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Can nanoparticles be useful for antiviral therapy?

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Abstract. In this paper, optical properties of the system consisting of mesoparticles (small dielectric particles) and nanoparticles (quantum dots) of various shapes have been considered. This system can be characterized by resonant absorption of electromagnetic waves and used for developing the new approach to antiviral therapy.

Keywords: nanoparticle (quantum dot), mesoparticle (small dielectric particle – virus), local field effects, resonant absorption.

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1. Introduction

For centuries, medical researchers and doctors around the world have raced to cure the serious maladies, for example, cancer, and they have had some success. The last decades give medical researchers and doctors new approaches and methods allowing to treat patients for an illness with driblet medicine delivered directly to diseased organ [1]. Most of the temporal exotic methods in modern medicine are connected with using the nanoparticles or nanosystems [2]. The nanoparticles are used both for drug delivery [3] and for therapy [4]. These treatments with nanoparticles were based on action of nanoparticles on cells [5].

Because electrodynamic properties of nanoparticles are strongly dependent on the shape of nanoparticles, one can show that the system consisting of mesoparticles and quantum dots (nanoparticles) can be characterized by resonant absorption of electromagnetic waves [6]. This property of nanoparticles can be used for developing the new approach to antiviral therapy. To demonstrate it, we will follow our previous work [6] and consider optical properties of quantum dots (QD), the role of which will be played by the nanoparticles and mesoparticles in the form of viruses. Then, to simulate behavior of QD optical properties in inhomogeneous field of mesoparticle, one can consider two particles in the external long-range field $\mathbf{E}^{(0)}(\mathbf{R},\omega)$. It can be supposed that the nanoparticle (QD) is characterized by spatial quantization and small dielectric particle is considered here as mesoparticle. The term mesoparticle in the problem means that dimensions of the particle are much smaller than the wavelength of probing field, and local-field effects begin to play an essential role in formation of electrodynamic properties. On the other hand, the mesoparticle is chosen to be which the spatial quantization effects can not be observed. The origin point of Cartesian coordinate system is connected with the centre of QD with OZ-axis directed through particles centres (Fig. 1).

It is clear that the total field acting on QD differs from $\mathbf{E}^{(0)}(\mathbf{R},\omega)$. The same one may affirm about the total field acting on the mesoparticle. Indeed, the external field acting on QD consists of two parts – the external (with respect to the whole system) field $\mathbf{E}^{(0)}(\mathbf{R},\omega)$ and field reradiated by the mesoparticle. On the other hand, the external field acting on the mesoparticle consists of the external field $\mathbf{E}^{(0)}(\mathbf{R},\omega)$ and the field reradiated by QD. To calculate the effective susceptibilities of the particles one should establish connection between the external and local fields.

Equation connecting the local field and currents induced by external field inside QD is Lippmann-Schwinger equation [7] and has the form

$$E_i(\mathbf{R},\omega) = E_i^{(0)}(\mathbf{R},\omega) - \\ - i\mu_0\omega \int_{V_q} d\mathbf{R}' G_{ik}(\mathbf{R},\mathbf{R}') J_k(\mathbf{R}',\omega)\,, \qquad (1)$$

where $G_{ik}(\mathbf{R},\mathbf{R}')$ is a Green's function of medium in which QD is embedded. In the frame of pseudo-vacuum Green's function formalism [7], the Green function of the system "vacuum + mesoparticle" can be written in the form

$$G_{ik}(\mathbf{R},\mathbf{R}') = G_{ij}^{(0)}(\mathbf{R},\mathbf{R}') - \\ - k_0^2 \int_{V_{mp}} d\mathbf{R}'' G_{ik}^{(0)}(\mathbf{R},\mathbf{R}'') X_{kl}^{(mp)}(\mathbf{R}'',\omega)\, G_{lj}^{(0)}(\mathbf{R}'',\mathbf{R}')\,, \qquad (2)$$

where $G_{ij}^{(0)}(\mathbf{R},\mathbf{R}')$ is the electrodynamic Green function of the medium in which the mesoparticle and QD are located. The effective susceptibility of mesoparticle $X_{kl}^{(mp)}(\mathbf{R},\omega)$ can be calculated using the method developed earlier (see, for example [8]).

Taking into account that the local current can be related with the local field by constitutive equation [9], one can solve the self-consistent equation (1) and find the connection between the local field at the quantum dot and external field acting on the system

$$E_i(\mathbf{R},\omega) = \Lambda_{ij}^{(QD)}(\mathbf{R},\omega) E_j^{(0)}(\mathbf{R}',\omega)\,, \qquad (3)$$

where $\Lambda_{ij}^{(QD)}(\mathbf{R},\omega)$ is the local-field factor [7] of the QD interacting with mesoparticle. On the other hand, solution of Eq. (1) means that one have known the relation between the local current inside the QD and external field acting on the system

$$J_i(\mathbf{R},\omega) = -i\omega\, X_{ij}^{(QD)}(\mathbf{R},\omega) E_j^{(0)}(\mathbf{R},\omega)\,, \qquad (4)$$

with $X_{ij}^{(QD)}(\mathbf{R},\omega)$ being the effective susceptibility of the QD.

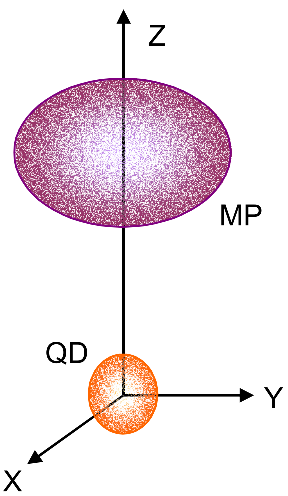

Fig. 1. Sketch of the problem.

By analogy to that discussed above, one can write for the mesoparticle equation relating the local field and currents induced by the external field inside mesoparticle

$$E_i(\mathbf{R},\omega) = E_i^{(0)}(\mathbf{R},\omega) - \\ - i\mu_0\omega \int_{V_{mp}} d\mathbf{R}' \Re_{ik}(\mathbf{R},\mathbf{R}') J_k(\mathbf{R}',\omega)\,, \qquad (5)$$

where $\Re_{ik}(\mathbf{R},\mathbf{R}')$ is the Green function of medium in which mesoparticle is embedded. In the frame of pseudo-vacuum Green's function formalism [7], the Green function of the system "vacuum + quantum dot" can be written in the form

$$\Re_{ik}(\mathbf{R},\mathbf{R}') = G_{ij}^{(0)}(\mathbf{R},\mathbf{R}') - \\ - k_0^2 \int_{V_{mp}} d\mathbf{R}'' G_{ik}^{(0)}(\mathbf{R},\mathbf{R}'') X_{kl}^{(QD)}(\mathbf{R}'',\omega)\, G_{lj}^{(0)}(\mathbf{R}'',\mathbf{R}')\,. \qquad (6)$$

Then, one can find the relation between the local field at the mesoparticle and external field acting on the system

$$E_i(\mathbf{R},\omega) = \Lambda_{ij}^{(mp)}(\mathbf{R},\omega) E_j^{(0)}(\mathbf{R},\omega)\,, \qquad (7)$$

where $\Lambda_{ij}^{(mp)}(\mathbf{R},\omega)$ is the local-field factor [7] of the mesoparticle interacting with QD. The relation between the local current inside the mesoparticle and external field acting on the system is

$$J_i(\mathbf{R},\omega) = -i\omega\, X_{ij}^{(mp)}(\mathbf{R},\omega) E_j^{(0)}(\mathbf{R},\omega)\,. \qquad (8)$$

One should note that both effective susceptibilities of the QD and mesoparticle are dependent on shapes and dimensions of the particles.

The next step should be calculations of the absorption properties of the system under consideration. Then, one should to calculate the energy absorbed by the system "QD+virus", which can be defined via dissipative function as Joule heat absorbed by unit of volume of the system per unit of time. After the cycle, averaging the dissipative function can be written in the form [6]

$$Q(\omega) = \frac{1}{2}\left\langle E_i^*(R) J_i(R,\omega) + E_i(R) J_i^*(R,\omega)\right\rangle_{DQ} + \\ + \frac{1}{2}\left\langle E_i^*(R) J_i(R,\omega) + E_i(R) J_i^*(R,\omega)\right\rangle_{mp}\,, \qquad (9)$$

where $\langle\ldots\rangle_{QD}$ and $\langle\ldots\rangle_{mp}$ mean averaging over the volumes of QD and mesoparticle, respectively. Using Eqs (3)-(4) and (7)-(8), one can write

$$Q_{QD}(\omega) = -i\omega\frac{1}{2}\left\langle \left[\Lambda_{ij}^{(QD)}(\mathbf{R},\omega)\right]^* X_{ik}^{(QD)}(\mathbf{R},\omega) - \\ - \Lambda_{ik}^{(QD)}(\mathbf{R},\omega)\left[X_{ij}^{(QD)}(\mathbf{R},\omega)\right]\right\rangle_{DQ} I_{(jk)}(\mathbf{R}_{QD},\omega)\,, \qquad (10)$$

and

$$Q_{QD}(\omega) = -i\omega\frac{1}{2}\left\langle \left[\Lambda_{ij}^{(mp)}(\mathbf{R},\omega)\right]^* X_{ik}^{(mp)}(\mathbf{R},\omega) - \\ - \Lambda_{ik}^{(mp)}(\mathbf{R},\omega)\left[X_{ij}^{(mp)}(\mathbf{R},\omega)\right]\right\rangle_{mp} I_{(jk)}(\mathbf{R}_{mp},\omega)\,, \qquad (11)$$

where

$$I_{(jk)}(\mathbf{R},\omega)=\left[E_j^{(0)}(\mathbf{R},\omega)\right]^{*}E_j^{(0)}(\mathbf{R},\omega) \qquad (12)$$

is the intensity of external field acting on the QD and mesoparticle.

As a result, taking into account that the external field can be considered as the long-range field, one can generalized Eq. (9) in the form

$$I(\omega)=\Re_{ij}(\omega)I_{ij}^{(0)}(\omega)\,, \qquad (13)$$

where the absorption tensor $\Re_{ij}(\omega)$ depends both on the dimensions and shapes of the particles. Moreover, this tensor has a resonant behavior. This resonant behavior was demonstrated for the system consisting of spherical nanoparticle and quantum dot [6]. The occurrence of the resonance is related with local-field enhancement and, very probable, to occurrence of the "collective" mode leading to strong narrow absorption line in *g*-aggregates.

The idea is based on strong resonance interaction between the mesoparticle (virus) and quantum dot which are depended on shaping of the particles we can propose the method of antiviral therapy. Additionally one should to note that long-range interaction between the QD and virus can lead to potential $Ar^m - Br^m$ $(m > n)$ type which has a minimum at the distance about of QD linear dimension. It means that interactions between the particles can lead to occurring the stable binding state "QD-virus". Then, injection into living organism the quantum dots of determined shape, can lead to occurring the bound system "QD-virus". Radiation of the system with the electromagnetic field of fixed (resonant) frequency leads to resonant absorption the energy of the field by the system "QD-virus" can leads to destroying the viral nucleocapsid. As a result, the infectious ability of the virus will decrease. Thereof, this method could have some antiviral therapeutic effect.

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