

*Full Length Research Paper*

# Exact dielectric constant of inhomogeneous crystal and its influence on propagation of electromagnetic (EM) wave: A quantum mechanical approach

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**We present an exact treatment of electromagnetic wave propagation in a crystal medium with varying dielectric constant via quantum mechanical approach. Quantum mechanical equation involving dielectric constant was defined for incoming linearly polarized monochromatic electromagnetic wave derived from a re-normalized relativistic Lagrangian equation,  $H = H_0 + H_{perturb}$ . Considering that the spatial waveform of the field inside the field medium is not sinusoidal, we applied the Fourier transform to obtain the dispersion relation and as such, the group velocity  $v_g$  of the waveform using the mean energy flux and energy density. The frequency of the forward propagating field and the reflected field that depicts the interaction of the field with the crystal, which on other hand explains the frequency range at which the crystal exhibit anti-reflection behavior, was also determined.**

**Key words:** Dielectric constant, quantum mechanical approach, inhomogeneous crystal, group velocity, Lagrangian equation, Fourier transforms.

## INTRODUCTION

The problem of wave propagation in a crystal medium with varying dielectric constant has received great attention since the early stage of electromagnetism. The first analytical results were obtained by Rayleigh for waves whose velocity inside the medium depends linearly on the coordinate (Rayleigh, 1880). Later, the linear profile for  $\epsilon(\omega)$  (Hartree, 1931),  $z$  being the direction of propagation of the electromagnetic wave as well as an exponential and in more general, the Epstein profile (Epstein, 1952) were used for the analysis of radio wave propagation in the ionosphere. The study of electromagnetic wave propagating in a spatially inhomogeneous medium is complicated (Budden, 1966; Wait, 1970; Born and Wolf, 1970). At a Later year after the exact analytic solutions for optical fields in homogeneous media were found only for a few specific geometries, such as the cholesteric liquid crystal (Peterson, 1983; Oldano et al., 1983). A number of schemes

have been proposed for the computation of the optical effect of layered inhomogeneous media. Such schemes include the Abelé  $2 \times 2$  matrix method (Abelé, 1950), the Jones  $2 \times 2$  propagation matrix (Jones, 1941; Azzam and Bashara, 1972) and  $2 \times 2$  propagation matrix for electromagnetic waves propagating obliquely in layered inhomogeneous uniaxial media (Ong, 1993).

This present work is aimed at studying the behaviour of electromagnetic wave propagating through a crystal with varying dielectric constant using a quantum mechanical approach.

## THEORETICAL FRAMEWORK

### Formulation of quantum mechanical equation involving dielectric constant

We begin by defining the dielectric constant  $\epsilon(\omega)$  via the relation

$$\epsilon E = E + 4\lambda\rho \quad (1)$$

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$$\text{Where } \rho = \rho e_z = N \bar{\rho} e_z \quad (2)$$

and  $N$  is the density of the molecular constituent of the thin film while  $\bar{\rho}$  is the part of the dipole moment. If we consider an incoming plane monochromatic linearly polarization electromagnetic wave not influenced by molecular polarization, we can assume that

$$E = A_0 E \sin(\omega t) e_z \quad (3)$$

with a related potential  $\phi(z, t)$  satisfying

$$E = \text{grad} \phi(z, t) \quad (4)$$

with a regularized field. The theoretical Hamiltonian,  $H$  derived in the usual way from a renormalized relativistic Langrangian (Walthout, 1998; Wilson et al., 1994) enable us to write that:

$$H = H_0 + H_{\text{perturb}} \quad (5)$$

where  $H_0$  is the usual free Hamiltonian and  $H_{\text{perturb}}$  is the perturbed term of the Hamiltonian represented by the field propagating through the crystal.

The Schrodinger equation for molecular electrons of the crystal ions is of the form

$$\left[ \hat{H}_0 - i\hbar \frac{\delta}{\delta t} \right] \Psi_2^1 = e_z \sin \omega t \Psi_2^1 \exp(-i/\hbar E_0 t) \quad (6)$$

Neglecting  $\exp(-i/\hbar E_0 t)$  with a common factor, and  $e^{i\omega t}$  and  $e^{-i\omega t}$  which are linearly independent coming out during the solution of Equation 6, we have

$$\hat{H}_0 \omega_+ - (E_0 + \hbar \omega) \omega_+ = \frac{e_z}{2i} \Psi_0 \quad (7a)$$

$$\hat{H}_0 \omega_- - (E_0 - \hbar \omega) \omega_- = \frac{e_z}{2i} \Psi_0 \quad (7b)$$

Since  $E_0 + \hbar \omega$  and  $E_0 - \hbar \omega$  are not eigenvalue of  $\hat{H}_0$ , otherwise  $\omega$  would be termed absorption frequency, then we assumed  $E_j$  ( $j = 0, 1, 2, \dots$ ) to be the eigenvalue of  $\hat{H}_0$  and  $\Psi_j(z)$ , the related eigeftion. With this,  $\omega_+$  is expanded to be

$$\omega_+ = \sum_{j=0}^{\infty} C_j^+ \Psi_j \quad (8)$$

which enabled us to write that

$$\hat{H}_0 \Psi_j = E_j \Psi_j \quad (9)$$

Using Equation 7a and b in Equation 8, we obtain that:

$$\omega_+(z) = \frac{e_z}{2i} \sum_{j=1}^{\infty} \frac{\langle \Psi_j | z | \Psi_0 \rangle}{E_j - E_0 + \hbar \omega} \Psi_j(z) \quad (10)$$

and

$$\omega_-(z) = \frac{e_z}{2i} \sum_{j=1}^{\infty} \frac{\langle \Psi_j | z | \Psi_0 \rangle}{E_j - E_0 - \hbar \omega} \Psi_j(z) \quad (11)$$

Therefore we can write the wave function as

$$\Psi(z, t) = \Psi_0(z) + \frac{cA_0}{zi} \sum_{j=1}^{\infty} \langle \Psi_j | z | \Psi_0 \rangle \left( \frac{e^{-i\omega t}}{E_j - E_0 + \hbar \omega} - \frac{e^{-i\omega t}}{E_j - E_0 - \hbar \omega} \right) e^{-i(\hbar E_j t)} \quad (12)$$

and this means that the dipole moment in the direction of the field is

$$\bar{p} = \frac{c^2 A_0}{2i} \sum_{j=1}^{\infty} \left| \langle \Psi_j | z | \Psi_0 \rangle \right|^2 \sin \omega t \frac{2(E_j - E_0)}{(E_j - E_0)^2 - \hbar^2 \omega^2} \quad (13)$$

Since it is the electric field component of light wave that we are considering, the atoms or the molecules are said to be partly polarized with

$$\hbar \omega_j = E_j - E_0 \quad (14)$$

$$f_j = \frac{2m_e}{\hbar} \left| \langle \Psi_j | z | \Psi_0 \rangle \right|^2 \omega_j \quad (15)$$

To obtain the dielectric constant, we use

$$\varepsilon(\omega) A_0 e_z \sin \omega t = A_0 e_z \sin \omega t + e_z \frac{8\lambda N c^2}{\hbar} \sum_{j=1}^{\infty} \left| \langle \Psi_j | z | \Psi_0 \rangle \right|^2 \frac{\omega_j}{\omega_j^2 - \omega^2} A_0 e_z \sin \omega t \quad (16)$$

$$= \left[ 1 + \frac{4\pi N c^2}{m_e} \right] \sum_{j=1}^{\infty} \frac{f_j}{(\omega_j^2 - \omega^2)} A_0 e_z \sin \omega t \quad (17)$$

Hence, we obtain from Equation 17 that the dielectric constant is:

$$\varepsilon(\omega) = 1 + \frac{4\pi N}{m_e} c^2 \sum_{j=1}^{\infty} \frac{f_j}{\omega_j^2 - \omega^2} \quad (18)$$

**REFLECTIVE BEHAVIOUR OF A WAVE PROPAGATING IN A CRYSTAL WITH SLOWLY VARYING REFRACTIVE INDEX**

Variation of refractive index in a medium cause a variation of frequency of propagating electromagnetic wave or field with the field propagating through a crystal of thickness  $z'$  and then if the interface with vacuum is  $z = 0$  and extends to  $z = z'$ . If the field arrives at the crystal surface at  $t = 0$  and that

$$f(t) = \begin{cases} 0 & \text{for } t < 0 \\ \sin\left(\frac{2\pi}{t}\right) & \text{for } t \geq 0 \end{cases} \tag{19}$$

Using the standard Fourier transform theory, the dispersion relation is obtained to be:

$$k^2 = \frac{\omega^2}{c^2} \left[ 1 + \frac{Ne^2 / \epsilon_0 m}{\omega_0^2 - \omega^2 - ig\omega_0} \right] \tag{20}$$

which can be written as;

$$k^2 = \frac{\omega^2}{c^2} n^2(\omega) \tag{21}$$

Hence, the spatial waveform of the field inside the film medium is not sinusoidal and is formed due to interference of forward and backward waves. As a result, the group velocities  $v_g$  of these waveforms have to be determined by means of energy flux (poynting vector) P and energy density W (Ginzburg, 1967). We recall that:

$$\left. \begin{aligned} v_g &= \frac{\rho}{\omega}; \left[ \rho = \frac{c}{4\pi} E \wedge H' \right] \\ W &= \frac{1}{8\pi} (\epsilon |E|^2 + |H|^2) \end{aligned} \right\} \tag{22}$$

which can be solved (Petite and Shvartsburg, 2005). The spatial structure of the field inside the film is already said to be formed by the interference of forward wave directed towards the plane of the film  $z = 0$ , and backward one, reflected from the plane  $z = z'$ . Let us further recall that the spatial component of the electric field  $E_x$  and the magnetic field  $H_y$ , propagating along the  $z$ -direction is given by

$$E_x = \frac{i\omega}{c\sqrt{u}} \exp i \left( \frac{\omega n_0}{c} \eta - \omega \tau \right) \tag{23}$$

$$H_y = \frac{i\omega n_0 \sqrt{u}}{c} (N - iG) \exp i \left( \frac{\omega \eta_0}{c} \eta - \omega \tau \right) \tag{24}$$

One can present in a simple term Equations 23 and 24 as:

$$E_x = \frac{i\omega C}{\sqrt{uc}} (e^{iq\eta} + Qe^{-iq\eta}) \tag{25}$$

$$H_y = iq c \sqrt{ui} \left( \frac{iuz}{2qu^2} (e^{iq\eta} + e^{-iq\eta}) e^{-q\eta} - Qe^{-iq\eta} \right) \tag{26}$$

Where Q is a dimensional parameter describing the reflectivity at the boundary  $z = z'$ . If the reflective coefficient of the film R is introduced, we can write the continuity at the boundary of the plane as  $z = 0$

$$E(1+R) = \frac{i\omega C}{c} [1+Q] \tag{27}$$

$$E(1-R) = \frac{i\omega n_0 CN}{c} \left[ \frac{ib_i}{2qa_1} (1+Q)(1-Q) \right] \tag{28}$$

with parameters C, q, N,  $\eta$  and  $p^2$  defined as shown below.

$$C = \frac{-icE(1+R)}{1+Q} \tag{29}$$

$$q = \frac{\omega n_0 N}{c} \tag{30}$$

$$N = \sqrt{\frac{1-c^2 p^2}{\eta_0 \omega^2}} \tag{31}$$

$$p^2 = \frac{1}{4a_1^2} + \frac{b_1}{a_2^2} \tag{32}$$

where  $b_1$  and  $b_2$  are the free parameter of the model and;  $a_1$  and  $a_2$  are the characteristic spatial scales of

$$G = \frac{Cb_1}{2\omega n_0 a_1} \left[ 1 + \frac{4b_2 a_1}{b_1 a_2^2} \right] \tag{34}$$

**RESULTS AND DISCUSSION**

Comparing the result of this work with the one obtained

using classical approach, when  $\chi < 1$  where  $\chi$  is a damping term which is neglected as obtained by Fitzpatrick (2007), we find out that the dielectric constant is a frequency dependant function. From Equation 18, it is observed that at low frequencies below the smallest frequency  $\omega_j$ , all the terms is the sum which is positive and even the refractive index  $n(\omega)$  which is related to the dielectric constant as  $\sqrt{\varepsilon(\omega)}$ , is greater than unity. It will be observed that as  $\omega$  increases to high values such that it is greater than  $\omega_j$ , negative sum occurs and hence  $n(\omega)$  is less than unity.

This depicts the fact that at high frequencies, electromagnetic wave propagated through ionic crystal medium with phase velocity is greater than the velocity of light in vacuum. This implies that  $\omega \approx \omega_j$ .

One also observes that the expression relating  $\omega$  in Equation 10 and 11 depicts the frequency of the forward propagating field with the reflected field interaction propagating in the crystal. This of course affects the amplitude of the reflected wave at the interface  $z = z'$  and thus changes the structure of the poynting vector and the energy density, and consequently the group velocity,  $V_g$ . Another interesting phenomenon is the dispersion introduced by such crystal which is frequency dependent as shown in Equation 21. Here, one observes that, if the refractive index is considered to have positive imaginary component that might lead to attenuation of the wave as it propagates through the crystal, the reflection coefficient of crystal is of low intensity over a large frequency range. The antireflection property of the crystal material is observed in the frequency range to vary only with the length of the scales  $a_1$  and  $a_2$ .

## CONCLUSION

In this work, we have presented a number of properties, which can be studied, with the help of exact solution of electromagnetic wave propagations applied to crystal media and presenting spatial variation of its dielectric constant. Though quantum mechanical approach was used, they contain enough parameters to describe the dielectric constant of a crystal and how the refractive index relates to the dielectric constant of the crystal.

This formalism allowed the understanding of how the dielectric constant variation influences the various properties of the crystals such as reflection coefficient, anti-reflectance and refractive index. It was shown that when used close to their cut-off frequency, in the propagation mode, such crystal might have some exceptional negative dispersion relation. With this knowledge, it is possible to design a system with specific dispersion or reflection properties in any frequency range.

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