Wave-vector-space method for wave propagation in bounded media

B. Chen and D. F. Nelson
Physics Department, Worcester Polytechnic Institute, Worcester, Massachusetts 01609
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A method for solving wave propagation problems in bounded media that operates entirely in wave-vector space is presented. No boundary conditions are used in the solution in contrast to the real-space method. The transmission/reflection problem of an electromagnetic wave on a dielectric half-space is solved as an illustration of the method. The dispersion relations of vacuum and medium, Snell's law, the reflection angle law, and the Fresnel reflection/transmission formulas are obtained from these procedures. Applications to wave-vector dispersion problems, where the method appears to be essential, are pointed out.

I. INTRODUCTION

Electromagnetic-wave-propagation problems in bounded media are quite standardly handled in a real-space formulation. Waves inside and outside the medium are found whose propagation constants are determined by the dispersion relations which result from substituting the waves into the electric field wave equation. The waves inside and outside are then joined with the use of the boundary conditions on the Maxwell fields, **E**, **H**, **D**, and **B**, at the medium surface. These conditions produce the Fresnel reflection/transmission coefficient relations between the amplitudes of the incident, reflected, and transmitted waves. They also relate the inside and outside propagation constants through Snell's law of refraction and the reflection law of equal angles of incidence and reflection.

The standard real-space method meets considerable difficulty when applied to wave-vector dispersion[1] problems. These are problems in which the polarization of the medium depends on spatial derivatives of the electric field as well as on the field itself. The dependence on the first spatial derivative of the electric field leads to optical activity[2] while dependence on the second spatial derivative leads to resonant wave-vector dispersion as present near the frequency of an exciton transition. Calculation of the transmission and reflection in the latter case leads to the so-called "additional boundary condition" or ABC problem.[3,4] Here "additional" refers to a boundary condition on the polarization or the electric field (or their derivatives) that supplements the usual Maxwell boundary conditions. The origin (microscopic or macroscopic) and nature of the ABC have remained in controversy for thirty-five years. Several real-space approaches[5–8] showed that a condition equivalent to an ABC could be obtained by an extinction theorem type of development. However, these approaches simply assumed that the bulk nonlocal constitutive relation held right up to the surface. This so-called "dielectric approximation" was at first thought to be the natural macroscopic assumption, but was later found to violate energy conservation.[9] The wave-vector-space method presented here is conveniently applied to the exciton problem at a fundamental level that derives the nonlocal constitutive relation for a bounded medium and thus avoids the dielectric approximation. Furthermore, the new wave-vector-space method[10,11] uses no boundary conditions to solve the problem and thus sidesteps the entire question of an ABC. By transformation of the appropriate steps back to real space, however, the form of the ABC implicitly used and needed for a real-space calculations can be found.

The procedures of the wave-vector-space method are sufficiently unfamiliar and novel that we believe it useful to present them here in the context of a familiar problem, the Fresnel reflection/transmission problem of a light wave impinging on a dielectric half-space. The electric field wave equation is first transformed to wave-vector (**k**) space by taking a spatial Fourier transform. A single (vector) equation results and replaces the two spatial forms of the wave equation for inside and outside the medium. The **k**-space electric field transform is thus continuous everywhere. Thus there is no need for boundary conditions and none are used in the **k**-space method. The form of the electric field transform is found by examining the poles of it in the complex **k** space implied by the transformed wave equation. The necessity of the wave equation remaining finite and thus meaningful at the poles of the **E**-field transform determines the dispersion relations of the medium and the vacuum. Transmission and reflection coefficients are introduced into the **E**-field transform as required by the asymptotic forms of a transmission/reflection problem. After substitution of the transform into the wave equation a nontrivial solution can be seen to exist only if Snell's law of refraction and the reflection law of equality of incident and reflected angles are both true. Use of the dispersion relations then recasts the wave equation into a polynomial in the wave-vector components. For the half-space problem treated here only the component of the wave vector k_z normal to the surface appears. Since k_z is the independent variable of the **E**-field transform, each term of the polynomial is linearly independent and so must vanish separately. These conditions determine the transmission and reflection coefficients which for the illustrative problem treated here are the familiar Fresnel formulas.

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II. TRANSFORMED WAVE EQUATION

The real space form of the electric field wave equation for linear propagation in a dielectric crystal is

$$\nabla \times [\nabla \times \mathbf{E}(\mathbf{x},t)] + \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\{[\overleftrightarrow{I} + \overleftrightarrow{\chi}(\mathbf{x},t)] \cdot \mathbf{E}(\mathbf{x}),t\} = 0. \quad (1)$$

For simplicity we consider either a cubic crystal or an isotropic amorphous medium for which the linear electric susceptibility is $\overleftrightarrow{\chi} = \overleftrightarrow{I}\chi$. Since we are concerned with spatial dependences, we simply assert that for single frequency propagation ($E \sim e^{-i\omega t}$) Eq. (1) can be recast as

$$\nabla \times [\nabla \times \mathbf{E}(\mathbf{x},\omega)] - \frac{\omega^2}{c^2}[1 + \chi(\mathbf{x},\omega)]\,\mathbf{E}(\mathbf{x},\omega) = 0. \quad (2)$$

We consider a homogeneous half-space of matter bounded by the $z = 0$ plane. The spatial dependence of the susceptibility is thus

$$\chi(\mathbf{x},\omega) = \Theta(z)\chi(\omega)\,, \quad (3)$$

where $\Theta(z)$ is the unit step function defined by

$$\Theta(z) = \begin{cases} 1 & (z > 0) \\ 0 & (z < 0). \end{cases} \quad (4)$$

The **k**-space Fourier transform of a general function $\mathbf{F}(\mathbf{x})$ (with frequency dependence omitted from here on) is

$$\mathbf{F}(\mathbf{k}) = \frac{1}{(2\pi)^3}\int \mathbf{F}(\mathbf{x})\,e^{-i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x} \quad (5)$$

and its inverse transform is

$$\mathbf{F}(\mathbf{x}) = \int \mathbf{F}(\mathbf{k})\,e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k}. \quad (6)$$

The **k**-space transform of $\Theta(z)$ can be calculated to be

$$\Theta(\mathbf{k}) = \frac{\delta(k_x)\,\delta(k_y)}{2\pi i}\frac{1}{k_z - i\eta}, \quad (7)$$

where η is an infinitesimal positive quantity introduced to obtain convergence of the transform and $\delta(k)$ is the Dirac delta function.

The inverse transforms of **E** and Θ of the form of Eq. (6) are introduced into Eq. (2) as modified by Eq. (3) with the result

$$\int\left\{\mathbf{k} \times [\mathbf{k} \times \mathbf{E}(\mathbf{k})] + \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{k})\right\}e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k} + \frac{\omega^2}{c^2}\chi\iint\frac{\delta(k'_x)\,\delta(k'_y)}{2\pi i(k'_z - i\eta)}\mathbf{E}(\mathbf{k}'')\,e^{i(\mathbf{k}'+\mathbf{k}'')\cdot\mathbf{x}}d\mathbf{k}'d\mathbf{k}'' = 0. \quad (8)$$

Substituting $\mathbf{k} = \mathbf{k}' + \mathbf{k}''$ in the second integral and carrying out the k'_x and k'_y integrations, we find

$$\int\left\{\mathbf{k} \times [\mathbf{k} \times \mathbf{E}(\mathbf{k})] + \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{k}) + \frac{\omega^2}{c^2}\chi\left[\frac{1}{2\pi i}\int\frac{\mathbf{E}(k_x,k_y,k'_z)}{k_z - k'_z - i\eta}dk'_z\right]\right\}e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k} = 0. \quad (9)$$

The electric field transform $\mathbf{E}(\mathbf{k})$ can be written as a sum of two functions, $\mathbf{E}^{(+)}\mathbf{k}$ having poles only in the upper half complex **k** plane, and $\mathbf{E}^{(-)}(\mathbf{k})$ having poles only in the lower half complex **k** plane,

$$\mathbf{E}(\mathbf{k}) = \mathbf{E}^{(+)}(\mathbf{k}) + \mathbf{E}^{(-)}(\mathbf{k})\,. \quad (10)$$

As discussed more fully in the Appendix, there are no poles on the real axis, i.e., between the upper and lower halves of the complex **k** plane. Those poles arising from the propagation characteristics of the medium are necessarily displaced into the upper half-plane by $i\eta$ while those arising from the propagation characteristics of the vacuum are necessarily displaced into the lower half-plane by $-i\eta$. For these reasons we speak of $\mathbf{E}^{(+)}(\mathbf{k})$ as the part of the transform arising from the medium and $\mathbf{E}^{(-)}(\mathbf{k})$ as the part arising from the vacuum.

The Appendix contains the proof of a very important theorem which states

$$\frac{1}{2\pi i}\int\frac{\mathbf{E}(k_x,k_y,k'_z)}{k_z - k'_z - i\eta}dk'_z = \mathbf{E}^{(+)}(\mathbf{k})\,. \quad (11)$$

Note that the left side of Eq. (11) is exactly the bracketed integral in Eq. (9) and so allows introduction of $\mathbf{E}^{(+)}(\mathbf{k})$ there. Now it is clear that the integral over **k** in Eq. (9) can vanish in general only if its integrand vanishes. After expanding the vector triple product and introducing Eq. (10) we obtain

$$(k_0^2 - k^2)\,\mathbf{E}^{(-)}(\mathbf{k}) + \mathbf{k}\left[\mathbf{k}\cdot\mathbf{E}^{(-)}(\mathbf{k})\right] + \left(\kappa k_0^2 - k^2\right)\mathbf{E}^{(+)}(\mathbf{k}) + \mathbf{k}\left[\mathbf{k}\cdot\mathbf{E}^{(+)}(\mathbf{k})\right] = 0, \quad (12)$$

where the vacuum wave vector is $k_0 \equiv \omega/c$ and the relative dielectric constant is $\kappa(\omega) \equiv 1 + \chi(\omega)$. Equation (12) is the transformed wave equation. Note that the only medium property, κ, is associated with $\mathbf{E}^{(+)}$ as expected from the above discussion. Note also that we have only one wave equation, not one for the medium and one for the vacuum as a real-space treatment has.

III. DETERMINING THE ELECTRIC FIELD TRANSFORM

As discussed in the Appendix the **E**-field transform can be expected to have a pole in the complex plane for each propagating mode, in the upper half-plane for medium modes and in the lower half-plane for vacuum modes. Clearly the transformed wave equation (12) must remain meaningful (finite) at each of these poles. The behavior of Eq. (12) at the poles must be examined in two steps: first, the scalar product terms two and four and, second, terms one and three that involve one field component at a time.

To isolate the scalar product terms we form a scalar product of the whole equation (12) with $\mathbf{k}$ and so obtain

$$\mathbf{k}\cdot\mathbf{E}^{(-)}(\mathbf{k})+\kappa\mathbf{k}\cdot\mathbf{E}^{(+)}(\mathbf{k})=0, \tag{13}$$

which is just the transformed $\nabla\cdot\mathbf{D}=0$ Maxwell equation. Consider $\mathbf{k}$ approaching a pole $\mathbf{k}_L$ in the lower half-plane. Since $\mathbf{E}^{(+)}$ has no poles there by definition, the second term in Eq. (13) is finite there and, since the first term is equal to the negative of the second term, the first term must also be finite at the pole $\mathbf{k}_L$. Thus, the pole in $\mathbf{E}^{(-)}$ at $\mathbf{k}_L$ must be canceled out by the combination of factors present in the scalar product. The cancellation shows that the pole must be first order. An analogous argument can be made as $\mathbf{k}$ approaches a pole $\mathbf{k}_U$ in the upper half-plane to show that $\mathbf{k}\cdot\mathbf{E}^{(+)}$ remains finite there and that its poles are also first order.

Next we consider the entire transformed wave equation (12) as $\mathbf{k}\to\mathbf{k}_L$. The third and fourth terms have no poles in the lower half-plane and we just showed that the second term is finite there. Since only an individual component of $\mathbf{E}^{(-)}$ appears in the first term, the only possible cancellation of its pole is the vanishing of the coefficient

$$k_0^2-k^2=0. \tag{14}$$

We interpret this required relation as the dispersion relation of the vacuum with two solutions,

$$(k_L)_z=\pm\left[k_0^2-k_x^2-k_y^2\right]^{1/2}\equiv\pm k_V, \tag{15}$$

corresponding to two poles, one for forward propagation and one for backward propagation. We have expressed the solution (15) for the z component of $\mathbf{k}$ because as we see presently the orientation of the matter surface ($z=0$) makes only the component k_z a true variable in the $\mathbf{E}$-field transform, k_x and k_y being fixed by the problem definition.

A completely analogous argument applied to the approach of $\mathbf{k}$ to an upper half-plane pole $\mathbf{k}_U$ leads to requiring the coefficient of the third term in Eq. (12) to vanish,

$$k_0^2\kappa-k^2=0. \tag{16}$$

This is the dispersion relation of the medium with its two solutions,

$$(k_U)_z=\pm\left[k_0^2\kappa-k_x^2-k_y^2\right]^{1/2}\equiv\pm k_M, \tag{17}$$

again corresponding to two poles for the two directions of propagation. Again the poles are determined to be first order.

The two parts of the $\mathbf{E}$-field transform can now be written as

$$\mathbf{E}^{(+)}(\mathbf{k})=\frac{1}{2\pi i}\left[\frac{\mathbf{t}^{(+)}(k_x,k_y)}{k_z-k_M-i\eta}+\frac{\mathbf{r}^{(+)}(k_x,k_y)}{k_z+k_M-i\eta}\right], \tag{18a}$$

$$\mathbf{E}^{(-)}(\mathbf{k})=\frac{1}{2\pi i}\left[-\frac{\mathbf{t}^{(-)}(k_x,k_y)}{k_z-k_V+i\eta}-\frac{\mathbf{r}^{(-)}(k_x,k_y)}{k_z+k_V+i\eta}\right], \tag{18b}$$

$\mathbf{t}^{(+)},\mathbf{t}^{(-)},\mathbf{r}^{(+)}$, and $\mathbf{r}^{(-)}$ being as yet arbitrary functions.

IV. FRESNEL FORMULAS FOR OBLIQUE INCIDENCE

We consider oblique incidence from the vacuum side onto the matter half-space. We take the plane of incidence as the xz plane so that $k_y=0$ and take the known angle of incidence with respect to the surface normal as θ_i, the (unknown) angle of reflection as θ_r, and the (unknown) angle of refraction as ϕ. Also causality allows us to take $\mathbf{r}^{(+)}=0$ because there can be no backward wave in the medium for incidence from the vacuum. With the problem thus specified we have

$$\mathbf{t}^{(-)}(k_x,k_y)=E_0\mathbf{e}_1\delta(k_x-k_0\sin\theta_i)\,\delta(k_y), \tag{19a}$$

$$\mathbf{r}^{(-)}(k_x,k_y)=E_0r\mathbf{e}_2\delta(k_x-k_0\sin\theta_r)\,\delta(k_y), \tag{19b}$$

$$\mathbf{t}^{(+)}(k_x,k_y)=E_0t\mathbf{e}_3\delta(k_x-k_0n\sin\phi)\,\delta(k_y), \tag{19c}$$

$$\mathbf{r}^{(+)}(k_x,k_y)=0, \tag{19d}$$

where $n\equiv k/k_0=\sqrt{\kappa}$ is the refractive index from Eq. (16), E_0 is a given incident electric field amplitude, r is a reflection coefficient, t is a transmission coefficient, and $\mathbf{e}_1,\mathbf{e}_2$, and $\mathbf{e}_3$ are as yet undetermined unit vectors.

Equations (18) and (19) can now be substituted into Eq. (12). Clearly it is then required that the arguments of the three Dirac delta functions involving k_x must be equal. Otherwise integration of the equation over a range of k_x including, for instance, the reflected wave $k_x=k_0\sin\theta_r$, but not the incident wave $k_x=k_0\sin\theta_i$, would violate causality. Thus we have

$$k_x=k_0\sin\theta_i=k_0\sin\theta_r=k_0n\sin\phi, \tag{20}$$

which yields the law of reflection

$$\theta_i=\theta_r\equiv\theta, \tag{21}$$

and Snell's law of refraction

$$\sin\theta=n\sin\phi. \tag{22}$$

These allow the values of k_z at the poles, Eqs. (15) and (17), to be reexpressed as

$$k_V=k_0\cos\theta, \tag{23}$$

$$k_M=k_0n\cos\phi. \tag{24}$$

With the Dirac delta functions dropped, Eq. (12) is recast as

$$-\left[\left(k_0^2-k^2\right)\mathbf{e}_1+\mathbf{k}\left(\mathbf{k}\cdot\mathbf{e}_1\right)\right]\frac{1}{k_z-k_0\cos\theta}$$
$$-\left[\left(k_0^2-k^2\right)\mathbf{e}_2+\mathbf{k}\left(\mathbf{k}\cdot\mathbf{e}_2\right)\right]\frac{r}{k_z+k_0\cos\theta}$$
$$+\left[\left(k_0^2\kappa-k^2\right)\mathbf{e}_3+\mathbf{k}\left(\mathbf{k}\cdot\mathbf{e}_3\right)\right]\frac{t}{k_z-k_0 n\cos\phi}=0, \tag{25}$$

where for the manipulations that follow we let $\eta\to 0$.

A. s polarization

Consider first that the incident **E**-field polarization is perpendicular to the xz plane, the so-called s polarization. Thus we can set

$$\mathbf{e}_1=\mathbf{e}_2=\mathbf{e}_3=\widehat{y} \tag{26}$$

and denote the reflection and transmission coefficients as r_s and t_s, respectively. If the conditions (26) are substituted into Eq. (25) and $k_x=k_0\sin\theta$ and $k_y=0$ regarded as parameters fixed by initial conditions, then Eq. (25) reduces to a first-order polynomial in k_z, the only remaining transform variable,

$$(t_s-1-r_s)\,k_z+(nt_s\cos\phi-\cos\theta+r_s\cos\theta)\,k_0=0. \tag{27}$$

This can vanish, in general, only if the coefficients of the two terms vanish. Thus we have

$$t_s=1+r_s, \tag{28}$$
$$nt_s\cos\phi=(1-r_s)\cos\theta. \tag{29}$$

These are easily solved for r_s and t_s,

$$r_s=-\frac{n\cos\phi-\cos\theta}{n\cos\phi+\cos\theta}, \tag{30}$$
$$t_s=\frac{2\cos\theta}{n\cos\phi+\cos\theta}, \tag{31}$$

which are the familiar Fresnel formulas for the reflection coefficient r_s and transmission coefficient t_s for s polarization. If the results are collected, the inverse electric field transform found by Eq. (6), and the time dependence added, the real-space solution for s polarization throughout all space (medium and vacuum) is found to be

$$\mathbf{E}^{(s)}(\mathbf{x},t)=\widehat{y}E_0[\theta(-z)\,e^{i(k_0x\sin\theta+k_0z\cos\theta-\omega t)}+\theta(-z)\,r_s e^{i(k_0x\sin\theta-k_0z\cos\theta-\omega t)}+\theta(z)\,t_s e^{i(k_0nx\sin\phi+k_0nz\cos\phi-\omega t)}]. \tag{32}$$

B. p polarization

Consider next that the incident **E**-field is polarized in the xz plane of incidence, the so-called p polarization, so that

$$e_{1y}=e_{2y}=e_{3y}=0. \tag{33}$$

For the p-polarization case we denote the reflection and transmission coefficients by r_p and t_p, respectively. Equation (25) has both x and z components in this case,

$$-\left[\left(k_0^2-k_z^2\right)e_{1x}+k_xk_ze_{1z}\right]\frac{1}{k_z-k_0\cos\theta}-\left[\left(k_0^2-k_z^2\right)e_{2x}+k_xk_ze_{2z}\right]\frac{r_p}{k_z+k_0\cos\theta}+\left[\left(k_0^2\kappa-k_z^2\right)e_{3x}+k_xk_ze_{3z}\right]\frac{t_p}{k_z-k_0n\cos\phi}=0, \tag{34}$$

$$-\left[\left(k_0^2-k_x^2\right)e_{1z}+k_zk_xe_{1x}\right]\frac{1}{k_z-k_0\cos\theta}-\left[\left(k_0^2-k_x^2\right)e_{2z}+k_zk_xe_{2x}\right]\frac{r_p}{k_z+k_0\cos\theta}+\left[\left(k_0^2\kappa-k_x^2\right)e_{3z}+k_zk_xe_{3x}\right]\frac{t_p}{k_z-k_0n\cos\phi}=0. \tag{35}$$

We cannot determine the ratio of x and z components of $\mathbf{e}_1$, by using $\mathbf{e}_1\cdot\mathbf{k}=0$ (and similarly for $\mathbf{e}_2$ and $\mathbf{e}_3$) because k_z is the variable of the transformed wave equation, not a parameter. However, that ratio can be determined by a further examination of the pole cancellation in the divergence equation (13). In the more developed notation of Eqs. (34) and (35) it is equivalent to the sum of Eq. (34) multiplied by k_x and Eq. (35) multiplied by k_z

$$-\frac{k_0^2\left(k_xe_{1x}+k_ze_{1z}\right)}{k_z-k_0\cos\theta}-\frac{k_0^2\left(k_xe_{2x}+k_ze_{2z}\right)}{k_z+k_0\cos\theta}\Phi+\frac{\kappa k_0^2\left(k_xe_{3x}+k_ze_{3z}\right)}{k_z-k_0n\cos\phi}=0. \tag{36}$$

With k_x determined by Eq. (20) the three poles of

Eq. (36) can be canceled only if $e_{1x}/e_{1z} = -\cot\theta$, $e_{2x}/e_{2z} = +\cot\theta$, and $e_{3x}/e_{3z} = -\cot\phi$ with one exception. If $\kappa(\omega) = 0$, which is true at all longitudinal-optic phonon frequencies, the pole at $k_z = k_0 n\cos\phi$ can be canceled at these specific frequencies. Since we are seeking propagating wave solutions for an arbitrary frequency, we are not concerned with these special frequencies.

We are now able to write

$$\mathbf{e}_1 = -\cos\theta\widehat{x} + \sin\theta\widehat{z}, \tag{37}$$

$$\mathbf{e}_2 = \cos\theta\widehat{x} + \sin\theta\widehat{z}, \tag{38}$$

$$\mathbf{e}_3 = -\cos\phi\widehat{x} + \sin\phi\widehat{z} \tag{39}$$

for the p-polarization case. These expressions along with the k_x values of Eq. (20) can be substituted into the two component equations (34) and (35) and polynomials in k_z found similarly to the s polarization case. However, the polynomials are of high degree, a great deal of algebraic manipulation is required, and much redundancy in the conditions obtained results from this approach. A much better approach is to form first the transverse portion of Eqs. (34) and (35) by subtracting the product of Eq. (35) with k_x from the product of Eq. (34) with k_z,

$$-\frac{\left(k_0^2 - k^2\right)\left(k_z e_{1x} - k_x e_{1z}\right)}{k_z - k_0\cos\theta} - \frac{\left(k_0^2 - k^2\right)\left(k_z e_{2x} - k_x e_{2z}\right)}{k_z + k_0\cos\theta} + \frac{\left(\kappa k_0^2 - k^2\right)\left(k_z e_{3x} - k_x e_{3z}\right)}{k_z - k_0 n\cos\phi} = 0, \tag{40}$$

and then insert Eqs. (20) and (37)–(39). Because the pole cancels now from each term, only a second degree polynomial,

$$k_z^2\left[t_p\cos\phi - (1-r_p)\cos\theta\right] + k_z k_0\left[n t_p - (1+r_p)\right] + k_0^2\left[t_p n^2\sin^2\phi\cos\phi - (1-r_p)\sin^2\theta\cos\theta\right] = 0, \tag{41}$$

results. Since k_z is the variable of the transformed wave equation, Eq. (41) can be satisfied only if the coefficient of each term separately vanishes. This yields two independent conditions

$$t_p\cos\phi = (1-r_p)\cos\theta, \tag{42}$$

$$n t_p = 1 + r_p. \tag{43}$$

The third condition resulting from Eq. (41) is seen to be redundant by the use of Snell's law, Eq. (22). Equations (42) and (43) can now be solved for

$$r_p = \frac{n\cos\theta - \cos\phi}{n\cos\theta + \cos\phi}, \tag{44}$$

$$t_p = \frac{2\cos\theta}{n\cos\theta + \cos\phi}, \tag{45}$$

which are the familiar Fresnel formulas for the reflection coefficient r_p and the transmission coefficient t_p for p polarization. If the results are collected, the inverse electric field transform found by Eq. (6), and the time dependence added, the real-space solution for p polarization throughout all space is found to be

$$\mathbf{E}^{(p)}(\mathbf{x},t) = E_0[\theta(-z)\left(-\cos\theta\widehat{x} + \sin\theta\widehat{z}\right)e^{i(k_0 x\sin\theta + k_0 z\cos\theta - \omega t)} + \theta(-z)\,r_p\left(\cos\theta\widehat{x} + \sin\theta\widehat{z}\right)e^{i(k_0 x\sin\theta - k_0 z\cos\theta - \omega t)} + \theta(z)\,t_p\left(-\cos\phi\widehat{x} + \sin\phi\widehat{z}\right)e^{i(k_0 n x\sin\phi + k_0 n z\cos\phi - \omega t)}]. \tag{46}$$

V. DISCUSSION

A new **k**-space method of solving wave propagation problems in bounded media is presented here. We chose the familiar problem of Fresnel reflection and transmission to illustrate its unfamiliar methods. There is no advantage to the use of the **k**-space method for this classic problem of local optics. However, for problems of nonlocal optics where wave-vector dispersion occurs, we have found the method to be essential to handle the effects of the medium surface correctly.[10,11] In that work we applied the **k**-space method to the transmission/reflection problem near an exciton resonance where resonant second-order wave-vector dispersion occurs. Our treatment of that problem[10,11] derived the nonlocal constitutive relation of the bounded medium and thus revealed the needed correction to the previously used dielectric approximation. Since we can see no way that the form of this correction to the dielectric approximation could be anticipated when assuming the constitutive relation of the real-space method, we believe the use of our wave-vector-space method is essential. Based on this observation we expect the **k**-space method to find important applications in wave propagation problems of bounded media, other than optics, where wave-vector dispersion occurs.

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APPENDIX

Consider an analytic function $f(k)$ of a single complex variable k where k is a component, such as k_z, of a vector variable **k**. Generalization of the proof that follows to a function of the vector variable **k** is straightforward. The function $f(k)$ must possess poles or else be a constant by Lionville's theorem, an uninteresting exception. Express

$f(k)$ as a sum of two parts,

$$f(k) = f^{(+)}(k) + f^{(-)}(k), \tag{A1}$$

$f^{(+)}(k)$ being the part containing all poles of $f(k)$ that lie in the upper half $[\mathrm{Im}(k) > 0]$ complex k plane and $f^{(-)}(k)$ being the part containing all poles in the lower half-plane $[\mathrm{Im}(k) < 0]$. We need not be concerned with the possibility of poles on the real axes for reasons discussed presently. We express the functions of Eq. (A1) as

$$f^{(+)}(k) = \sum_{u=1}^{M} \frac{p_u(k)}{(k - k_u)^{n_u}}, \tag{A2}$$

$$f^{(-)}(k) = \sum_{l=1}^{N} \frac{p_l(k)}{(k - k_l)^{n_l}}, \tag{A3}$$

where there are M poles in the upper half-plane, the uth pole occurs at k_u and is of order n_u, $p_u(k)$ is a polynomial in k, and similar quantities are defined in Eq. (A3) for the lower half-plane. Since for any long wavelength phenomenon $f(k) \to 0$ as $k \to \infty$ at least as fast as $1/k$, the polynomial $p_u(k)$ must be of $n_u - 1$ degree or lower and similarly for $p_l(k)$. Under the conditions described we assert the truth of the theorem

$$\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{f(k')dk'}{k - k' - i\eta} = f^{(+)}(k), \tag{A4}$$

where η is an infinitesimal positive quantity. To prove it, consider first the series expressing $f^{(+)}(k)$,

$$\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{1}{k - k' - i\eta} \sum_{u=1}^{M} \frac{p_u(k')}{(k' - k_u)^{n_u}} dk'. \tag{A5}$$

This can be evaluated by contour integration. Since all poles $k' = k_u$ lie in the upper half-plane and the other pole of the integrand lies in the lower half-plane at $k' = k - i\eta$, we choose the contour as the perimeter of a semicircle with the real axis forming the straight side and the semicircular arc extending into the lower half-plane. The contribution along this arc vanishes as its radius becomes infinite because the integrand approaches zero at least as fast as $1/k^2$ as $k \to \infty$. Thus the real integral is equal to the residue at the pole $k' = k - i\eta$. Thus we have

$$\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{f^{(+)}(k')dk'}{k - k' - i\eta} = \sum_{u=1}^{M} \frac{p_u\,(k - i\eta)}{(k - i\eta - k_u)^{n_u}} = f^{(+)}(k), \tag{A6}$$

where $\eta \to 0$ is used in the last step. Next consider the series expressing $f^{(-)}(k)$,

$$\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{k - k' - i\eta} \sum_{l=1}^{N} \frac{p_l(k')}{(k' - k_l)^{n_l}} dk'. \tag{A7}$$

Since all the poles $k' = k_l$ and $k' = k - i\eta$ lie in the lower half-plane, the integral (A7) is most easily evaluated with a semicircular contour in the upper half-plane. Since it encloses no poles and the contour integral again vanishes on the semicircular arc, the real integral (A7) vanishes, giving

$$\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{f^{(-)}(k')dk'}{k - k' - i\eta} = 0. \tag{A8}$$

Adding Eqs. (A6) and (A8) yields the desired theorem (A4).

In order to get an intuitive feel for the poles of, say, the electric field transform and for why poles do not arise on the real axis, consider just the spatial portion of a normally incident vacuum wave on a half-space medium occupying $z > 0$,

$$E\,(\mathbf{x}) = \Theta\,(-z)\, e^{ik_0 z}, \tag{A9}$$

where the step function is defined in Eq. (4). The $\mathbf{k}$-space transform by Eq. (5) is

$$E\,(\mathbf{k}) = -\frac{1}{2\pi i} \frac{\delta\,(k_x)\,\delta\,(k_y)}{k_z - k_0 + i\eta} \quad (\eta > 0). \tag{A10}$$

Note that to obtain a convergent transform an infinitesimal damping constant had to be inserted and that it necessarily displaces the pole from the real axis into the *lower* half complex $\mathbf{k}$ plane for this vacuum wave. Note also that the real part of the pole coordinate k_0 is just the free wave propagation constant of the vacuum. Lastly, note the transform behaves as $1/k_z$ as $k_z \to \infty$. Next consider just the transmitted wave in the medium

$$E\,(\mathbf{x}) = \Theta\,(z)\, e^{ink_0 z}. \tag{A11}$$

Its $\mathbf{k}$-space transform is then

$$E\,(\mathbf{k}) = \frac{1}{2\pi i} \frac{\delta\,(k_x)\,\delta\,(k_y)}{k_z - nk_0 - i\eta} \quad (\eta > 0). \tag{A12}$$

Note that the pole of the transmitted wave in the medium has necessarily been displaced from the real axis into the *upper* half complex $\mathbf{k}$ plane and that the real part of the pole coordinate $k_0 n$ is just the free wave propagation constant of the medium.

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[1] We use the term *wave-vector dispersion* in preference to *spatial dispersion* because of its analogy to the term *frequency dispersion* which is universally preferred over *temporal dispersion*.

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