^{iqd}\gamma_2'(-q)-\bar{\mathcal{E}}\tilde{\alpha}-\tilde{\mathcal{E}}\tilde{\beta}, \quad \text{(B22)}$$

where

$$\gamma_2'(q)=B\frac{1}{2\pi i}\int_c \frac{1}{\sin(Kd)}\frac{(K-q)iK}{(K^2-k_1^2)(K^2-k_2^2)(K+iP)}(1-e^{iqd}e^{iKd})dK$$

$$=Be^{iqd}\left[-\frac{i(k_1+q)}{(k_1^2-k_2^2)(P+ik_1)}-\frac{i(k_2+q)}{(k_2^2-k_1^2)(P+ik_2)}+\frac{2P(P-iq)}{(P^2+k_1^2)(P^2+k_2^2)}\right], \quad \text{(B23)}$$

Substitution of the above results, (B14)–(B23), into (B12) leads to the final expression of $\mathcal{E}(Z)$ in the semi-infinite medium in the same form as (4.8)–(4.10), which is obtained by the proper limiting procedure. Since $f(X)\to 0$ for $X\to\infty$, $\bar{\mathcal{E}}f(Z)$ and $\tilde{\mathcal{E}}f(\bar{Z})$ describe the field in the regions $Z\sim 0$ and $Z\sim d$, respectively. The part $\bar{\mathcal{E}}f(Z)$ coincides with the result of DA-DS, as discussed in Sec. IV.

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