Dielectric Permeability of Nanocylinder

S. Jaćimovski, V. Sajfert, D. Raković and B. Tošić

1. Introduction

Our goal is to investigate dielectric permeability tensor $\varepsilon_{\alpha\beta}$, as well as tensors of nonlinear polarization of the nanocylinder. In nonlinear optics, the vector of electrical induction $D$ is the series of different degrees of electric field components. The coefficient in the first term of this series is dielectric permeability tensor, while in other terms appear higher tensors of third range, fourth range etc.

The idea of Dzyalosinski and Pitaevski [1], for equating the phenomenological value of the vector potential from Maxwell’s equations with its nonequilibrium average value, is the bridge connecting optical phenomenology with micro characteristic of molecular crystals. The micro characteristic of crystals enters the retarded and advanced Green’s functions and correct use of Paulion Green’s function. It turned out that refraction and absorption indices depend on configuration coordinates, having maximal values at boundary cross-sections and minimal value at central cross-section of the nanocylinder broken symmetry structure. Although it was expected that boundary conditions make higher refractive and absorptive characteristics of the nanocylinder, this appeared not to be possible because Paulion Green’s function is not proportional to the exciton concentration.

PACS numbers: 78.20Ci, 78.40Me

2. Correct expression for Paulion Green’s function

We shall consider here the linear infinite chain of molecules. The procedure derived for linear chain can be then extended for two and three dimensional structures.

The excitonic Hamiltonian of an ideal molecular chain, $H_{\text{exc}} = \sum_{n} \Delta W_{n} (P_{n+1}^{+} P_{n} + P_{n}^{+} P_{n-1})$, is the nearest neighbours approximation, can be written as follows:

\[
H_{p} = \Delta \sum_{n} P_{n}^{+} P_{n} - W \sum_{n} P_{n}^{+} (P_{n+1} + P_{n-1})
- F \sum_{n} P_{n}^{+} P_{n} (P_{n+1}^{+} + P_{n+1} + P_{n-1}^{+} + P_{n-1})
\]

Paulion Green’s function of the system is defined as:

* corresponding author; e-mail: stevo.jacimovski@kpa.edu.rs

(738)
\[
\langle P_n(t) \, \vert \, P^+_m(0) \rangle = \theta(t) \langle P_n(t) \, \vert \, P^+_m(0) \rangle .
\]
(2.2)

differentiating Eq. (2.2) with respect to \( t \) and using Fourier time-frequency transformation
\[
f(t) = \int_0^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} f(\omega),
\]
(2.3)
we obtain the following equation for Paulion Green’s function:
\[
(E - \Delta) \langle P_n \, \vert \, P^+_m \rangle_{\omega} = \frac{i\hbar}{2\pi} (1 - 2N_p)
- W \left[ \langle \langle P_{n+1} \, \vert \, P^+_m \rangle \rangle_{\omega} + \langle \langle P_{n-1} \, \vert \, P^+_m \rangle \rangle_{\omega} \right]
+ 2W \left( \langle \langle P^+_n \, P_n \, P_{n+1} \, \vert \, P^+_m \rangle \rangle_{\omega} \right)
+ \langle \langle P^+_n \, P_n \, P_{n+1} \, \vert \, P^+_m \rangle \rangle_{\omega}
- 2\langle \langle P^+_n \, P_{n+1} \, P_{n+1} \, P_n \, \vert \, P^+_m \rangle \rangle_{\omega}
+ \langle \langle P_{n-1} \, P_n \, P_{n+1} \, \vert \, P^+_m \rangle \rangle_{\omega} \right)
N_p \equiv \langle P^+ \rangle .
\]
(2.4)

The higher order Green’s function, containing four Pauli operators, will be decoupled by means of Tyablikov approximation [2, 5]
\[
\langle \langle P^+_n \, P_n \, P_{n+1} \, \vert \, P^+_m \rangle \rangle_{\omega} \approx N_{p0} = \langle \langle P \, \vert \, P^+_n \rangle \rangle_{\omega} .
\]
(2.5)

Tyablikov’s approximation physically means substitution of the scattering processes on real potential by the propagation of particles through the soft potential.

After inserting Eq. (2.5) into Eq. (2.4) for Paulion Green’s function, we have:
\[
(E - \Delta) \langle P_n \, \vert \, P^+_m \rangle_{\omega} = \frac{i\hbar}{2\pi} \delta_{n,m} (1 - 2N_p)
- (1 - 2N_{p0}) W \left[ \langle \langle P_{n+1} \, \vert \, P^+_m \rangle \rangle_{\omega} + \langle \langle P_{n-1} \, \vert \, P^+_m \rangle \rangle_{\omega} \right]
- 4F N_{p0} \langle \langle P_n \, \vert \, P^+_m \rangle \rangle_{\omega} .
\]
(2.6)

Further solving of Eq. (2.6) requires application of noncanonical transformation
\[
P_n = \frac{1}{\sqrt{N}} \sum_{k=0}^{\infty} e^{i\hbar \omega k} P_k ,
\]
(2.7)

which reduces Eq. (2.6) to
\[
\langle \langle P^+_n \rangle \rangle_{k,\omega} = \frac{i\hbar}{2\pi} \frac{1 - 2N_p}{\sqrt{e^{i\omega k} - 1}} .
\]

\[E^{(1)}_k = \Delta - 2W \cos ak + 4 (W \cos ak - F) N_{p0} .
\]
(2.8)

It should be noticed that correlator of Paulion Green’s function (2.8) leads to spurious error [5].

We shall not use Paulion Green’s function (2.8) due to the reasons [1–2] given in the Introduction. Instead, we shall use equivalent bozon Green’s function, which will be determined by means of the exact bozon representation for Pauli operators from [4]. In the considered case it is sufficient to use this exact representation in the approximations
\[
P = B - B^+ B B^+ B^+ ;
\]
\[
P^+ P = B^+ B - B^+ B^+ B B^+ .
\]
(2.9)

Inserting Eq. (2.9) into Eq. (2.6), by means of Wick’s theorem for bozons we obtain
\[
(1 - 4N_{p0}) (E - \Delta) \langle \langle B_n \, \vert \, B^+_m \rangle \rangle_{\omega}
+ (1 - 2N_{p0}) W \langle \langle B_{n+1} \, \vert \, B^+_m \rangle \rangle_{\omega}
+ (1 - 2N_{p0}) W \langle \langle B_{n-1} \, \vert \, B^+_m \rangle \rangle_{\omega}
= \frac{i\hbar}{2\pi} \delta_{n,m} (1 - 2N_p) - 4FN_{p0} \langle \langle B_n \, \vert \, B^+_m \rangle \rangle_{\omega} .
\]
(2.10)

We note that in Eq. (2.10) squares of bozon concentration are neglected.

Using Fourier transformation of Bose operator (which is canonical transformation for bozons), we obtain the following equation for bozon Green’s function \( \langle \langle B_k \, \vert \, B^+_k \rangle \rangle_{\omega} \):
\[
\langle \langle B_k \, \vert \, B^+_k \rangle \rangle_{\omega} = \frac{\hbar}{2\pi} (1 + 2N_{p0})
+ \frac{4}{\pi} \left( \frac{\theta}{4\pi W} \right)^{3/2} \sum_{n=1}^{\infty} e^{-n(\frac{\theta}{4\pi W})} n^{-3/2} .
\]
(2.11)

where
\[E^{(1)}_k = \Delta - 2W \cos ak + 4 (W \cos ak - F) N_{p0} .
\]
(2.12)

The energy of zero approximations is
\[E^{(0)}_k = \Delta - 2W \cos ak.
\]
(2.13)

Now we shall calculate zero order value \( N_{B0} \). Taking \( \cos ak \approx 1 - \frac{1}{4} a^2 k^2 + \frac{1}{24} a^4 k^4 \), we obtain:
\[
N_{B0} = \frac{1}{N} \sum_{k>0} \frac{1}{\sqrt{e^{i\omega k} - 1}}
= \left( \frac{\theta}{4\pi W} \right)^{1/2} \sum_{n=1}^{\infty} e^{-n(\frac{\theta}{4\pi W})} n^{-1/2}
+ \frac{\pi}{4} \left( \frac{\theta}{4\pi W} \right)^{3/2} \sum_{n=1}^{\infty} e^{-n(\frac{\theta}{4\pi W})} n^{-3/2} .
\]
(2.14)

For \( N_B \) we obtain the formula:
\[
N_B = \frac{1}{N} \sum_{k>0} \frac{1}{\sqrt{e^{i\omega k} - 1}} = N_{B0} - \left( \frac{C_{1/2}(\theta)}{\theta} \right)^{1/2}
- C_{3/2}(\theta) \left( \frac{\theta}{4\pi W} \right)^{3/2}
+ C_{5/2}(\theta) \left( \frac{\theta}{4\pi W} \right)^{5/2} N_{B0} ,
\]
(2.15)

where
\[C_{1/2}(\theta) = \frac{4(W - F)}{\theta} \sum_{n=1}^{\infty} e^{-n(\frac{\theta}{4\pi W})} n^{1/2} ,
\]
(2.16)

\[C_{3/2}(\theta) = \frac{\pi (W + F)}{\theta} \sum_{n=1}^{\infty} e^{-n(\frac{\theta}{4\pi W})} n^{-1/2} ,
\]
(2.17)

\[C_{5/2}(\theta) = \frac{\pi^2 W}{\theta} \sum_{n=1}^{\infty} e^{-n(\frac{\theta}{4\pi W})} n^{-3/2} .
\]
(2.18)

Besides, in accordance with Eq. (2.9) we can take
\[ N_p = N_B - 2N_{B0}^2. \]

Multiplying Eq. (2.8) and (2.11) we have
\[
\langle \langle P | P^+ \rangle \rangle_{k,\omega} \langle \langle B | B^+ \rangle \rangle_{k,\omega}
= \left( \frac{i\hbar}{2\pi} - E - E^{(1)}_k \right)^2 (1 - 2N_p)(1 + 2N_{B0})
= \left( \frac{i\hbar}{2\pi} - E - E^{(1)}_k \right)^2 (1 - 2(N_{B0} - N_B))
+ 4 \left( N_{B0}^2 - N_{B0}N_B + 8N_{B0}^3 \right). \tag{2.20}
\]

It was said that all contributions proportional to \(N_{B0}^2\) and higher degrees of \(N_{B0}^2\) are to be neglected in this analysis, so that we can write Eq. (2.20) as
\[
\langle \langle P | P^+ \rangle \rangle_{k,\omega} \langle \langle B | B^+ \rangle \rangle_{k,\omega} = \left( \frac{i\hbar}{2\pi} - E - E^{(1)}_k \right)^2 (1 - 2(N_{B0} - N_B)). \tag{2.21}
\]

Now we shall estimate the value \(2(N_{B0} - N_B)\). Taking only leading terms in \(N_B\) and \(N_{B0}\) in Eq. (2.10) we have:
\[
2(N_{B0} - N_B) = 2 \left( \frac{W-F}{\pi W} \right) \sum_{n=1}^{\infty} e^{-n(\Delta_{2W})}n^{-1/2}
 \times \sum_{n=1}^{\infty} e^{-n(\Delta_{2W})}n^{-3/2}. \tag{2.22}
\]

Since the maximal achieved exciton concentrations are of the order \(10^{-3}\) [2] we can take in Eq. (2.22) that \(e^{-\Delta_{2W}} = 10^{-3}\). This gives the estimation \(2(N_{B0} - N_B) \approx 10^{-6} \approx N_{B0}^2\). Consequently, the term \(2(N_{B0} - N_B)\) in Eq. (2.21) must be neglected and Eq. (2.21) becomes
\[
\langle \langle P | P^+ \rangle \rangle_{k,\omega} \langle \langle B | B^+ \rangle \rangle_{k,\omega} = \left( \frac{i\hbar}{2\pi} - E - E^{(1)}_k \right)^2 ,
\]
\[
\langle \langle P | P^+ \rangle \rangle_{k,\omega} = \langle \langle B | B^+ \rangle \rangle_{k,\omega} = \left( \frac{i\hbar}{2\pi} - E - E^{(1)}_k \right)^2 .
\]

So, the correct use of Paulion Green’s function is:
\[
\langle \langle P | P^+ \rangle \rangle_{k,\omega} = \left( \frac{i\hbar}{2\pi} - E - E^{(1)}_k \right)^2 ;
\]
\[
E^{(1)}_k = \Delta - 2W \cos ak + 4(W \cos ak - F) N_{\rho 0}. \tag{2.23}
\]

It should be pointed out that this correct use of Paulion Green’s functions does not lead to spurious errors, and that gives the correct expression for low temperature magnetization in the theory of magnetism.

### 3. Green’s functions of nanocylinder

Nanocylinder will be taken as a set of parallel discs normal to z axis. Number of discs \(M\) is of the order 10. Number \(N\) of molecules in disc is also maximally of the order 10. The discs will be labeled with integer \(m \in (0, M)\). The molecules in disc will be labeled with integer \(n \in (0, N)\) [6].

The boundary conditions are actual along z axis. In this direction the discs labeled with \(m = -1\) and \(m = M + 1\) are absent. So the boundary conditions can be written as:
\[
X_{n,0;n,-1} = X_{n,M;n,M+1}; \quad Y_{n,0;n,-1} = Y_{n,M;n,M+1};
\]
\[
Z_{n,0;n,-1} = Z_{n,M;n,M+1}. \tag{3.1}
\]

If we assume that one of molecules is excited by energy quant \(\Delta\), and take into account that interactions between neighbour molecules in one disc and interaction between corresponding molecules laying in neighbour discs differ, the Hamiltonian of nanocylinder we can written in the nearest neighbours approximation as follows:

\[
H = \sum_{n=0}^{N} \sum_{m=0}^{M} \Delta P_{nm}^{+} P_{nm} + \sum_{n=0}^{N} \sum_{m=1}^{M-1} \left( X_{n,m,n+1,m} + X_{n,m,n+1,m+1} + X_{n,m,m,n-1} + X_{n,m,m,n-1} \right) P_{nm}^{+} P_{nm}
\]
\[
- \sum_{n=0}^{N} \sum_{m=1}^{M-1} \left( P_{nm}^{+} Y_{n,m,n+1,m} P_{n+1,m} + Y_{n,m,n+1,m} P_{n+1,m} + Y_{n,m,m+1} P_{n+1,m+1} + Y_{n,m,m+1} P_{n+1,m+1} \right)
\]
\[
+ \sum_{n=0}^{N} \sum_{m=1}^{M-1} \left( Z_{n,m,n+1,m} P_{n+1,m} + Z_{n,m,n+1,m} P_{n+1,m} + Z_{n,m,m+1} P_{n+1,m+1} + Z_{n,m,m+1} P_{n+1,m+1} \right)
\]
\[
+ \sum_{n=0}^{N} \sum_{m=1}^{M-1} \left( P_{n+1,m} Y_{n+1,0;n+1,0} P_{n+1,0} + Y_{n+1,0;n+1,0} P_{n+1,0} + Y_{n,0,0} P_{n,0} \right)
\]
\[
+ \sum_{n=0}^{N} \sum_{m=0}^{M} \left( Z_{n,0;n+1,0} P_{n+1,0} + Z_{n,0;n+1,0} P_{n+1,0} + Z_{n,0;n+1,0} P_{n+1,0} + Z_{n,0;n+1,0} P_{n+1,0} \right)
\]
In this Hamiltonian $\Delta \approx 5$ eV is the energy of excitation of an isolated molecule [7–9], while $X$, $Y$, and $Z$ are matrix elements of the dipole-dipole interaction which are two orders of magnitude less than $\Delta$. The terms proportional to $Z$ characterize dynamical interaction of excitons.

It is important to note that system of molecules in disc is cyclically invariant. It means that for arbitrary physical characteristic $F$ the following is valid:

$$F_n = F_{n+(N+1)}.$$  \hspace{1cm} (3.3)

For further evaluation it is important to point out the cyclic rules $P_{n+(N+1)} = P_n$ and $e^{iak_n} = e^{iak(n+(N+1))}$, wherefrom $e^{iak(n+1)} = 1$. The last means that $k = \frac{2\pi\nu}{N+1}$, where $\nu$ is an integer. On this basis, Kronecker symbol can be expressed in terms of plane waves:

$$\delta_{k,q} = \frac{1}{N+1} \sum_{n=0}^{N} e^{i(q-k)n}$$

$$= \begin{cases} 
1 & \text{if } k = q \\
\frac{1 - e^{i(q-k)(N+1)}}{1 - e^{i(q-k)}} & \text{if } k \neq q
\end{cases}$$ \hspace{1cm} (3.4)

allowing that the system of discs molecules can be treated as an ideal structure.

Introducing notations

$$X_{n,m,n \pm 1,m} = C; \quad Y_{n,m,n \pm 1,m} = -D; \quad$$

$$X_{n,m,n \pm 1, m} = R; \quad Y_{n,m,n \pm 1, m} = -S;$$

$$Z_{n,n \pm 1, m} = -F; \quad Z_{n,n,n \pm 1} = -L,$$ \hspace{1cm} (3.5)

we can write the Hamiltonian (3.2) as:

$$H = \sum_{n=0}^{N} \sum_{m=1}^{M} \Delta P_{n,m}^+ P_{n,m}$$

$$+ \sum_{n=0}^{N} \sum_{m=1}^{M-1} \left[ 2(C + R) P_{n,m}^+ P_{n,m} - D \left( P_{n,m}^+ P_{n+1,m} + P_{n,m}^+ P_{n-1,m} \right) - S \left( P_{n,m}^+ P_{n,m+1} + P_{n,m}^+ P_{n,m-1} \right) \right]$$

$$- \sum_{n=0}^{N} \sum_{m=1}^{M-1} \left[ F P_{n,m}^+ P_{n,m} \left( P_{n+1,m}^+ P_{n+1,m} + P_{n-1,m}^+ P_{n-1,m} \right) \right.$$ 

$$+ \left. L P_{n,m}^+ P_{n,m} \left( P_{n+1,m}^+ P_{n+1,m} + P_{n-1,m}^+ P_{n-1,m} \right) \right]$$

$$+ \sum_{n=0}^{N} \sum_{m=0}^{N-1} \sum_{\nu=0}^{N-1} \left( P_{n,0}^+ D P_{n+1,0}^+ + D P_{n-1,0}^+ + R P_{n,1} \right)$$

$$+ \sum_{n=0}^{N} \sum_{m=0}^{N} \left( F P_{n,0}^+ P_{n+1,0}^+ + F P_{n-1,0}^+ P_{n-1,0}^+ + L P_{n,1}^+ P_{n,1}^+ \right)$$

$$+ \sum_{n=0}^{N} \sum_{m=1}^{N} \sum_{\nu=0}^{N} \left( P_{n,0}^+ D P_{n+1,1}^+ + D P_{n-1,1}^+ + R P_{n,M-1} \right)$$

$$+ \sum_{n=0}^{N} \sum_{m=1}^{N} \sum_{\nu=0}^{N} \left( F P_{n,0}^+ P_{n+1,1}^+ + F P_{n-1,1}^+ P_{n-1,1}^+ + L P_{n,M-1}^+ P_{n,M-1}^+ \right).$$ \hspace{1cm} (3.6)

Paulion Green’s function will be denoted as:

$$\Gamma_{n,m,n',m'}(t,t') = \theta(t-t') \left[ \left( P_{n,m}(t), P_{n',m'}^+ \right) \right]$$

$$\equiv \langle \langle P_{n,m}(t)|P_{n',m'}^+ \rangle \rangle.$$ \hspace{1cm} (3.7)

It will be determined by standard Green’s function solving procedure, although all problems pointed out in introduction stay open.

Differentiating Eq. (3.7) with respect to $t$, taking into account equations of motion, and using transformation

$$\Gamma_{n,m,m',n'}(\omega) = \frac{1}{N+1} \sum_{\nu} e^{i(n-n')\omega} \gamma_{m,m'}(\omega, \nu),$$ \hspace{1cm} (3.8)

with
and parameter \( \varphi \), we obtain the following system of three difference equation [10]:

\[
\begin{align*}
\hat{S}_{\gamma_{m+1,m}} + \hat{S}_{\gamma_{m-1,m}} + \hat{S}_{\gamma_{m,m}} &= \frac{i}{2\pi} (1 - 2N_{P0}) \delta_{m,m'} ; \quad 1 \leq m \leq M - 1 \\
\end{align*}
\]

and

\[
\begin{align*}
\hat{S}_{\gamma_{M-1,m}} + \hat{S}_{\gamma_{M,m}} &= \frac{i}{2\pi} (1 - 2N_{P0}) \delta_{m,m'} ; \quad m = 0 \\
\end{align*}
\]

and

\[
\begin{align*}
\hat{S}_{\gamma_{1,m}} + \hat{S}_{\gamma_{M-1,m}} + \hat{S}_{\gamma_{M,m}} &= \frac{i}{2\pi} (1 - 2N_{P0}) \delta_{m,m'} ; \quad m = M ,
\end{align*}
\]

where

\[
\begin{align*}
\hat{S} &= \hat{S}_{1} (1 - 2N_{P0}) ; \quad \hat{D} = \hat{D}_{1} (1 - 2N_{P0}) ; \\
\rho &= \rho_{1} - \Delta - 2D - 2R + 2\hat{D} \cos \tau_{\nu} ; \\
\langle B_{n,m}^{+} B_{n,m} \rangle^{(0)} &= N_{B0} \approx (P_{m}^{+} P_{m})^{(0)} = N_{P0} ; \\
\end{align*}
\]

\[
\begin{align*}
\langle B_{n,m}^{+} B_{n,m} \rangle = N_{B} .
\end{align*}
\]

By the substitution

\[
\gamma_{m,m'} (\omega, \nu) = \sum_{\sigma} A_{\sigma} (m', \nu, \omega) \delta(m) ,
\]

where

\[
A(m) = \sin (m + 1) \varphi \sigma - \frac{R - LN_{P0}}{S(1 - 2N_{P0})} \sin m \varphi \sigma ,
\]

and parameter \( \varphi \) satisfy the equation:

\[
\sin (M + 2) \varphi \sigma - \frac{R - LN_{P0}}{S(1 - 2N_{P0})} \sin (M + 1) \varphi \sigma
\]

\[
+ \left( \frac{R - LN_{P0}}{S(1 - 2N_{P0})} \right)^{2} \sin M \varphi \sigma = 0 ,
\]

the system of Eq. (3.10–3.12) reduces into one unique equation:

\[
\sum_{\sigma} \left( 2 \delta \cos \varphi + \rho \right) A_{\sigma} (m', \nu, \omega) \delta(m) = \frac{i}{2\pi} (1 + 2N_{B0}) \delta_{m,m'} , \quad m, m' \in (0, 1, 2, \ldots, N) .
\]

Parameter \( \varphi \) have real solutions of the Eq. (3.16), laying in the interval \((0, \pi)\). Parameter \( \varphi \) may not have values \( m = 0 \) or \( m = M \), since in these cases the Green’s function becomes \( \gamma \equiv 0 \). Also, in the system the autoreduction process takes place. It means, that \( m \) takes \( m + 1 \) values for \( m \) values of \( \sigma \). It means that we must in principle solve two problems: one problem is related to the subsystem of \( m \in (0, 30) \) and the second problem is related to the subsystem \( m \in (1, 31) \).

Taking that

\[
A_{\sigma} (m', \nu, \omega) = \chi (\omega, \nu) \delta(m') ,
\]

and

\[
\sum_{\sigma} A_{\sigma} (\omega, \nu) \Phi (m') = \delta_{m,m} ,
\]

since \( \chi_{\sigma}(\omega) \equiv \langle \langle P_{\sigma}^{+} \rangle \rangle \), we can finally write the expression for Fourier image of the Paulion Green’s function:

\[
\langle \langle P \rangle \rangle_{\sigma,\omega} = \frac{i}{2\pi E - E_{k}^{(1)}},
\]

where

\[
E_{k}^{(1)} = \Delta + 2C + 2R - 2D (1 - 2N_{B0}) \cos \tau_{\nu} .
\]

Now we shall look for bozon Green’s function of the nanocylinder. This bozon Green’s function is given by:

\[
G_{n,m,m',m'} (t, t') = \theta (t - t') \langle [B_{n,m}(t), B_{n,m}^{+}(t)] \rangle \equiv \langle \langle B_{n,m}(t) B_{n,m}^{+}(t) \rangle \rangle .
\]

By inserting Eq. (2.9) into Eq. (3.7), by absolutely same procedure we can determine the bozon Green’s function:

\[
\langle \langle B \rangle \rangle B_{\sigma, \omega} = \frac{i}{2\pi E - E_{k}^{(1)}} .
\]

Multiplying Eq. (3.23) and (3.20) we obtain:

\[
\langle \langle P \rangle \rangle_{\sigma, \omega} \langle \langle B \rangle \rangle_{\sigma, \omega} = \left( \frac{i}{2\pi E - E_{k}^{(1)}} \right)^{2} (1 - 2N_{P0})(1 + 2N_{B0})
\]

\[
+ 4 (N_{B0} - N_{B0} N_{B}) + 8N_{B0}^{3} .
\]

In the first section it was demonstrated that all terms added to unit on the right hand side of the Eq. (3.24) are of the order \( N_{B0}^{2} \), i.e. of the order \( 10^{-6} \). This is the reason to neglect all these terms. It means that \( \langle \langle P \rangle \rangle_{\sigma, \omega} \langle \langle B \rangle \rangle_{\sigma, \omega} \) reduces to

\[
\langle \langle P \rangle \rangle_{\sigma, \omega} \langle \langle B \rangle \rangle_{\sigma, \omega} = \left( \frac{i}{2\pi E - E_{k}^{(1)}} \right)^{2} .
\]

It means that Paulion Green’s function, which enters dielectric permeability and nonlinear polarizability tensor, is given by the Eq. (3.25).

4. Dielectric polarization of crystal

The dielectric permeability tensor \( \varepsilon_{\alpha \beta}(k, \omega) \) represents the relation between vacuum electrical field and its images in the material medium induction vector \( \mathbf{D} \). In Fourier components this relation is given by the equation

\[
\mathbf{D}_{k}(k, \omega) = \varepsilon_{\alpha \beta}(k, \omega) \mathbf{E}_{k}(k, \omega) .
\]

In accordance with Einstein convention, repeated index means summation. The system of Maxwell’s equations, where weak external currents are present and external charges are absent, can be written as follows:
\[ k \times B (k, \omega) = -\frac{\omega}{c} D (k, \omega) + \frac{4\pi}{1\varepsilon} j^\text{ext} (k, \omega), \quad (4.2) \]
\[ k \times D (k, \omega) = 0, \quad (4.3) \]
\[ k \times E (k, \omega) = \frac{\omega}{c} B (k, \omega), \quad (4.4) \]
\[ k \times B (k, \omega) = 0. \quad (4.5) \]

Since external charges are equal to zero the following conditions are valid:
\[ k \cdot D (k, \omega) = k \cdot B (k, \omega) = 0 \]
If we use Lorentz calibration of vector potential \( A (k, \omega) \), we obtain equations:
\[ B (k, \omega) = \text{rot} A (k, \omega), \quad (4.6) \]
\[ E (k, \omega) = -\frac{1}{c} \frac{\partial A (k, \omega)}{\partial t}. \quad (4.7) \]

By combining Maxwell’s Eq. (4.2), (4.4), and (4.1) with Eq. (4.7) we obtain
\[ E (k, \omega) = \frac{i \omega}{c} A (k, \omega). \quad (4.8) \]

Then we obtain the following relation between the vector potential and the external forces:
\[ \Delta_{\alpha\beta} (k, \omega) A_{\beta} (k, \omega) = \frac{4\pi}{\varepsilon} j^\text{ext} (k, \omega). \quad (4.9) \]

Consequently, the explicit relation for the vector potential components is \([2]\):
\[ \Delta_{\alpha\beta} (k, \omega) = k^2 \delta_{\alpha\beta} - k_\alpha k_\beta - \frac{\omega^2}{c^2} \varepsilon_{\alpha\beta} (k, \omega), \quad (4.10) \]
and
\[ A_{\beta} (k, \omega) = \frac{4\pi}{c} \Delta^{-1}_{\alpha\beta} (k, \omega) j^\text{ext} (k, \omega). \quad (4.11) \]

This phenomenological value will be equated with the non-equilibrium mean value vector potential. The interaction of the vector potential with the external currents is defined as follows. The non-equilibrium mean value vector potential we shall calculate by using S matrix of the system, i.e.:
\[ \langle A_{\alpha} (r, t) \rangle_n = \langle T e^{ikz} e^{-i\frac{\pi}{\varepsilon} \int_{-\infty}^{\infty} dt W(t')} \times A_{\alpha} (r, t') e^{i\frac{\pi}{\varepsilon} \int_{-\infty}^{\infty} dt' W(t')} \rangle. \quad (4.12) \]

In linear approximation in \( j^\text{ext} \), we obtain non-equilibrium value of vector potential.

Vector potential has not physical sense. It is only useful mathematical element of the theory. That is the reason for going over of vector potential components to components of electrical field, since electrical field components are measurable. The final connecting of phenomenological electromagnetic field and micro characteristic of physical medium is given by formula \([11–12]\):
\[ \Delta^{-1}_{\alpha\beta} (k, \omega) = -\frac{\varepsilon}{\varepsilon^2} \delta_{\alpha\beta} + i \frac{\varepsilon^2}{\varepsilon^2} \varepsilon_{\alpha\beta} (k) E_{\beta} (k) \times \left[ G^R (k, \omega) + G^A (k, \omega) \right], \quad (4.13) \]

where \( \Delta_{\alpha\beta} (k, \omega) \) is given by Eq. (4.10).

The obtained relation is complicated for analysis, so in practice it is used in homogenized approximation and with neglecting of space dispersion \([12]\). Then general Eq. (4.13) can be written in the form:
\[ \varepsilon^{-1}_{\alpha\beta} (k, \omega) = 1 + \frac{\varepsilon^2 E^2 (k)}{8\pi \varepsilon^2} \left( \frac{1}{1 - \frac{\omega^2}{\varepsilon \omega}} - \frac{1}{1 + \frac{\omega^2}{\varepsilon \omega}} \right). \quad (4.14) \]

Retarded Green’s function \( G^R (\nu, \omega) \) is given by formula
\[ G^R (\nu, \omega) = \frac{i}{2\pi} \sum_{\sigma = 1}^{M} \frac{\Psi_{\sigma} (m) \Phi_{\sigma} (m')}{\omega - \omega_{\nu}}. \quad (4.15) \]

Advanced Green’s function \( G^A (\nu, \omega) \) can be obtained from Eq. (4.15) by inversion \( \omega \rightarrow -\omega \). Consequently
\[ G^A (\nu, \omega) = \frac{i}{2\pi} \sum_{\sigma = 1}^{M} \frac{\Psi_{\sigma} (m) \Phi_{\sigma} (m')}{\omega + \omega_{\nu}}. \quad (4.16) \]

Putting Eq. (4.15) and (4.16) into Eq. (4.14) we obtain
\[ \varepsilon^{-1}_{\alpha\beta} (k, \omega) = 1 + \frac{\varepsilon^2 E^2 (k)}{8\pi \varepsilon^2} \left( \sum_{\sigma = 1}^{M} \frac{\Psi_{\sigma} (m) \Phi_{\sigma} (m')}{\omega_{\nu}} \right) \times \left( \frac{1}{1 - \frac{\omega^2}{\varepsilon \omega}} - \frac{1}{1 + \frac{\omega^2}{\varepsilon \omega}} \right). \quad (4.17) \]

The obtained result points out that dielectric permeability \( \varepsilon \) of the nanocylinder depends on the configuration variables \( m \) and \( m' \), and this is the main difference compared to permeability of the ideal structure. With suitable choice of the functions \( \Psi \) and \( \Phi \), we can influence the magnitude of permeability.

Ending these analyzes, we should say that after construction of the high-power lasers it was registered that material equation is not linear relation between vectors \( D \) and \( E \). Vector \( D \) is infinite series containing products of electrical fields components. The coefficient of this series is called tensor of nonlinear polarizability. Relation \( D_\alpha = \varepsilon_{\alpha\beta} E_\beta \) is only first term of the series \([12]\):
\[ D_\alpha = \varepsilon_{\alpha\beta} E_\beta + \varepsilon_{\alpha\beta\gamma} E_\gamma E_\beta + \varepsilon_{\alpha\beta\gamma\delta} E_\alpha E_\beta E_\gamma E_\delta + \ldots \]

The tensors \( \varepsilon_{\alpha\beta\gamma} \) and \( \varepsilon_{\alpha\beta\gamma\delta} \) are so called nonlinear polarizability tensors. In the last formula, as well as in all formulas of this section, repeated index denotes a summation.

5. Conclusion

Nanostructures are physical objects of great potential practical interest. Here we investigated what could be expected from nanocylinders in the linear and nonlinear optics.

Dielectric properties of nanocylinder of finite length were therefore analyzed. Defining the correct value of Paulion Green’s functions, we determined dielectric permeability of the nanocylinder in \( z \)-direction, and found that it depends on configuration coordinates. The expressions for transformation functions \( \Psi \) and \( \Phi \) give possibility to change behaviour of the nanocylinder polarizability.
It was expected that boundary conditions make higher refractive and absorptive characteristics of the nanocylinder, but this was not possible because Paulion Green’s function is not proportional to the exciton concentration. Although negative, this conclusion represents the main result of our analysis.

Acknowledgments

This paper was in part supported by the Serbian Ministry of Science and Technology: Grant No 141044 and by Vojvodina Academy of Sciences and Arts and by the Provincial Secretariat for Science and Technological Development of the Autonomous Province of Vojvodina (114-451-01336/2007-02).

References