The mathematical model of quantum dots pair orientation under laser radiation field

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Abstract

One approach for the formation of structures with complex geometries at the nanoscale is the step-by-step assembly. In this case, it is necessary to be able to estimate the time required to establish orientational equilibrium for a preformed pair of particles. This process is statistical in nature and depends on the mechanism of interaction of the ensemble with the external field. The orientation of particles in an alternating field is associated with certain relaxation times, which depend on the viscosity and temperature of the medium, as well as on the geometric structure of the samples. This paper proposes an mathematical model of the process of establishing the distribution of nanoparticles pairs orientations taking into account the friction force, thermal motion, and the orienting laser field. A statistical orientation distribution was obtained for CdTe particles in the field of moderate laser radiation, and the average time for establishing orientational equilibrium was estimated.

Keywords: mathematical methods, nanostructure fabrication, relaxation process.

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Introduction

In recent years, elements and devices based on nanostructures with controllable properties, consisting of quantum dots, have been actively developed and investigated [1 – 4]. In this regard, it becomes necessary to create a cheap method for their production, which allow to reproduce the same topology. Self-organization of nanoparticles can be the basis for this method [5 – 6]. The selectivity of self-organization can be achieved through chemical [7 – 8] or physical [9] principles. And as it was shown in [10 – 12] self-assembly of nanoparticles under the action of laser field can be an universal method for the formation of nanostructures with specific properties for application in nanophotonics and sensorics.

The authors of the present paper suggested an universal method of nanostructures' formation under action of external quasiresonant field due to the self-organization of nanoparticles [10, 11]. The first experiments [13] have shown the fundamental possibility of pair formation from colloidal quantum dots. Numerical calculations [14] have shown the possibility of creating more complex structures using step-by-step self-assembly. However, for its experimental implementation, it is necessary to solve a number of questions, in particular, to estimate the time of establishing the orientational equilibrium of a particles pair in the field of laser radiation.

Within the framework of this work, an original mathematical model of the orientation of a particles pair in the field of laser radiation has been constructed and the time of establishing the orientational equilibrium has been estimated.

1. Object of the study

1.1. The model of dipole pair

In our study a structure consisting of two spherical CdTe nanoparticles of radius R is considered (Figure 1). We assume that the line connecting the centers of mass of these particles is codirectional with the Ox axis and the external light field is uniform and directed at an angle to the line connecting the centers of mass of the particles that make a pair in the Oxy plane.

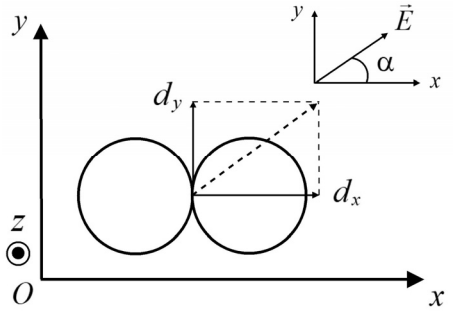

Fig. 1. Projection onto the Oxy plane of the position of a dipole pair

Assume that a pair of particles is characterized by a dipole moment $\vec{d}$, which is determined by the superposition of dipole moments $\vec{d}_i$ for i–th particle that is part of the pair. It is known [14] that the vector of the induced dipole moment $\vec{d}_i$ of a single nanoparticle with resonant frequency $\omega_{0,i}$ has the form

$$\vec{d}_i = \left|d_{12}\right|_i^2 \left(\vec{E} + \vec{E}_j\right) \Big/ \hbar\left(\Omega + i\Gamma_i\right), \quad (1)$$

where for i–th particle: $|d_{12}|$ is the module of electric dipole matrix element of the transition between states 1 and 2 [11]; $\Omega = \omega_{0,i} - \omega$ is the detuning of external field frequency from the resonance; ω is frequency of external radiation; Γ_i is the homogeneous linewidth [11]. Also $\hbar$ is Planck constant, and $\vec{E}_j$ is the field created by j–th particle of the pair at the point of location of i–th one where $j \neq i$:

$$\vec{E}_j = \left(3\left(\vec{d}_j, \vec{r}\right) - \vec{d}_j r^2\right) \Big/ r^5. \quad (2)$$

Here $\vec{r}$ is the vector connecting the centers of mass of the particles. We assume the particles to be the same with the following parameters: $|d_{12}|_0 = |d_{12}|_1 = |d_{12}|$; $\Gamma_0 = \Gamma_1 = \Gamma$; $\omega_{0,1} = \omega_{0,2} = \omega_0$. Taking into account that a pair of particles is located in the Oxy plane and the vector $\vec{r}$ is codirectional with the Ox axis, it follows from (1) and (2) that the components of the dipole moment of a pair of particles located according to fig. 1 can be written as

$$\begin{aligned} d_x &= 2E\omega_s r^3 \cos\alpha \times \\ &\times \left[\frac{\Omega - 2\omega_s}{\left(\Omega - 2\omega_s\right) + \Gamma^2} - i\frac{\Gamma}{\left(\Omega - 2\omega_s\right) + \Gamma^2}\right], \\ d_y &= 2E\omega_s r^3 \sin\alpha \times \\ &\times \left[\frac{\Omega + \omega_s}{\left(\Omega + \omega_s\right) + \Gamma^2} - i\frac{\Gamma}{\left(\Omega + \omega_s\right) + \Gamma^2}\right], \\ d_z &= 0. \end{aligned} \quad (3)$$

Here $\omega_s = |\mathrm{d}_{12}|^2 / r^3\hbar$ is the value of the frequency shift of the resonance of a particle due to its interaction with another one [11]. Note that (3) holds only if the vector $\vec{r}$ is directed along the Ox axis and the external field vector $\vec{E}$ is located in the Oxy plane. At the same time, the relaxation process of a pair assumes that the pair can be oriented arbitrarily. Take into account the interaction of the pair's dipole with an external field by introducing into consideration the local coordinate system (CS) $Ox'y'z'$, rigidly fixed to the pair (fig. 2) in such a way that the vector is always directed along the Ox' axis; the origin of the local CS is located at the center of mass of the pair and coincides with the origin for the inertial CS. Assume also that in the local CS the pair is always located in the $Ox'y'$ plane, and the Oy', Oz' axes complete the local CS to the right triplet. Thus, at the initial moment of time in the local CS $Ox'y'z'$, the components of the dipole moment vector are specified according to (3).

Let us identify the further spatial rotation of the pair with the rotation of the moving CS rigidly fixed to the pair. For a connection between the moving (local) and inertial coordinate systems, the Euler angles [15] φ, θ, ψ which are called the angles of precession, nutation and proper rotation, respectively (fig. 3) are considered.

In this case, the transition matrix A from an inertial CS to local one is written in the form presented in Appendix. Then the vector of the dipole moment in the inertial stationary SC can be obtained according to the following expression

$$\vec{d} = A^{-1} \begin{pmatrix} d_x^{loc} & 0 & 0 \\ 0 & d_y^{loc} & 0 \\ 0 & 0 & d_z^{loc} \end{pmatrix} A\vec{E}, \quad (4)$$

where the components d_x^{loc}, d_y^{loc}, d_z^{loc} are determined according to (3).

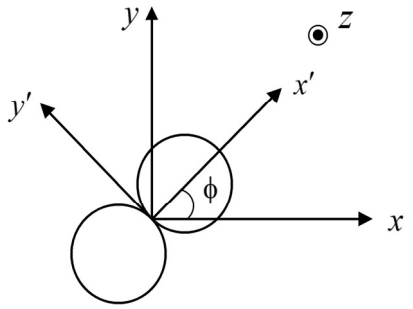

Fig. 2. Position of the local and inertial coordinate systems at the initial moment of time

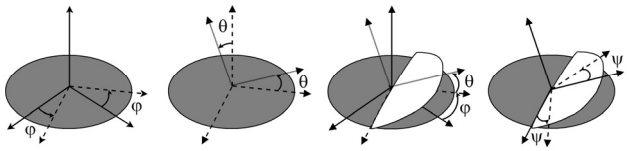

Fig. 3. Euler angles

1.2. Parameters of the model

Let us consider a pair of similar particles, the position of the center of mass of which is fixed relative to each other. Each particle is described by the value of its mass m, radius R, resonance frequency ω_0, radius vector of the center of mass of an particle $\vec{r}_i$, as well as the quantities $|d_{12}|^2$ and Γ. For a bonded pair, we define the following quantities: the radius vector of the center of mass of the pair $\vec{r}_p$, its angular velocity $\vec{w}$, and the modulus of the induced dipole moment $\vec{d}$ in an external field $\vec{E}$ with frequency ω. Also assume that a local CS rigidly fixed with a pair. The rotation of the pair will be identified with the rotation of the local CS. In the local (moving) coordinates system, define the value of the dipole moment $\vec{d}^{loc}$ and the moment of inertia J. Hereinafter, the superscript of a vector $\vec{\cdot}^{loc}$ means that the vector is defined in the local CS, and the value of the vector quantity without $\vec{\cdot}$ denotes the modulus of this vector. The interaction of a pair with an external field is simulated in a viscous medium characterized by temperature T, density ρ and viscosity μ.

For numerical simulation, we considered a pair of CdTe particles of radius of $R = 3$ nm. According to the data given in [14], let us choose following parameters as the starting data:

$$T = 300\mathrm{K},\ \left|d_{12}\right|^2 = 1.91 \cdot 10^{-44}\,\mathrm{J \cdot m^3},$$
$$\lambda_0 = 2\pi/\omega_0 = 525\mathrm{nm},\ m = 2.12 \cdot 10^{-23}\,\mathrm{kg}.$$

As the resonant frequency for an isolated quantum dot, the frequency of the first exciton transition is chosen, taking into account the size quantization. As the parameters of the medium, we define intensity of laser field equal to $I=10^6$V/cm^2; we also consider the interaction of a pair in an aqueous solution with a density $\rho=996.8$ kg/m^3 and dynamic viscosity $\eta=0.8902$ mPa·s. Further, to describe the rotation of a pair in a viscous fluid, we will approximate the pair with a cylinder of radius R and height $4R$. For the cylinder determine the value of the moment of inertia J in the local CS:

$$J=\begin{pmatrix} \frac{mR^2}{2} & 0 & 0 \\ 0 & \frac{19mR^2}{12} & 0 \\ 0 & 0 & \frac{19mR^2}{12} \end{pmatrix}.$$

Since the Ox' axis is the axis of symmetry for the cylinder, the Ox', Oy', Oz' axes coincide with the principal axes for the body of revolution, and the components J_{vv}, J_{zz} are equal.

2. The function of orientation distribution

The algorithm of the step-by-step formation of complex structures assumes that the previously formed pair is oriented in some way in space. In the absence of an orienting external light field, the orientation of the pair in space is equally probable in directions due to thermal motion. In the presence of an electric field, a moment of forces $[\vec{E}\times\vec{d}]$ acts on the induced dipole, and tends to rotate it so that the interaction energy of the dipole with the field is minimal. The expression for the potential energy of an electric dipole in a uniform electric field of magnitude $E=E_0\cos\omega t$ with frequency ω is determined as $-(\vec{E}\cdot\vec{d})$. For a dipole whose components are determined according to (3), and the dipole-field system is determined by Figure 1, the expression for the potential energy of a pair, depending on its orientation, takes the form

$$W(\alpha)=-2E_0^2\omega_s r^3\times \\ \times\left[\cos^2\alpha\frac{\Omega-2\omega_s}{(\Omega-2\omega_s)^2+\Gamma^2}-\sin^2\alpha\frac{\Omega+\omega_s}{(\Omega+\omega_s)^2+\Gamma^2}\right]. \quad (5)$$

An expression of the form (5) is easy to analyze. Thus, the energy of interaction of the induced dipoles with the field has two maxima and two minima. For low frequencies, both terms in (5) take negative values. When the frequency of external field approaching the resonant frequency of an isolated particle, the term at the cosine is the first to respond to a change in frequency and its sign becomes positive. At higher frequencies, the positive contribution of the first term increases with a decrease in the negativity of the second, and the energy takes on a positive value. Ultimately, since the denominator of each term grows faster than the numerator, the energy takes on a value close to zero.

If we know the energy of interaction of a dipole pair with an external field, the distribution of a large number of pairs that do not interact with each other can be statistically estimated through the Boltzmann distribution [16]:

$$f(\alpha)=A\exp(-W(\alpha)/kT), \quad (6)$$

where k is the Boltzmann constant, T is the temperature of the medium, and A is the normalization factor. Figure 4 shows the results of a numerical calculation of the interaction energy (5) of a pair, the parameters of which are determined in Section 1.2., with an external field, depending on the wavelength of the incident radiation and the angle α specifying the direction of the vector $\vec{E}$ in the $Ox'y'$ plane of the local CS.

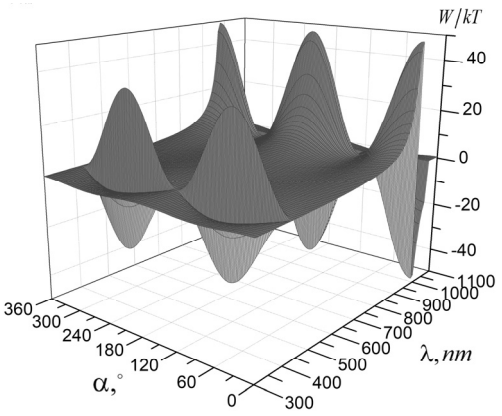

Fig. 4. The energy of the dipole interaction of a pair with an external field as a function of the angle of orientation α of its polarization and the wavelength of the external field λ

The distribution function (6) corresponding to the calculated energy (fig. 4) is shown in fig. 5.

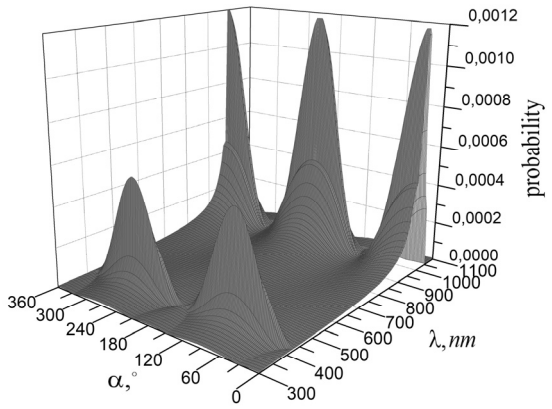

Fig. 5. Distribution function for the system of a pair of particles relative to the field strength vector depending on the angle of its orientation α and wavelength λ

Fig. 4 and 5 show that the maxima of the orientation distribution function of a pair are determined by those parameters α and λ that correspond to the minima of the potential energy of interaction of a pair of particles with the field in the long-wave and short-wave regions. In the

short-wavelength region of the spectrum, the maximum probability is reached at $\lambda = 430$ nm. In this case, the pair is oriented orthogonally to the vector of polarization of the electric field. The opposite situation is observed in the long-wavelength region of the spectrum, where the pair is located along the polarization vector (at $\lambda = 990$ nm). This is explained by the fact that when the particles are in the low frequency region, the system is reoriented along the direction of the field, since in this direction the natural vibrations of the system are phase matched. The energy of interaction with this orientation will be minimal. In the opposite case, approaching the high-frequency resonance of the system, the particle oscillation frequency is higher, and the potential interaction energy is lower.

Thus, the expression (6) makes it possible to estimate the assumed probability of orientation of a pair after switching on the laser field in a local CS rigidly fixed to the pair. Obviously, when the laser field is switched on, the establishment of the orientational equilibrium determined by (6) will not occur instantaneously, but will be associated with a certain relaxation process due to the rotation of the pair in a viscous liquid. The time of establishing orientational equilibrium is one of the characteristics of the self-organization process of large structures, since, firstly, this parameter should be taken into account when assessing the total assembly time, and secondly, as shown in [14], when organizing the self-assembly process, the orientation of the preformed pair has great value. Therefore, the following sections of this work will be devoted to mathematical modeling of the relaxation process of a pair and a numerical estimate of the time to establish orientational equilibrium.

3. Mathematical model of relaxation process

The rotational motion of a pair which is characterized by an induced dipole moment $\vec{d}$ in a uniform constant laser field $\vec{E}$ in a viscous fluid is determined by the action of the moment of forces $\vec{N}$:

$$\vec{N} = \left[\vec{d} \times \vec{E}\right] + \vec{M}^{rot}, \tag{7}$$

where $[\vec{a} \times \vec{b}]$ is the vector product, M^{rot} is the moment of rotation caused by the forces of hydrodynamic resistance to the rotation of the structure.

$$\vec{M}^{rot} = \left[\vec{F} \times \vec{r}\right]. \tag{8}$$

According to [17], the magnitude of the viscous drag force $\vec{F}^R$ for flowing around a cylinder is determined by the equality:

$$F^R = CF\rho v^2/2, \tag{9}$$

where C is the dimensionless drag coefficient, F is the projection area of the body onto the plane normal to the direction of motion, v is the body's velocity relative to the fluid. As before, for numerical simulation, approximate the pair with a cylinder of radius R and height $4R$. With this assumption, at low Reynolds numbers, the coefficient $C \approx 1.2$ [17]. As the midsection, choose the circular projection of the cylinder $F = \pi R^2$, as the smallest possible. Thus, estimate the force of viscous resistance $\vec{F}^R$ as

$$\vec{F}^R = \tilde{C}\vec{w}, \tag{10}$$

where $\tilde{C} = 0.6\pi\rho R^4 w$. The interaction of particles with the environment with fluctuating density usually leads to a random change in their trajectory. To take into account Brownian motion, we consider a random force described by the Gaussian distribution. Assume that a pair of particles undergoes a random force action over a time period Δt. Before each step of integration, the values of the projections of the random force $\vec{F}^G$ on the coordinate axes are selected from the Gaussian distribution with zero mean and standard deviation $\sigma^2 = 12\pi\eta RkT/\Delta t$. Then the force of hydrodynamic rotation $\vec{F}$ is defined as the superposition of the forces of viscous resistance and a random force $\vec{F} = \vec{F}^R + \vec{F}^G$.

We associate the rotation of the pair with the rotation of the local CS fixed to it. The rotation of a particle in a local coordinate system is determined by the equation of moments [15]:

$$\frac{d\vec{L}}{dt} + \left[\vec{w}^{loc} \times \vec{L}\right] = \vec{N}^{loc}. \tag{11}$$

Here $\vec{L}$ is the angular momentum of the dipole pair, which is defined in the form $\vec{L} = J\vec{w}^{loc}$; $\vec{N}^{loc}$ is the rotational moment determined in the local CS. Since $dJ^i/dt = 0$, then (11) can be rewritten in the form of dynamic Euler equations [15]

$$\begin{cases} \dfrac{dw_x^{loc}}{dt} + w_y^{loc} w_z^{loc} \dfrac{J_z - J_y}{J_x} = \dfrac{N_x^{loc}(\vec{r})}{J_x}, \\ \dfrac{dw_y^{loc}}{dt} + w_x^{loc} w_z^{loc} \dfrac{J_x - J_z}{J_y} = \dfrac{N_y^{loc}(\vec{r})}{J_y}, \\ \dfrac{dw_z^{loc}}{dt} + w_x^{loc} w_y^{loc} \dfrac{J_y - J_x}{J_z} = \dfrac{N_z^{loc}(\vec{r})}{J_z}. \end{cases} \tag{12}$$

Equations (12) characterize the change in the angular velocity in the local CS $Ox'y'z'$. Note that the second term in the first equation of system (12) is identically equal to zero due to the change in the local CS with respect to the inertial one is characterized by the system of equations (13) [15].

$$\begin{cases} \dfrac{d\varphi}{dt} = \dfrac{1}{\sin\theta}\left(w_x^{loc}\sin\psi + w_y^{loc}\cos\psi\right), \\ \dfrac{d\psi}{dt} = w_z^{loc} - \cot\theta\left(w_x^{loc}\sin\psi + w_y^{loc}\cos\psi\right), \\ \dfrac{d\theta}{dt} = w_x^{loc}\cos\psi - w_y^{loc}\sin\psi. \end{cases} \tag{13}$$

Thus, the rotational motion of the pair is described by the combined system of differential equations (12) and

(13). Integration of the resulting system in the general case can be performed only numerically.

4. Numerical modelling

For the numerical solution of the systems of equations (12) and (13), the explicit numerical Runge-Kutta method of the 4th order [18] was used. A cube with an edge of 20 nm was considered as a computational domain. At the initial moment of time $t=t_0$ the angular velocity of the pair w is close to zero, and the Euler angles φ, θ, ϕ was set in a random way so that $\varphi\in[0;2\pi]$, $\theta\in[0;\pi/12]$, $\varphi\in[0;\pi/12]$. The criterion for stopping the iterative process $w^k<\varepsilon$ is considered the damping of the rotation speed at a time $t_k=\tau k$ with a time step τ. The time interval $T=t_k$ at which the stopping criterion was performed is the time of establishing the orientational equilibrium.

Fig. 6 shows a numerical calculation of the time to establish the orientational equilibrium for different frequencies of the external field. Thus, it follows from the figure that for resonance frequencies of 990 and 430 nm, the most probable time for establishing orientational equilibrium is 0 – 4 ns (average – 2.62 ns for 990 nm, 3.15 ns for 430 nm), and for frequencies lying between resonances the most the likely settling time range is 4 – 6 ns.

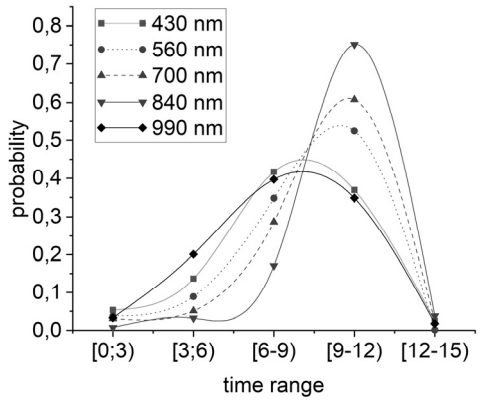

Fig.6. The probability of the time of establishing the orientational equilibrium falling into the time interval for different frequencies of the external field

In this case, the distribution of the relaxation time for the resonant frequencies is more uniform and, for the most part, is determined by the initial orientation of the pair.

Conclusions

The work is devoted to the numerical analysis of the process of establishing the orientational equilibrium of particles pairs in a laser field. Consideration of the orientation of a pair in conjunction with a local CS rigidly fixed to it allows one to transfer well-analyzed analytically models that are valid under certain restrictions to the general case.

It is shown that the process of establishing orientational equilibrium can be described by six ordinary differential equations, which makes it possible to both numerically estimate the settling time and predict the position of a pair after a given time interval, including in the absence of external radiation.

The obtained results make it possible to estimate the time of orientational equilibrium, which is important when implementing the method of step-by-step assembly of nanoparticles in a laser radiation field. A feature of this method is the ability to form structures from colloidal quantum dots of different chemical composition, but with optical resonances. This approach can be used to obtain structures sensitive to the local environment (sensors) and, in the future, as elements of optoelectronic systems.

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Appendix

The form of transition matrix A from an inertial coordinate system to local one:

$$A=\begin{pmatrix} \cos\varphi\cos\psi-\sin\varphi\cos\theta\sin\psi & -\cos\varphi\sin\psi-\sin\varphi\cos\theta\cos\psi & \sin\varphi\sin\theta \\ \sin\varphi\cos\psi+\cos\varphi\cos\theta\sin\psi & -\sin\varphi\sin\psi+\cos\varphi\cos\theta\cos\psi & -\cos\varphi\sin\theta \\ \sin\theta\sin\psi & \sin\theta\cos\psi & \cos\theta \end{pmatrix}.$$

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