

# Novel Mathematical Approach for Random 3D Spin System Under the Influence of External Field. Generalization of Clausius-Mossotti Equation

Ashot S. Gevorkyan and Arax A. Gevorkyan

Institute for Informatics and Automation Problems of NAS of RA  
e-mail: g.ashot@sci.am

## Abstract

A dielectric medium consisting of roughly polarized molecules has been treated as a 3D disordered spin system. For investigation of statistical properties of this system on scales of space-time periods of standing electromagnetic wave a microscopic approach has been developed. Using the Birgoff ergodic hypothesis the initial 3D spin problem is reduced to two conditionally separate 1D problems along external electromagnetic field propagation. The first problem describes a quantum dynamics of disordered  $N$ -particles system with relaxation, while the second one describes statistical properties of steric disordered spin chain system. Based on developed in both problems constructions, the coefficient of polarizability related to collective orientational effects was calculated. The Clausius-Mossotti equation for dielectric constant was generalized on the micrometer space and nanosecond time scales.

## 1 Formulation of the problem

Let us consider the fundamental problem of applied physics, space-time modulation of dielectric constant in some types of amorphous materials.

In this subsection we shall give a mathematical formulation for the dielectric constant, where the generation of collective orientation effects is possible in the presence of standing low electromagnetic field. A particular attention will be devoted to an investigation of dispersion properties of dielectric permittivity function.

The starting point in our discussion will be the Clausius-Mossotti relation for dielectric constant. It is known that in isotropic media (as well as in crystals of cubic symmetry) the dielectric constant is well described by the Clausius-Mossotti equation [1, 2, 3]:

$$\frac{\epsilon_s - 1}{\epsilon_s + 2} = \frac{4\pi}{3} \sum_m N_m^0 \alpha_m^0, \quad (1)$$

where  $N_m^0$  is the concentration of particles (electrons, atoms, ions, molecules) with given  $m$  types of polarizability and  $\alpha_m^0$  correspondingly are polarizability coefficients. It follows from this formula that the static dielectric constant  $\epsilon_s$  depends on the polarizability properties of particles as well as on their topological order. In the external field the homogeneity and

isotropy of the medium is often lost. Then, it is expected that formula (1) will be applicable after slight generalization.

The object of our investigation is solid state dielectrics of the amorphous silicon dioxide  $\alpha - \text{SiO}_2$  type. According to numerical *ab initio* simulations [4], the structure of this type compound is well described by 3D random network FIG. 1.



FIG 1. The structure of amorphous silicon dioxide ( $\alpha - \text{SiO}_2$ ) is described by 3D random network with covalent bonds.

Every silicon vertex (gold sphere) has 4 edges and every oxygen vertex (red sphere) has 2 edges.

The red and brown lattice points in this figure correspond to different atoms, while the links between them correspond to covalent bonds. The redistribution of charges in outer electronic shells takes place because of the asymmetry of the bound atoms. As a result, some atoms acquire positive charge, while the others - the negative ones. Thus, a compounds of this type may be considered as a disordered 3D system of rigid dipoles (hereinafter termed as 3D disordered spin system, FIG. 2).

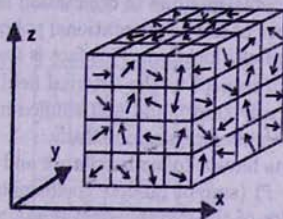


FIG 2. The amorphous silicon dioxide (see FIG. 1.) may be represented as a 3D lattice where by one rigid dipole (spin) is randomly put in every lattice sell.

For description of amorphous media 3D lattice with the lattice constant  $d_0(T) = \{m_0/\rho_0(T)\}^{1/3}$  is used, where  $m_0$  is the molecule mass,  $\rho_0$  is the density and  $T$  is the temperature. The lattice contains one random spin per elementary cell. Note that inside the cell it has random direction as well as random location.

Suppose now that with the help of external electromagnetic filed a standing wave is formed in the medium:

$$E(x; E_0, \Omega, \lambda_s, \varphi_0) = E(x; g) = 2E_0 \sin(\varphi_0) \cos(kx), \quad \varphi_0 = \Omega t_0, \quad (2)$$

where  $\varphi_0$  and  $t_0$  are respectively the initial phase and time,  $\Omega$  is the wave frequency,  $k = 2\pi/\lambda_s$  and  $\lambda_s$  is the wavelength, the symbol  $g$  shows the parameters of standing wave (controlling parameters)  $(E_0, \Omega, \lambda_s, \varphi_0)$ .



Here a natural question follows, how does the dielectric constant change on the scale of wavelength period and in time interval  $\Delta t \ll \Omega^{-1} \sim 10^{-9} \text{ sec}$ , when the relaxation time of molecular dipoles is  $\tau \sim 10^{-11} \div 10^{-12} \text{ sec} \ll \Omega^{-1}$ . This question is important since the processes associated with the Cerenkov and transition radiation produced in media are much faster than the above time scale. Note, that the time, during which a relativistic electron passes the wavelength ( $\lambda_s \sim 10^{-4} \text{ cm}$ ) of standing wave and the formation times of transition or Cerenkov photons in this layer is less than  $10^{-15} \text{ sec}$ . This time interval is essentially less than the time, during which the standing wave is steady-state. Since the wavelength is supposed to be much larger than the inter-dipole distance  $\lambda_s \gg d_0$ , the Clausius-Mossotti relation is still true. In this case the main problem is to calculate the polarizability coefficient related to orientation effects.

Taking into account the external field, one can express the polarization of matter at an arbitrary point as the macroscopic self-consistent relation:

$$\vec{P}(\vec{r}, d_0(T)) = \sum_{\vec{l}} \vec{p}(\vec{l} - \vec{r}) = \sum_{\vec{l}} \left[ \sum_m n_m \alpha_m (\vec{l} - \vec{r}) \vec{E}_{loc}(\vec{l} - \vec{r}) \right], \quad \vec{l} \equiv l(l_x, l_y, l_z), \quad (3)$$

where  $\vec{l}$  is 3D lattice vector,  $\vec{p}$  is respectively the dipole moment of molecule. The second equation in (3) contributes to the value of dipole moment (spin). Note, that the number of the carriers of given polarization type in an elementary cell is  $n_m \sim (d_0(T))^{-3}$ ,  $\alpha_m$  being coefficients of the polarizability of corresponding types with due regard for external field and  $\vec{E}_{loc}$  is the local field, i.e. the effective field that induces the polarization at the site of an individual molecule. The contribution of each effect to the net dipole moment per molecule is linear, that is actually verified by experiments. Under the action of external field the polarization of different types arise in media. However, simple analysis shows that the values of polarizability coefficients due to orientation effects essentially exceed the others.

Note that the coefficient of elastic orientational polarizability in amorphous media  $\alpha_{dip}(\vec{l} - \vec{r})$  is a random function of cell location. This fact is due to random orientation of local field strengths  $\vec{E}_{loc}(\vec{l} - \vec{r})$  with respect to the external field  $\vec{E}(x; g)$ . Therefore, all terms in the right side of (1) are basically known and well studied in literature (see, e.g., [1, 2, 3]) except from those connected with the orientation effects.

The orientation effects have a collective nature and are characterized by average value of random sum  $\sum_{\vec{l}} \alpha_{dip}(\vec{l} - \vec{r})$  (sum of random coefficients of orientational polarizability).

Multiplying both sides of the external field relation (3), we have:

$$\vec{P}(\vec{r}, g) \vec{E}(x, g) = -\delta U(\vec{r}, g) = \sum_m n_m \left[ \sum_{\vec{l}} \alpha_m (\vec{l} - \vec{r}) \vec{E}_{loc}(\vec{l} - \vec{r}) \right] \vec{E}(x; g), \quad (4)$$

where  $-\delta U(\vec{r}, g)$  describes the potential energy of amorphous matter in the external field. The statistical properties of medium in the direction of wave propagation will be considered later.

Taking into account formula (4), one can obtain the following expression for the part of potential energy of 3D spin system that is related with orientation effects in the external field:

$$-\delta U_{dip}(\vec{r}, g) = \sum_{\vec{l}} \alpha_{dip}(\vec{l} - \vec{r}) \vec{E}_{loc}(\vec{l} - \vec{r}) \vec{E}(x; g). \quad (5)$$

Let us separate a layer with volume  $V = L_x \times L_y \times L_z$  in the infinite crystal lattice, where  $L_x \sim (\lambda_s) \gg d_0(T)$  and  $(L_y, L_z) \rightarrow (\infty, \infty)$ . It is easy to see that this volume is filled with infinite number of  $L_x$ -site random 1D steric spin chains FIG. 3.

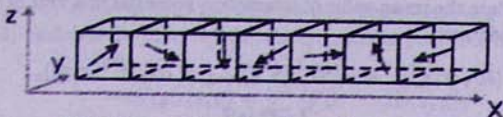


FIG 3. The steric 1D random spin chain system.

An important problem is now to calculate the mean value of the interaction potential between the spin layer and the external field.

Formally the following expression may be written for that:

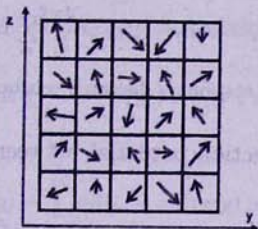
$$\begin{aligned}
 -\delta U_V(\vec{r}, \mathbf{g}) &= -\sum_{\vec{l}_\perp} \delta U_{L_\perp}(\vec{l}_\perp | \vec{r}, \mathbf{g}), \\
 -\delta U_{L_\perp}(\vec{l}_\perp | \vec{r}, \mathbf{g}) &= \sum_{l_x} \alpha_{dip}(\vec{l} - \vec{r}) \vec{E}_{loc}(\vec{l} - \vec{r}) \vec{E}(\mathbf{x}; \mathbf{g}), \quad \vec{l}_\perp \equiv \vec{l}_\perp(l_x, l_y), \quad (6)
 \end{aligned}$$

where  $-\delta U_{L_\perp}(\vec{l}_\perp | \vec{r}, \mathbf{g})$  is the interaction potential between the 1D steric spin chain and external field. First, we take the mean value of the potential  $-\delta U_V(\vec{r}, \mathbf{g})$  on  $(y, z)$  plane:

$$\lim_{S_\perp \rightarrow \infty} \frac{1}{S_\perp} \int \delta U_V(\mathbf{x}, \mathbf{g}) dS_\perp = \lim_{S_\perp \rightarrow \infty} \frac{1}{S_\perp} \int \sum_{\vec{l}_\perp} \delta U_{L_\perp}(\vec{l}_\perp | \mathbf{x}, \mathbf{g}) dS_\perp = \langle \delta U_{L_\perp}(\mathbf{x}, \mathbf{g}) \rangle_1,$$

where  $S_\perp = L_y \times L_z$  and  $\langle \dots \rangle_1$  is the averaging over all possible stable steric 1D spin chain configurations.

Taking into account the fact that the distribution of spins in  $(y, z)$  plane is random but isotropic (see FIG. 4), it is simple to prove that in the limit of  $S_\perp \rightarrow \infty$  it passes into the full self-averaging of the spin system.

FIG 4. The projection of 3D disordered spin system on the plane  $(y, z)$ .

It means that we can use Birgoff ergodic hypothesis [5] and in the expression  $\langle \delta U_{L_\perp}(\mathbf{x}, \mathbf{g}) \rangle_1$  may change the integration by  $(y, z)$  plane on the integration by spin chain's energy distribution:

$$\langle \delta U_{L_\perp}(\mathbf{x}, \mathbf{g}) \rangle_1 = \langle \delta U_{L_\perp}(\varepsilon | \mathbf{x}, \mathbf{g}) \rangle_\varepsilon = \frac{\int_{-\infty}^0 \delta U_{L_\perp}(\varepsilon | \mathbf{x}, \mathbf{g}) Z(\varepsilon; \mathbf{g}) d\varepsilon}{\int_{-\infty}^0 Z(\varepsilon; \mathbf{g}) d\varepsilon}, \quad (7)$$

where  $-\delta U_{L_\perp}(\varepsilon | \mathbf{x}, \mathbf{g})$  shows the interaction potential energy between some 1D steric spin chain with energy of  $\varepsilon$  and external field (2), and  $Z(\varepsilon; \mathbf{g})$  denotes the energy distribution function (partition function) of 1D steric spin chain configurations. The definition of distribution function will be given in section III. Note that in (7) only the negative values of  $\varepsilon$  were taken into account, because only for these values the spin chains might be stable.



Now we can calculate the mean value of interaction potential in a unit of volume between standing wave and medium:

$$-\langle \delta U_V(\vec{r}, \mathbf{g}) \rangle_V = -\langle \delta U_{L_x}(x, \mathbf{g}) \rangle_{(x, \uparrow)} = \bar{\alpha}_{ch} \langle \vec{E}^2(x, \mathbf{g}) \rangle_x, \quad (8)$$

$$\langle \delta U_{L_x}(x, \mathbf{g}) \rangle_{(x, \uparrow)} = \frac{1}{L_x} \int_{-L_x/2}^{+L_x/2} \langle \delta U_{L_x}(\varepsilon|x, \mathbf{g}) \rangle_\varepsilon d\varepsilon, \quad (8)$$

where the bracket  $\langle \dots \rangle_x$  means the integration over  $x$  on a scale  $L_x$ , parameter  $\bar{\alpha}_{ch}$  will be named a collective polarization coefficient of 1D steric spin chains:

$$\bar{\alpha}_{ch} = -\frac{\langle \delta U_{L_x}(x, \mathbf{g}) \rangle_{(x, \uparrow)}}{\langle \vec{E}^2(x, \mathbf{g}) \rangle_x}. \quad (9)$$

Note that  $\bar{\alpha}_{ch}$  is a complex value and describes the averaged 1D spin chain polarizability with due regard for the lattice relaxation. When  $E_0 \rightarrow 0$ , it is simple to show that  $\bar{\alpha}_{ch} \rightarrow 0$ .

Now one can write down the expression for sum in the right part of relation (1), in which the spin chain orientation effects in the external field are taken into account:

$$\sum_m N_m \alpha_m = \sum_m N_m^0 \alpha_m^0 + N_{ch} \bar{\alpha}_{ch} = \sum_m N_m^0 \alpha_m^0 - \frac{\langle \delta U_{L_x}(x, \mathbf{g}) \rangle_{(x, \uparrow)}}{d_0^3 N_x \langle \vec{E}^2(x, \mathbf{g}) \rangle_x}, \quad (10)$$

where  $N_{ch} = d_0^{-3} N_x^{-1}$  is the concentration of 1D steric spin chains. As it follows from (10), in areas where the field strength is small the orientation correction vanishes. In other words, on wavelength scale (2) the external field creates alternating inhomogeneities with different dielectric constants. These layers are stable on nanosecond scale  $\Delta t \sim 10^{-10} \text{ sec} = 0.1 \text{ ns}$ .

Using (10) we can generalize the Clausius-Mossotti equation on the space-time scale of standing wave taking into account the orientation effects:

$$\frac{\epsilon_{st}(\mathbf{g}) - 1}{\epsilon_{st}(\mathbf{g}) + 2} = \Lambda(\mathbf{g}), \quad \text{where} \quad \Lambda(\mathbf{g}) \simeq \frac{4\pi}{3} \left[ \sum_m N_m^0 \alpha_m^0 - \frac{\langle \delta U_{L_x}(x, \mathbf{g}) \rangle_{(x, \uparrow)}}{d_0^3 N_x \langle \vec{E}^2(x, \mathbf{g}) \rangle_x} \right]. \quad (11)$$

Note that  $\epsilon_{st}$  is the label of stationary dielectric constant.

## 2 The average interaction potential between 1D steric spin chain and external field

Considering the fact that the external field is low i.e.  $|\vec{E}(l_x - x)| \ll |\vec{E}_{loc}(l_x - x)| \cong |\vec{E}_{int}(l_x - x)|$ , we can expand the dipole angular momentum in a Taylor series:

$$\vec{p}(l_x - x) \simeq \vec{p}^0(l_x - x) + \delta \vec{p}(l_x - x), \quad \delta \vec{p}(x) \sim \vec{E}(x, \mathbf{g}), \quad (12)$$

where  $|\delta \vec{p}(x)| \ll |\vec{p}^0(x)|$ , as well as  $\vec{E}_{int}(x - l_x)$  and  $\vec{p}^0(x - l_x)$  are respectively the field strength and dipole angular momentum of the molecule, located in the  $l_x$ -th cell in the absence of the external field. When the coordinate  $x$  is outside of  $l_x$ -th cell, the field vanishes. Their values inside the cell are constant. Based on the above discussion with due regard for (6) for interaction potential  $-\delta U_{L_x}(\varepsilon|x, \mathbf{g})$  one can write the following relation:

$$-\delta U_{L_x}(\varepsilon|x, \mathbf{g}) = \sum_{l_x=0}^{L_x} \vec{p}^0(l_x - x) \vec{E}(x, \mathbf{g}) + \sum_{l_x=0}^{L_x} \delta \vec{p}(l_x - x) \vec{E}(x, \mathbf{g}). \quad (13)$$

As in the absence of external field the spin system is not polarized, we conclude that the first sum in (13) vanishes. In other words, the interaction potential has the following form:

$$-\delta U_{L_x}(\varepsilon|x, \mathbf{g}) = \sum_{l_x=0}^{L_x} \delta \vec{p}(l_x - x) \vec{E}(x; \mathbf{g}). \quad (14)$$

Now turn to the equation of motion for the 1D steric spin chain with relaxation in 3D spin lattice in the external field. Remember that the interaction potential  $-\delta U_{L_x}(\varepsilon|x, \mathbf{g})$  (see (7) and (14)) between 1D disordered spin chain and external field does not allow for the relaxation with environmental spin chains. The allowance for the relaxation effects is possible only after solution of the dynamical problem. The resulting interaction potential in this case will be complex, the imaginary part of which characterizes the relaxation processes in the 3D lattice.

Taking into account the above considerations one can describe the quantum motion in 1D disordered spin chain by the stochastic Schrödinger equation (see for example [5]):

$$\lambda \delta U_{L_x}(\varepsilon|x, \mathbf{g}) = \lambda \varepsilon + \Psi^{-1}(d_t)^2 \Psi, \quad (15)$$

where

$$t = x/d_0, \quad \lambda = 2\mu/(\hbar^2 d_0^2), \quad \mu = m_0/N^{1/(N-1)}, \quad (d_t)^2 = d^2/dt^2,$$

$\mu$  is a spin chain effective mass,  $N_x$  is the number of particles (molecules) in the chain,  $t$  denote the natural parameter of evolution along the spin chain. In the equation (15) the interaction potential  $-\delta U_{L_x}(\varepsilon|x, \mathbf{g})$  is a random complex function. Its detailed description is given in what follows.

Substituting

$$\Psi(t) = \exp\left(\int_0^t \Xi(t') dt'\right), \quad (16)$$

into (16) we obtain the following nonlinear complex stochastic differential equation (SDE) (Langevin equation) [6, 7]:

$$\Xi_t + \Xi^2 + \lambda(\varepsilon - V) + \lambda f(t) = 0, \quad \Xi(t) = \theta(t) + i\vartheta(t), \quad \Xi_t = d\Xi/dt, \quad (17)$$

where

$$\sum_{l_x=0}^{L_x} \vec{p}(l_x - x) \vec{E}(x; \mathbf{g}) = \sum_{l_x=0}^{L_x} \delta \vec{p}(l_x - x) \vec{E}(x; \mathbf{g}) = V + f(t). \quad (18)$$

In formulas (17) and (18) we denoted by  $V$  the mean value of the sum, and by  $f(t)$  its complex random part. Based on an analysis of different polarization mechanisms in the spin glass medium, it is concluded that under the influence of external field (2) with frequency  $\Omega \sim 10^9 \text{ Hz}$  the main contribution is made by the elastic dipole orientation effect. Recall that in this case the thermal polarization of dipole is not essential due to the large relaxation time  $\tau \sim 10^{-4} \div 10^{-5} \text{ sec}$  [1], [8]. Note that the coefficient of elastic dipole polarization at low external fields is determined by [9]:

$$\alpha_{dip}(l_x - x) = \Lambda^{-1} (p^0 \sin[\beta(l_x - x)])^2 = \frac{p^0}{E_{int}^0} \sin^2[\beta(l_x - x)],$$

$$\delta \vec{p}(l_x - x) = \alpha_{dip}(l_x - x) \vec{E}(x; \mathbf{g}), \quad (19)$$



where  $\beta(l_z - x)$  is the angle between the external  $\vec{E}(x; \mathbf{g})$  and the internal  $\vec{E}_{int}^0(l_z - x)$  fields,  $\Lambda(l_z) = \vec{p}^0(l_z) \vec{E}_{int}^0(l_z) \cong p^0 E_{int}^0$  is the dipole energy in the field  $\vec{E}_{int}^0$ . Following the heuristic argumentation of Debye [1] one can write down the expression for the elastic dipole polarization, in which the spin (molecule) relaxation process in the glass is taken into account:

$$\alpha_{dp}(l_z - x) = \frac{\alpha_{dp}(l_z - x)}{(1 - i\Omega\tau)} \cong \frac{p^0 \sin^2[\beta(l_z - x)]}{E_{int}^0(1 - i\Omega\tau)}, \quad (20)$$

where  $\tau$  is the spin relaxation time in the glass. It is very small in the above media  $\tau \sim 10^{-11} \div 10^{-12}$  sec (see, e.g., [1]).

So, the equation (15) with generalized coefficient of elastic dipole polarizability (19) will describe the motion of 1D random steric spin chain in the external field with relaxation.

After substitution of (20) in (18) and simple calculations we obtain:

$$V = -\frac{1 + i\Omega\tau}{1 + (\Omega\tau)^2} \frac{N_x p^0 E_0^2}{4d_0^3 E_{int}^0} \left( 1 - \frac{\sin(2kL_z)}{2kL_z} \right), \quad (21)$$

where  $\bar{E}_0(\varphi_0) = 2E_0 \sin \varphi_0$ .

Now we can investigate the properties of random function  $f(t)$ . From relations (19) and (20) it is easy to find the random strength:

$$f(t) = -\frac{1 + i\Omega\tau}{1 + (\Omega\tau)^2} \cdot \frac{p^0 \bar{E}_0^2}{4d_0^3 E_{int}^0} \xi(t), \quad \xi(t) = \left( 1 + \cos(2k_t t) \right) \sum_{l_z=0}^{L_z} \cos 2\bar{\beta}(l_t - t), \quad (22)$$

$$\bar{\beta}(l_t - t) = \beta(l_z - x), \quad k_t = \hbar^{-1} \sqrt{2\mu} k, \quad l_t = \hbar l / \sqrt{2\mu}.$$

If the phase  $\beta$  is homogeneously distributed in the interval  $[0, \pi]$  for the random function  $\xi$ , we can write the following mean value and autocorrelation function:

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t) \xi(t') \rangle = 4\delta(t - t'), \quad (23)$$

For real and imaginary components of complex random function  $f(t)$  the following autocorrelation functions [10] may be written:

$$\langle f^r(t) f^r(t') \rangle = \frac{1}{2} \left[ \frac{1}{1 + (\Omega\tau)^2} \right]^2 \left( \frac{N_x p^0 \bar{E}_0^2}{4d_0^3 E_{int}^0} \right)^2 \langle \xi(t) \xi(t') \rangle = 2D^r \delta(t - t'), \quad (24)$$

$$\langle f^i(t) f^i(t') \rangle = \frac{1}{2} \left[ \frac{\Omega\tau}{1 + (\Omega\tau)^2} \right]^2 \left( \frac{N_x p^0 \bar{E}_0^2}{4d_0^3 E_{int}^0} \right)^2 \langle \xi(t) \xi(t') \rangle = 2D^i \delta(t - t'), \quad (25)$$

where  $f^r(t) = \text{Re} f(t)$  and  $f^i(t) = \text{Im} f(t)$ .

For further investigation, it is convenient to represent the complex equation (17) as a system of two real equations:

$$\dot{\theta} + \theta^2 - \vartheta^2 + \lambda(\varepsilon - V^r + f^r(t)) = 0, \quad (26)$$

$$\dot{\vartheta} + 2\theta\vartheta + \lambda(-V^i + f^i(t)) = 0, \quad (27)$$

where  $\dot{\theta} = d_t \theta$ ,  $\dot{\vartheta} = d_t \vartheta$ ,  $V^r = \text{Re} V$  and  $V^i = \text{Im} V$ .

Now the problem is to find the evolution equation for the conditional probability:

$$Q(\theta, \vartheta, t | \theta_0, \vartheta_0, t_0) = \langle \delta(\theta(t) - \theta(t_0)) \delta(\vartheta(t) - \vartheta(t_0)) \rangle \Big|_{\{\theta_0 = \theta(t_0); \vartheta_0 = \vartheta(t_0)\}}, \quad (28)$$

describing the probability that the trajectory ( $\theta \equiv \theta(t)$ ,  $\vartheta \equiv \vartheta(t)$ ) starting at the initial moment of natural parameter  $t_0$  from the point  $(\theta_0, \vartheta_0)$ , will be at an arbitrary moment  $t$  in the vicinity of point  $(\theta, \vartheta)$ . Subject to SDE system (26), (27) the Fokker-Plank equation is easily found [?] (see also [6]):

$$\frac{\partial Q}{\partial t} = D^r \frac{\partial^2 Q}{\partial \theta^2} + D^i \frac{\partial^2 Q}{\partial \vartheta^2} + [\theta^2 - \vartheta^2 + \lambda(\varepsilon - V^r)] \frac{\partial Q}{\partial \theta} + [2\theta\vartheta - \lambda V^i] \frac{\partial Q}{\partial \vartheta} + 4\theta Q, \quad (29)$$

where  $Q \equiv Q(\varepsilon|\theta, \vartheta; t)$ .

Note, that the solution of equation (29) must satisfy the initial condition:

$$Q(\varepsilon|\theta, \vartheta; t)|_{t=t_0} = \delta(\theta - \theta_0)\delta(\vartheta - \vartheta_0), \quad (30)$$

where initial phases  $\theta_0$  and  $\vartheta_0$  are equal to zero. More interesting for us from here on will be the stationary limit of solution (29) clearly followed for values  $t \gg \Delta t = O(1)$ , that is equivalent to condition  $t \rightarrow \infty$ . In this case Eq. (29) is transformed to the following stationary form:

$$\left\{ D^r \frac{\partial^2}{\partial \theta^2} + D^i \frac{\partial^2}{\partial \vartheta^2} + [\theta^2 - \vartheta^2 + \lambda(\varepsilon - V^r)] \frac{\partial}{\partial \theta} + [2\theta\vartheta - \lambda V^i] \frac{\partial}{\partial \vartheta} + 4\theta \right\} Q_s = 0, \quad (31)$$

where  $Q_s \equiv Q_s(\varepsilon|\theta, \vartheta) \equiv \lim_{t \rightarrow \infty} Q(\theta, \vartheta, t)$  and  $t_{N_s} = N_s$ .

The (31) is an elliptic differential equation, for which there are no real characteristics. The solution of equation (31) must satisfy the boundary conditions:

$$Q_s|_S = \frac{\partial Q_s}{\partial n}|_S = 0, \quad |n| = (\theta^2 + \vartheta^2)^{1/2}, \quad (32)$$

where  $n$  is the normal to curve  $S$ .

Now we can calculate the mean value of interaction potential between 1D spin chain with energy  $\varepsilon$  and external field taking into account its relaxation in the 3D lattice.

Since in the stationary limit the interaction potential has a form:

$$\delta U(\varepsilon|x, g)|_{x \rightarrow \infty} \rightarrow \delta U(\varepsilon|\theta, \vartheta) = \lambda\varepsilon + \theta^2 - \vartheta^2 - i2\theta\vartheta, \quad (33)$$

(see (15) and (17)), we can find the mean value of interaction potential after averaging (33) over the stationary distribution  $Q_s(\varepsilon|\theta, \vartheta)$ :

$$\langle \delta U_{L_s}(\varepsilon|x, g) \rangle_x = \frac{1}{\lambda R} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} [(\lambda\varepsilon + \theta^2 - \vartheta^2) - i2\theta\vartheta] Q_s(\varepsilon|\theta, \vartheta) d\theta d\vartheta, \quad (34)$$

where  $R = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} Q_s(\varepsilon|\theta, \vartheta) d\theta d\vartheta$  denotes the normalization constant.

### 3 Statistical mechanics of the steric 1D random spin chain

Prior to turning to the calculation of effective stationary dielectric constant, two important problems have to be solved. The first one is the calculation of partition function  $Z(\varepsilon; g)$  for a steric 1D random spin chain with energy  $\varepsilon$ , whereas the second one consists in determination of the thickness of layers on the scale of this chain (i.e., the fragmentation of media on layers with different dielectric constants).



First, let us consider the statistical properties of 1D steric spin chain. As is shown, the (a-SiO<sub>2</sub>) compound can be described by canonical model continuous random networks of atoms and bonds [11],[4] (see Fig. 1). It means that the Heisenberg spin glass Hamiltonian is suitable for description of 3D disordered spin system [12]. Note that this permits to use the ergodic hypothesis (see (7)) and reduces 3D spin lattice dynamical problem to the problem of 1D complex Schrödinger-Langevin type stochastic differential equation (see (15), (17)), as well to construct the statistical mechanics of steric 1D disordered spin chain system. It is easy to see that this type of reduction is somewhat conditional because both the problems are interrelated.

For further investigations it is appropriate to consider the spin glass Hamiltonian of type:

$$H(N_z; \mathbf{g}) = - \sum_{ij}^{N_z} J_{ij}(r_{ij}) \vec{S}_i \vec{S}_j + p^0 \sum_i^{N_z} \vec{E}_i \vec{S}_i, \quad \vec{S}_i \equiv \frac{\vec{p}_i^0}{p^0}, \quad (35)$$

where  $r_{ij} = |i-j|d_0(T) + \eta_{ij}$  is the distance between 1D spins  $\vec{S}_i$  and  $\vec{S}_j$  (classical unit length vectors),  $\eta_{ij}$  is its random part, subject to Gaussian distribution with zero mean value and unit variance,  $J_{ij}$  is the nearest-neighbor interaction constant that depends on the distance between spins. It may be positive or negative, the external field  $\vec{E}_i$  being defined by means of formulas (2).

Our purpose now is to construct the energy distribution function of spin chains  $Z(\varepsilon; \mathbf{g})$ . However, the difficulty here is that the time scale on which the statistical study of system is made, is very short ( $10^{-10} \text{ sec} = 0,1 \text{ nsec}$ ), while the characteristic thermal relaxation time in amorphous media [1] is of the order  $\Omega_T^{-1} \sim 10^{-4} \div 10^{-3} \text{ sec}$ , where  $\Omega_T$  is the frequency of thermal fluctuations. This means that in our problem the temperature and related thermodynamical constructions become meaningless. Nevertheless, some structural similarity between the gas and amorphous media is evident. In this case the steric 1D spin chain will correspond to an atom in gas. Since in the equilibrium state the average value of energy per atom in the gas is  $\frac{3}{2}kT$ , the corresponding value in this case will be the energy of chain in the equilibrium state (the energy of chain without the external field). However, the system under study has a specific feature. The point is that the equilibrium state in gas is characterized by one temperature, whereas the spin system in the equilibrium state can be at any negative energy. These energies coincide with local minima of the non-perturbed Hamiltonian [12, 13]. In other words, in this case the phase space may be decomposed uniquely into micro-canonical states associated with different thermodynamic equilibrium states [14].

The Hamiltonian (35) in the absence of external field can be rewritten in spherical coordinate system as follows:

$$H_0(d_0(T), N_z) = \sum_{(ij)=1, i \neq j}^{N_z} J_{ij}(r_{ij}) (\cos \psi_i \cos \psi_j \cos(\phi_i - \phi_j) + \sin \psi_i \sin \psi_j), \quad (36)$$

For determination of local minimums one has to solve the following algebraic equations:

$$\Phi_{\psi_i}(\Theta) = \frac{\partial H}{\partial \psi_i} = \sum_{j=1}^{N_z} J_{ij}(r_{ij}) (-\sin \psi_i \cos \psi_j \cos(\phi_i - \phi_j) + \cos \psi_i \sin \psi_j) = 0,$$

$$\Phi_{\phi_i}(\Theta) = \frac{\partial H}{\partial \phi_i} = - \sum_{j=1}^{N_z} J_{ij}(r_{ij}) \cos \psi_i \cos \psi_j \sin(\phi_i - \phi_j) = 0,$$

$$\Phi_{r_{ij}}(\Theta) = \frac{\partial H}{\partial r_{ij}} = \sum_{j=1}^{N_s} \frac{\partial J_{ij}}{\partial r_{ij}} (\cos \psi_i \cos \psi_j \cos(\phi_i - \phi_j) + \sin \psi_i \sin \psi_j) = 0, \quad (37)$$

where  $\Theta_i = (\psi_i, \phi_i)$  are angles of  $i$ -th spin ( $\psi_i$  is the polar and  $\phi_i$  azimuthal angles),  $\Theta = (\Theta_1, \Theta_2, \dots, \Theta_{N_s})$  respectively describe the angular part of spin configuration. Now suppose that the non-perturbed Hamiltonian for fixed averaged distance between spins  $d_0(T)$  has  $n$  local minima of function  $\varepsilon_j(d_0(T))$ , each of which corresponds the  $M_j$  spin configurations  $\{\Theta^{(i)}\}$ , where  $i = 0, 1, \dots, M_j$ . The number of all configurations that relates to the local equilibrium states  $M_{full} = \sum_{j=1}^N M_j$ . Accordingly, the weight of every equilibrium state may be defined by formulas:

$$P_j(\varepsilon_j; d_0(T)) = M_j / M_{full}, \quad \sum_{j=1}^N P_j(\varepsilon_j; d_0(T)) = 1. \quad (38)$$

Thus, we propose to use the following statistical weight instead of the canonical distribution at multi-equilibrium state:

$$W_j(H; \mathbf{g}) = P_j(\varepsilon_j; d_0(T)) \exp\left\{-\frac{H(N_s; \mathbf{g})}{\varepsilon_j(d_0(T))}\right\}, \quad (39)$$

where  $\varepsilon_j$  is the energy of spin chain in the absence of external field. Remember, that the multicanonical ensemble was introduced in the [15] as an approach to simulate a strong first-order phase transitions.

Now, taking into account (36)-(39), the expression for energy distribution function for  $N_s$  spin system (this expression can be explained as a local partition function in the aforementioned multicanonical thermodynamics) is written as

$$Z(\varepsilon; \mathbf{g}, \mathbf{q}) = P(\varepsilon; d_0(T)) \int \frac{d\Omega_1}{4\pi} \dots \frac{d\Omega_{N_s}}{4\pi} \exp\left\{-\frac{H(N_s; \mathbf{g})}{\varepsilon(d_0(T))}\right\}, \quad (40)$$

where  $\mathbf{q}$  describes the set of random distances  $\eta_{ij}$  and random angles  $\beta_i$ , accordingly  $d\Omega_i$  is an element of solid angle  $\Omega_i$  containing the unit vector  $\vec{S}_i$ .

The energy distribution function of spin chain may be essentially simplified on assumption that in Hamiltonian (35) only the nearest-neighboring spins interact, i.e.  $J_{ij} \equiv 0$  if  $|j-i| > 2$ . In this case the multidimensional integral can be taken exactly as follows. The integration starts from the end of the chain. When integrating over  $d\Omega_i$  we take the direction of the vector  $(J_{i(i-1)}\vec{S}_i + p^0\vec{E}_i)$  as a polar axis. Then it is easy to obtain the following expression:

$$Z(\varepsilon; \mathbf{g}, \mathbf{q}) = P(\varepsilon; d_0(T)) \prod_{i=1}^{N_s} \left[ \frac{1}{2} \int_0^\pi \exp\{K_i \cos \psi\} \sin \psi d\psi \right] = P(\varepsilon; d_0(T)) \prod_{i=1}^{N_s} \frac{\sinh K_i}{K_i},$$

$$K_i = \frac{1}{\varepsilon} [J_{i(i-1)}^2 + 2p^0 E_i J_{i(i-1)} \cos \beta_i + (p^0)^2 E_i^2], \quad (41)$$

where  $\beta_i$  is the random angle between the vectors  $\vec{S}_{i-1}$  and  $\vec{E}_i$ . Assuming that the distribution of spin  $\vec{S}_i$  around field  $\vec{E}_i$  direction is isotropic, one can perform an integration over the angle  $\beta_i$ . After simple integration with the help of formula [16]:

$$Ei(ax) = \int \frac{e^{ax}}{x} dx = \ln|x| + \sum_{k=1}^{\infty} \frac{(ax)^k}{k!k}, \quad a \neq 0,$$



we find:

$$Z(\varepsilon; \mathbf{g}, \eta) = P(\varepsilon; d_0(T)) \prod_{i=1}^{N_x} \left[ \frac{1}{2} \int_0^\pi \frac{\sinh K_i}{K_i} \sin \beta_i d\beta_i \right] \\ = P(\varepsilon; d_0(T)) \prod_{i=1}^{N_x} \frac{1}{4a_i} \left[ \{Ei(b_i + a_i) - Ei(-b_i - a_i)\} - \{Ei(b_i - a_i) - Ei(-b_i + a_i)\} \right], \\ a_i = \frac{2}{\varepsilon} p^0 Ei J_{(i-1)i}, \quad b_i = \frac{1}{\varepsilon} [J_{(i-1)i}^2 + (p^0)^2 E_i^2]. \quad (42)$$

In (42) the symbol  $\eta$  describes a set of random distances,  $Ei(x)$  is the exponential integral function. It is simple to see that despite the fact that every member in parentheses near values  $E_i^+ = J_0/p^0$  or  $E_i^- = -J_0/p^0$  has a singularity, their sum is an analytical function.

In [17] it was suggested for the first time that the spin glass may be described by the Hamiltonian of the type (35), where spins are put onto the nodes of regular lattice, but the disorder is introduced by means of suitable distribution  $W(J_{(i-1)i})$  of exchange bonds. A standard choice is the Gaussian Edwards-Anderson model [17]:

$$W(J_{(i-1)i}) = \frac{1}{\sqrt{2\pi(\Delta J_{(i-1)i})^2}} \exp\left\{-\frac{(J_{(i-1)i} - J_0)^2}{2(\Delta J_{(i-1)i})^2}\right\} \\ J_0 = \langle J_{(i-1)i} \rangle_{av}, \quad (\Delta J_{(i-1)i})^2 = \langle J_{(i-1)i}^2 \rangle_{av} - \langle J_{(i-1)i} \rangle_{av}^2. \quad (43)$$

Remember that for this model  $J_0$  and  $\Delta J_{(i-1)i}$  are independent on the distance and scaled with spin number  $N_x$  as:

$$\langle J_{(i-1)i} \rangle_{av} = J_0 \propto N_x^{-1}, \quad \Delta J_{(i-1)i} \propto N_x^{-1/2}, \quad (44)$$

to ensure a sensible thermodynamic limit. Eq.s (43) and (44)  $\langle \dots \rangle_{av}$  describe the averaging procedure. Now the averaging of function (42) over the distribution (43) is made to find the partition function at some equilibrium energy  $\varepsilon$  of disordered spin chain:

$$Z(\varepsilon; \mathbf{g}) = P(\varepsilon; d_0(T)) \langle Z(\varepsilon, J; \mathbf{g}) \rangle_J, \quad \langle Z(\varepsilon, J; \mathbf{g}) \rangle_J = \prod_{i=1}^{N_x} \int dJ_{(i-1)i} W(J_{(i-1)i}) G(\varepsilon, J_i; \mathbf{g}), \\ G(\varepsilon, J_i; \mathbf{g}) = \frac{1}{2a_i} \left[ \{Ei(b_i + a_i) - Ei(-b_i - a_i)\} - \{Ei(b_i - a_i) - Ei(-b_i + a_i)\} \right]. \quad (45)$$

When an allowance is made for the facts that on the scale of half-wavelength  $N_x \gg 1$  and  $G(\varepsilon, J_i; \mathbf{g})$  is an analytical function for computation of integrals in partial partition function (43), the Laplace asymptotic method [18] may be used:

$$Z(\varepsilon, \mathbf{g}) \approx P(\varepsilon; d_0(T)) \prod_{i=1}^{N_x} \frac{1}{4a_i^0} \left[ \{Ei(b_i^0 + a_i^0) - Ei(-b_i^0 - a_i^0)\} - \{Ei(b_i^0 - a_i^0) - Ei(-b_i^0 + a_i^0)\} \right], \\ a_i^0 = \frac{1}{\varepsilon} 2p^0 Ei J_0, \quad b_i^0 = \frac{1}{\varepsilon} [J_0^2 + (p^0)^2 E_i^2]. \quad (46)$$

$Z(\varepsilon, \mathbf{g}) \rightarrow P(\varepsilon; d_0(T))$  takes place.

In analogy to conventional thermodynamics, the Helmholtz type free energy for steric 1D random spin chain system may be specified at the local equilibrium state with energy  $\varepsilon$ . In this case the free energy per one spin in the equilibrium state is defined as:

$$F(\varepsilon; \mathbf{g}) = -\frac{1}{N_s} \ln Z(\varepsilon; \mathbf{g}). \quad (47)$$

All macroscopic thermodynamic properties of steric 1D random spin chain may be obtained by means of free energy derivatives. Simple examination of the expression for free energy shows that for low fields  $E_1 \sim 1/N_s$  the free energy of spin system is essentially changed. Moreover the multicanonical thermodynamic allows first-order phase transitions in the 1D disordered spin-glass model for low external field which is very important.

Particularly, the order parameter for a disordered spin-glass medium is described by  $\sum_i p_i^z$  and in the absence of external field on the scale of standing wave period it is equal to zero, where  $p_i^z$  is the projection of spin on the direction of external field propagation. It becomes non-zero for a weak external field  $E_1 \sim |E_c^\pm|$  due to the symmetry breaking. In this case the nanoparticles (spin chains) with the *super spins* (macropolarizations) are generated on the microscale space and nanoscale time.

#### 4 Dielectric constant of neighboring layers

Now we will examine the question of dividing the dielectric medium into regions with extremely different polarizations. Remember that in the absence of external field the polarized medium has zero macroscopic polarization on the space scale  $10^{-4} \div 10^{-5} \text{ cm}$ .

When the external field in the medium (on the wavelength scale of standing electric field) is turned on the orientation effects are amplified and, as a result, the initiation of macroscopic polarization proves possible. Assuming that the collective orientation effects induced in regions of media, where the voltage of external field  $E$  is of the order of critical value  $E_c$ , we can divide the wavelength scale of external field into four regions. In the first and third regions the macroscopic polarization of medium is zero, whereas in the second and forth regions it is different from zero (see FIG. 5). Note that the height of these layers may be computed with the help of numerical experiments.

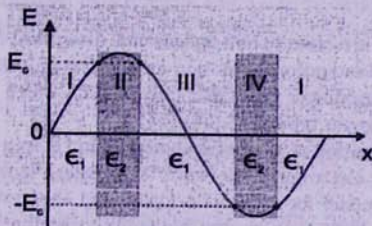


FIG 5. The regions with different polarizations and corresponding different dielectric constants on the single wavelength  $\lambda_s$  scale.

Now we may calculate the stationary dielectric constant at the half-wavelength scale of external electromagnetic field in time intervals  $\Delta t \ll 2\pi/\Omega$ .



Using (11), we obtain:

$$\epsilon_{st}(\mathbf{g}) = \frac{1 + 2\Lambda(\mathbf{g})}{1 - \Lambda(\mathbf{g})}. \quad (48)$$

Remember, that here we have taken into account the contribution from the elastic dipole polarization only. It is easy to see that the nominator of expression (48) has no singularities and is bounded by the imaginary part of the potential increment (34). The important characteristic is the difference of dielectric constants in the neighboring layers. Taking into account the relations (11) and (48) we get:

$$\delta\epsilon_{st}(\mathbf{g}) = \epsilon_{st}(\mathbf{g}) - \epsilon_{st}(0) = (1 - \epsilon_{st}(0)) + \frac{3\Lambda(\mathbf{g})}{1 - \Lambda(\mathbf{g})}. \quad (49)$$

Recall that the difference of dielectric constants of neighboring layers (49) is near to the critical value of external field  $E_c$  when the first order phase transition which can have extremely high profile takes place in the system.

## 5 Concluding remarks

In the present article a new microscopic approach has been developed for studying the properties of stationary dielectric constant on a micrometer space and nanosecond time scales. It was allowed generalized the Clausius-Mossotti equation.

Mathematically the problem is solved as follows. The dielectric medium in the external electromagnetic field is modelled as a 3D spin glass system under the influence of external field. Note that all general changes of properties of media take place in the wavelength scale of external field. This aim in view we have investigated in detail the layer of medium that consisted of disordered 1D spin chains with the length of the order of wavelength. Taking into account the fact that in infinite  $(x, y)$  plane the distribution of spin chains is isotropic we can use the Birgoff ergodic hypothesis (see (6)-(7)) and conditionally reduce the initial 3D spin glass problem to 1D + 1D problem. It means that it becomes possible to investigate two 1D problems separately, only in this case the parameters of the first 1D problem ought to be taken into account during the solution of the second 1D problem.

In this work we adduced all formal definitions made with a view to allow for the contribution of orientation effects in calculation of stationary and frequency-depending dielectric constants.

The first 1D problem is related to one-dimensional disordered  $N$ -particle quantum system with relaxation. The investigation of motion in this system takes place in the framework of complex Langevin-Schrödinger type SDE (15) or (17), which can be transformed to 2D system of nonlinear Langevin type SDE (26)-(27).

For probability distribution of interaction potential in 1D spin chain with definite energies  $\epsilon$  and external standing electromagnetic wave the Fokker-Plank equation (29) is obtained using the white noise model for stochastic forces and the system of SDE (26)-(27). In the long-range distance limit  $t \rightarrow \infty$ , the probability distribution  $Q(\epsilon|\theta, \vartheta; t)$  tends to its stationary limit  $Q_s(\epsilon|\theta, \vartheta)$  that satisfies the elliptic differential equation (31).

The second 1D problem includes the calculation of 1D random spin chain system energy distribution  $Z(\epsilon, \mathbf{g})$  in an external field.

To do this, the classical spin-glass Heisenberg type Hamiltonian is investigated (35). At the first step, the non-perturbed Hamiltonian (36) is used and the system of algebraic

equations (37) is found for computation of all possible stable spin configurations on the spin chain scale. Then, the statistic weight  $P_j(\varepsilon_j; d_0(T))$  for certain energies  $\varepsilon_j$  of stable non-perturbed spin chain is found simply by means of formula (38). Using formulae (38)-(43), the partition function  $Z(\varepsilon; g)$ , that gives the energy distribution in the spin chain system after introduction of external field, is defined (44). The Helmholtz free energy (47) is constructed and it is shown that the 1D random spin chain system is subjected to a weak external field  $E_i$  and the order  $E_c \pm \sim 1/N_x$  can be drastically changed (see FIG. 6), and moreover a first order phase transition can occur in the system at these conditions.

The mean value of complex interaction potential  $\langle \delta U_{Lx}(x, g) \rangle_{x=1}$  between steric 1D spin chain and external field is found from formula (7) taking into account expressions (38) and (47). An averaging potential is used for computation of polarizability coefficients related with the orientation effects (9) and correspondingly for generalization of Clausius-Mossotti equation (11). Remember that Eq. (11) makes sense only on the microscale space and nanoscale time. It is easy to see that the value of stationary dielectric constant strongly depends on initial electrostatic dielectric constant  $\epsilon_s$  of media. In particular, it may be shown that in the spin glass media with static dielectric constants  $\epsilon_s < 4$  under the external field the value of stationary dielectric constant can be changed no more than 3-4 times. The analysis in case of  $\epsilon_s > 4$  shows that the value of  $Re(\Lambda(g)) \rightarrow 1$  and correspondingly the stationary dielectric constant can be a complex function  $\epsilon_{st}(g)$  depending on parameters of external field  $g$ . Moreover, for a set of some parameters of weak external field one can assert that  $\epsilon_{st}(g)$  has a large imaginary part (see (49)).

Obviously, in the vicinity of this value critical effects take place. In this case owing to the allowance for relaxation processes in the lattice the system becomes ordered and is characterized by the macroscopic classical polarization.

Finally, it is important to note that in this work an original mathematical approach for reducing the problem of dynamical 3D disordered spin system in the external field to the two conditionally separate 1D problems is developed. This scheme may be used for elaboration of new highly effective parallel algorithms that is very important for systematic investigations of the above problem by means of numerical simulation method.

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**Նոր մաթեմատիկական մոտեցում չկարգավորված 3D  
սպինային համակարգի համար արտաքին դաշտի ազդեցության տակ:  
Կլաուզիուս-Մոսսոտիի հավասարման ընդհանրացումը**

**Ա. Ա. Գևորգյան և Ա. Ա. Գևորգյան**

**Ամփոփում**

Կոչտ բևեռացմամբ մոլեկուլներ պարունակող դիէլեկտրիկ միջավայրերը ներկայացվում է որպես չկարգավորված 3D սպինային համակարգ: Զարգացված է միկրոսկոպիկ պատկերացում կամգում էլեկտրոմագնիսական ալիքի տարածա-ժամանակային պարբերության վրա այդ համակարգի վիճակագրական հատկությունները ուսումնասիրելու համար: Օգտագործված է Բիրգոֆֆի երգողիկ հիպոթեզը և սկզբնական 3D սպինային խնդիրը, արտաքին էլեկտրոմագնիսական դաշտի տարածման ուղղությամբ ձևափոխված է երկու պայմանականորեն անկախ 1D խնդիրների: Առաջին խնդիրը մկարագրում է չկարգավորված N-մասնիկանի համակարգի խնդիրը հաշվի առնելով միջավայրի ռելակսացիան, այն դեպքում երբ երկրորդը՝ մկարագրում է տարածական սպինային շղթայի վիճակագրական հատկությունները: Հիմնվելով երկու խնդիրներում զարգացված կառուցվածքների վրա հաշված է խմբային ուղղորդվածության երևույթով պայմանավորված բևեռացվածության գործակիցը: Կլաուզիուս-Մոսսոտիի հավասարումը դիէլեկտրիկ հաստատունի համար ընդհանրացված է տարածա-ժամանակային մանոմասշտաբների վրա: