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# INTEGRAL EQUATIONS IN THE GENERAL THEORY OF LIGHT ABSORPTION AND SCATTERING

*The problem of light absorption and scattering has been reduced to the solution of a singular integral equation for the complex vector of electric field intensity inside a nanoparticle. The dipole approximation is chosen as the initial one. The results of computing experiments testify to an acceptable agreement between the approach proposed for the consideration of the electric field inside a spherical nanoparticle and the results available for the optical and emission properties of metal nanoclusters.*

*K e y w o r d s*: metal nanoclusters, optical properties, integral equation, computing experiment.

## 1. Introduction

Researches of the processes of light absorption and scattering by small particles have a long history (see, e.g., [1–3]). The interest in those objects (small particles) is associated with the fact that their optical and emission properties differ substantially from the analogous properties of massive materials. In particular, in metal nanoparticles, there emerge the so-called plasma resonances connected with collective oscillations of conduction electrons relatively to the nanocluster lattice. The number of plasma resonances, their frequencies, and decrements depend on the nanoparticle shape: there is one plasma resonance in the case of spherical nanoparticles, two in the case of spheroidal nanoparticles, and three in the case of ellipsoidal ones.

When metal clusters are irradiated with laser pulses, besides the excitation of plasma resonances, which results in the appearance of high local electric fields near the cluster surface, the heating of electrons in the conduction band also becomes possible. The electrons become "hot". As a result, various nonlinear optical effects may appear. The electron heating is favored by the features of the electron-lattice energy exchange in small clusters. Those features are reduced to a decrease (in a quasioscillatory way) of the intensity of electron-lattice energy exchange, when the nanocluster sizes diminish [4]. Such a weakening of the energy exchange arises, when the nanoparticle dimensions become smaller than the mean free path of electrons.

Metal nanoclusters (MNCs) and their ensembles find wide applications in science and engineering owing to their unique optical and emission properties. In particular, MNCs are deposited onto surfaces in order to change the reflective ability of a material [5]. Those nanostructures are used for the optical recording of information [6], in biosensorics and genetic engineering [7], to visualize cell structures [8], and, finally, in medicine to treat cancer [9]. The more detailed information about the properties and applications of nanostructures can be found, e.g., in [11–14].

## 2. Integral Relation between the Current Density and Electric Field Vectors: Ohm's Law in the Operator Form

The problem of light absorption and scattering by MNCs is reduced to the solution of Maxwell's equa-

tions with corresponding boundary conditions. In the case of spherical MNCs, the most general, consistent, and widely applied theory of light absorption and scattering is a theory developed by Mie [15]. However, his theory, as well as the theories of the overwhelming majority of other authors on this subject, is based on the assumption that the current density vector $\mathbf{j}(\mathbf{r},\omega)$ (here, $\mathbf{r}$ is the coordinate vector, and $\omega$ is the frequency) is connected with the vector of the internal electric field $\mathbf{E}(\mathbf{r},\omega)$ by the relation

$$\mathbf{j}(\mathbf{r},\omega) = \sigma(\omega)\,\mathbf{E}(\mathbf{r},\omega), \tag{1}$$

where $\sigma(\omega)$ is the electron conductivity of a metal cluster.

Ohm's law in the form (1) is valid for MNCs under certain conditions. First, this is a possibility to neglect the spatial dependence of the local internal electric field. For ellipsoidal MNCs, the local internal field is uniform, if the wavelength of the external electromagnetic field is much larger than the characteristic MNC dimensions. Second, this is a possibility to neglect the contribution of the surface electron scattering to the dissipation. This conditon is satisfied, if the MNC dimensions are much larger than the electron mean free path.

In the general case, the relation between the vectors of current density and electric field induced by this current should be found by solving the corresponding Boltzmann equation. The internal electric field $\mathbf{E}(\mathbf{r},\omega)$ forms the distribution function of electrons over their velocities $\mathbf{v}$'s. In the linear (in the field) approximation, this distribution function can be written as the sum

$$f(\mathbf{r},\mathbf{v},\omega) = f_0(\varepsilon) + f_1(\mathbf{r},\mathbf{v},\omega), \tag{2}$$

where $f_0(\varepsilon)$ is the Fermi distribution function, $\varepsilon$ the electron energy, and $f_1(\mathbf{r},\mathbf{v},\omega)$ the linear-in-the-field correction to the equilibrium Fermi distribution.

The function $f_1(\mathbf{r},\mathbf{v},\omega)$ satisfies the linearized Boltzmann equation

$$(\nu - i\,\omega)\,f_1 + \mathbf{v}\frac{\partial f_1}{\partial \mathbf{r}} + e\,\mathbf{E}(\mathbf{r},\omega)\mathbf{v}\frac{\partial f_0}{\partial \varepsilon} = 0. \tag{3}$$

In addition, it also has to satisfy boundary conditions. In the case of diffuse electron scattering at the surface $S$ of a metal cluster, the boundary condition looks like

$$f_1(\mathbf{r},\mathbf{v},\omega)|_S = 0 \quad \text{at} \quad v_n < 0. \tag{4}$$

Here, $v_n$ is the electron velocity component normal to the surface.

The aim of this work is to analyze the influence of the MNC shape on the processes of light absorption and scattering. For this purpose, it is enough to admit that the MNCs have the form of an ellipsoid. The expediency of this choice consists in that the results obtained for this shape can be extended (by deforming of the ellipsoid curvature radii) to a wide spectrum of shapes ranging from the disk to rod-like ones.

The solution of problem (3), (4) for the case of ellipsoidal nanoparticles can be written in the form [16, 17]

$$f_1(\mathbf{r},\mathbf{v},\omega) = -f_0'(\varepsilon)\int\limits_0^{t_0} d\tau\, e^{-\tilde{\nu}\tau} e\,\mathbf{E}(\mathbf{r}'-\mathbf{v}'\tau,\omega). \tag{5}$$

Here, $t_0$ is the characteristic of Eq. (3),

$$t_0(\mathbf{r}',\mathbf{v}') = \frac{1}{v'^2}\left\{\mathbf{r}'\mathbf{v}' + \sqrt{(R^2-r'^2)v'^2 + (\mathbf{r}'\mathbf{v}')^2}\right\}, \tag{6}$$

where $\mathbf{r}'$ and $\mathbf{v}'$ are the vectors of electron coordinates and velocity, respectively, in the deformed coordinate system (in which the ellipsoidal particle transforms into a spherical one). The coordinates in the deformed and undeformed systems are connected by the relations [16, 17]

$$x_i = \frac{R_i}{R}x_i', \quad v_i = \frac{R_i}{R}v_i', \tag{7}$$

where $R_i$ are the ellipsoid curvature radii, and $R = (R_1R_2R_3)^{1/3}$. In the case of spherical particle, $R$ is the sphere radius. In addition, the notation

$$\tilde{\nu} = \nu - i\omega \tag{8}$$

was introduced in Eq. (5).

Knowing the velocity distribution function of electrons in the form (2) and (5), it is possible to determine the relation between the current density and the field that induces it:

$$\mathbf{j}(\mathbf{r},\omega) = \frac{2\,e}{(2\pi\hbar)^3}\int \mathbf{v}\,f(\mathbf{r},\mathbf{v},\omega)\,d^3(mv) =$$
$$= 2\,e^2\left(\frac{m}{2\pi\hbar}\right)^3\int d^3v\,\mathbf{v}(-f_0'(\varepsilon))\int\limits_0^{t_0} d\tau\, e^{-\tilde{\nu}\tau}\,\mathbf{E}(\mathbf{r}'-\mathbf{v}'\tau,\omega),$$

where $m$ is the electron mass. This formula can be rewritten in the operator form

$$\mathbf{j}(\mathbf{r},\omega) = \Sigma(\mathbf{E})(\mathbf{r},\omega), \tag{9}$$

where $\Sigma(\mathbf{E}) \equiv -2e^2\left(\frac{m}{2\pi\hbar}\right)^3 \int d^3v \mathbf{v} f_0'(\varepsilon) \int_0^{t_0} d\tau e^{-\tilde{\nu}\tau} \times \times \mathbf{E}\left(\mathbf{r}' - \mathbf{v}'\tau, \omega\right)$ is a linear integral operator. Expression (9) generalizes relation (1) to the case of small clusters. In other words, we obtained Ohm's law for small clusters in the operator form. If we neglect the coordinate dependence of the internal electric field in Eq. (9), suppose that only one scattering mechanism (either in the bulk or at the surface) dominates, and account for the relation

$$f_0'(\varepsilon) = \frac{\partial f_0}{\partial \varepsilon} \approx -\delta(\varepsilon - \varepsilon_{\mathrm{F}}),$$

where $\varepsilon_{\mathrm{F}}$ is the Fermi energy, integral (9) can be calculated. As a result, we obtain Ohm's law [16, 19] in the form (1). In this case, the conductivity of a spherical nanoparticle looks like [16, 19]

$$\sigma^{(0)}(\omega) = \frac{n_0 e^2}{m} \begin{cases} \dfrac{\nu}{\omega^2 + \nu^2} & \text{at } \nu \gg \nu_s; \\ \dfrac{3}{2}\dfrac{\nu_s}{\omega^2}\left[1 - 2\dfrac{\nu_s}{\omega}\sin\dfrac{\omega}{\nu_s} + 2\left(\dfrac{\nu_s}{\omega}\right)^2 \times\right. & \\ \left. \times \left(1 - \cos\dfrac{\omega}{\nu_s}\right)\right] & \text{at } \nu \ll \nu_s. \end{cases} \quad (10)$$

Here, $\nu_s = \frac{v_{\mathrm{F}}}{2R}$ is the frequency of electron oscillations (from wall to wall), $v_{\mathrm{F}}$ the Fermi velocity, and

$$n_0 = \frac{1}{3\pi^2}\left(\frac{m\, v_{\mathrm{F}}}{\hbar}\right)^3$$

the electron concentration. In the case of elliptic nanoparticle, the conductivity becomes a tensor, provided that the electron mean free path is larger than the particle size [16, 17, 19]. The components of this tensor are quoted in the cited works.

Hence, for a simple expression describing the relation between the current and the field, like Ohm's law (1) or (10), to be applicable, while studying the optical properties of MNCs, two conditions have to be satisfied. First, the internal electric field has to be spatially uniform. This condition demands that the MNC dimensions should be much smaller than the wavelengths, at which the particle is irradiated. Second, if the particle is not spherical, the bulk scattering has to dominate; otherwise, the conductivity will be a tensor quantity. For the bulk scattering to dominate, the electron mean free path has to be much shorter than the nanoparticle size. If those conditions are not satisfied, Ohm's law for small clusters in the operator form (9) has to be used.

In the general case, the coordinate dependence of wave components both inside and outside the MNC can be found by solving Maxwell's equations with regard for relations (9) and the corresponding boundary conditions for the field components. From the viewpoint of obtaining the analytical results, this is rather a complicated mathematical problem. The method of hybrid numerical-analytical solution of integral equations derived on the basis of Maxwell's equations making allowance for a real relation between the current and the field [see Eq. (9)] is much more promising in this case, because there is no necessity to satisfy the boundary conditions for the field components in this approach.

## 3. Research of the Optical Properties of Metal Clusters on the Basis of Integral Equations

Consider a dielectric matrix with dielectric permittivity $\epsilon(\omega)$. The matrix includes a metal nanoparticle, in which external fields induce an electric charge with the density $\rho$ and a current with the density $\mathbf{j}$. The Fourier transforms of Maxwell's equations describing this system look like

$$\mathrm{rot}\,\mathbf{E}(\mathbf{r},\omega) = i\,k_0 \mathbf{B}(\mathbf{r},\omega), \quad (11)$$

$$\mathrm{div}\,\mathbf{B}(\mathbf{r},\omega) = 0, \quad (12)$$

$$\epsilon(\omega)\,\mathrm{div}\,\mathbf{E}(\mathbf{r},\omega) = 4\pi\rho(\mathbf{r},\omega), \quad (13)$$

$$\mathrm{rot}\,\mathbf{B}(\mathbf{r},\omega) = -i\,k_0\epsilon(\omega)\mathbf{E}(\mathbf{r},\omega) + \frac{4\pi}{c}\mathbf{j}(\mathbf{r},\omega). \quad (14)$$

where $c$ is the light speed, and $k_0 = \omega/c$. The charge and current densities can be expressed in terms of the polarization vector density:

$$\rho(\mathbf{r},\omega) = -\nabla\mathbf{P}(\mathbf{r},\omega), \quad (15)$$

$$\mathbf{j}(\mathbf{r},\omega) = -i\,\omega\,\mathbf{P}(\mathbf{r},\omega). \quad (16)$$

The differential equations (11)–(14) together with relations (15) and (16) can be reduced to integral equations (see, e.g., review [18]). In particular, for the electric component of an electromagnetic wave, the following equation holds:

$$\mathbf{E}(\mathbf{r},\omega) = \mathbf{E}_0(\mathbf{r},\omega) + \int \hat{S}_0(\mathbf{r},\mathbf{r}',\omega)\mathbf{P}(\mathbf{r}',\omega)\,d\mathbf{r}'. \quad (17)$$

Here, $\mathbf{E}_0(\mathbf{r},\omega)$ is the vector of electric field strength for the external wave (the field in the absence of a nanoparticle), and the susceptibility tensor $\hat{S}_0(\mathbf{r},\mathbf{r}',\omega)$ equals

$$\hat{S}_0(\mathbf{r},\mathbf{r}',\omega) = \left\{-k^2 T_1(\Re) - ikT_2(\Re) + T_3(\Re)\right\} \frac{e^{ik\Re}}{\epsilon(\omega)}, \tag{18}$$

where the notations

$$k^2 = k_0^2\epsilon(\omega), \quad \Re = \mathbf{r} - \mathbf{r}'$$

were introduced. In addition, $T_i(\Re)$ in Eq. (18) stand for the diad tensors

$$T_1(\Re) = \frac{1}{\Re^3}\{\Re\otimes\Re - I\Re^2\}, \tag{19}$$

$$T_2(\Re) = \frac{1}{\Re^4}\{3\Re\otimes\Re - I\Re^2\}, \tag{20}$$

$$T_3(\Re) = \frac{1}{\Re^5}\{3\Re\otimes\Re - I\Re^2\}, \tag{21}$$

where $I$ is the identity matrix.

Hence, in the general case, our task consists in the solution of a system of two equations in the vector form. These are Eq. (17) and the equation for the polarization vector density, which, according to Eqs. (16) and (9), has the form

$$\mathbf{P}(\mathbf{r},\omega) = -i\frac{2e^2}{\omega}\left(\frac{m}{2\pi\hbar}\right)^3 \int d^3v\,\mathbf{v} f_0'(\varepsilon) \times$$

$$\times \int\limits_0^{t_0} d\tau\, e^{-\tilde{\nu}\tau}\,\mathbf{E}(\mathbf{r}'-\mathbf{v}'\tau,\omega). \tag{22}$$

An alternative way consists in analyzing and solving the following integral equation for the complex vector of electric field strength:

$$\mathbf{E}(\mathbf{r},\omega) = \mathbf{E}_0(\mathbf{r},\omega) - i\,g\int d^3\mathbf{r}'\hat{S}_0(\mathbf{r},\mathbf{r}') \times$$

$$\times \int d^3v\,\mathbf{v} f_0'(\varepsilon) \int\limits_0^{t_0} d\tau\, e^{-\tilde{\nu}\tau}\,\mathbf{E}(\mathbf{r}'-\mathbf{v}'\tau,\omega), \tag{23}$$

where

$$g \equiv \frac{2e^2}{\omega}\left(\frac{m}{2\pi\hbar}\right)^3. \tag{24}$$

## 4. Approximate Solutions

As the zeroth approximation, let us assume that the spatial dependence of the wave electric field in a metal nanoparticle can be neglected. Formally, this assumption corresponds to the passage to the limit $k \to 0$ in Eq. (17).

Let $\mathbf{E}_0$ be directed along the axis $Oz$. Then the projection of Eq. (17) on this axis looks like (as $k \to 0$)

$$E = E_0 + \int d^3r'\{\hat{S}_0\}_{zz}P_z, \tag{25}$$

where

$$\{\hat{S}_0\}_{zz} = \left\{\hat{S}_0(\mathbf{r},\mathbf{r}',\omega)\right\}_{zz} = \frac{3\Re_z^2 - \Re^2}{\Re^5\epsilon(\omega)}. \tag{26}$$

In the case of spherical nanoparticle, according to Eq. (16), the projection of the dipole moment vector density on the axis $Oz$ equals

$$P_z = P = \frac{i}{\omega}\sigma\,E. \tag{27}$$

It is important to emphasize that the field $E$ and the dipole moment density $P$ in Eqs. (17) and (25) are complex-valued quantities. Therefore, the conductivity $\sigma$ in Eq. (27) is also complex-valued, unlike that in Eq. (10). In particular, for a spherical particle and the bulk scattering, from Eqs. (8) and (16), we obtain

$$P = i\frac{n_0e^2}{m\omega\tilde{\nu}}\sigma\,E = -\frac{\omega_p^2}{\omega^2+\nu^2}\frac{\omega-i\nu}{\omega}E, \tag{28}$$

where $\omega_p$ is the plasma frequency $\left(\omega_p^2 \equiv 4\pi\frac{n_0e^2}{m}\right)$.

Now, let us substitute Eqs. (26) and (28) into Eq. (25) and take into account that

$$\int d^3r'\frac{3\Re_z^2-\Re^2}{\Re^5} = V\begin{cases} -\frac{1}{R^3} & \text{at } z<R; \\ \frac{3z^2-r^2}{r^5} & \text{at } z>R. \end{cases} \tag{29}$$

Then, from Eq. (25), we obtain

$$E^{(0)} = \frac{E_0}{1+\frac{1}{3}\left(\frac{\epsilon_M(\omega)}{\epsilon(\omega)}-1\right)}. \tag{30}$$

Here,

$$\epsilon_M(\omega) = \epsilon(\omega) - \frac{\omega_p^2}{\omega^2+\nu^2}\frac{\omega-i\nu}{\omega} \tag{31}$$

is the dielectric permittivity. Formula (30) is a known result of the dipole approximation for the electric field inside a nanoparticle.

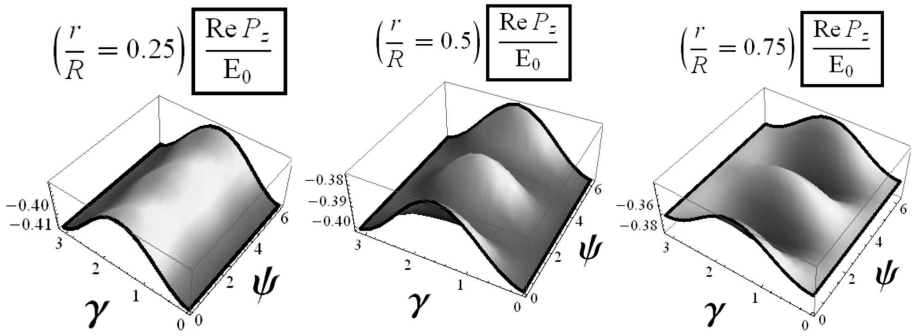


***Fig. 1.*** Real part of the projection of the dipole moment density vector on the axis $Oz$. For the input parameters, see Appendix

In the case where the surface scattering plays the dominating role, the result for $\epsilon_M(\omega)$ can be obtained from Eq. (31), by using the formal substitution $\nu \to \frac{3}{4}v_{\mathrm{F}}/R$.

Returning back to ellipsoidal metal nanoparticles, one should bear in mind that, if the nanoparticle size is smaller than the electron mean free path or has the same order, the conductivity in such particles becomes a tensor quantity [16,17]. It can be shown that, in this case, instead of Eq. (30), we obtain

$$E_j^{(0)} = \frac{E_{0j}}{1 + L_j\left(\frac{\epsilon_{jj}}{\epsilon(\omega)} - 1\right)}, \tag{32}$$

where $L_j$ is the depolarization factor, and $\epsilon_{jj}$ the diagonal component of the conductivity tensor.

## 5. Spatial Dispersion Effect

Let the spatial dependence of the external field $\mathbf{E}_0(\mathbf{r},\omega)$ in relation (30) look like

$$\mathbf{E}_0(\mathbf{r},\omega) = \mathbf{E}_0 e^{i\mathbf{k}\,\mathbf{r}}. \tag{33}$$

Then, taking result (30) into account, the following approximation is justified for the coordinate dependence of the electric field inside the particle:

$$\mathbf{E}^{(1)}(\mathbf{r}) = \frac{\mathbf{E}_0 e^{i\mathbf{k}\,\mathbf{r}}}{1 + \frac{1}{3}\left(\frac{\epsilon_M(\omega)}{\epsilon(\omega)} - 1\right)}. \tag{34}$$

Formula (34) is valid for spherical MNCs. In the case of ellipsoidal MNCs, a more general expression than formula (34) should be used:

$$E_j^{(1)}(\mathbf{r},\omega) = \frac{E_{0j} e^{i\mathbf{k}\,\mathbf{r}}}{1 + L_j\left(\frac{\epsilon_{jj}(\omega)}{\epsilon(\omega)} - 1\right)}. \tag{35}$$

Expressions for the diagonal elements $\epsilon_{jj}$ of the tensor of dielectric permittivity can be found in works [16, 17].

Now, let us substitute expression (35), if the MNC is ellipsoidal, or expression (34), if it is spherical, into Eq. (22). Then we obtain

$$\mathbf{P}(\mathbf{r},\omega) = -\,i\frac{2\,e^2}{\omega}\left(\frac{m}{2\pi\hbar}\right)^3 e^{i\mathbf{k}\,\mathbf{r}} \times$$
$$\times \int d^3v\, f_0'(\varepsilon)\,\mathbf{v}(\mathbf{v}\mathbf{E}^{(0)})\frac{1 - \exp[-(\tilde{\nu} + i\mathbf{k}\,\mathbf{v})t_0]}{\tilde{\nu} + i\mathbf{k}\,\mathbf{v}}. \tag{36}$$

Here, $\mathbf{E}^{(0)}$ is a constant complex amplitude of the electric field inside the metal nanoparticle. It is described by formula (30), if the MNC is spherical, and by formula (32), if it is ellipsoidal.

The angular and radial dependences of the real and imaginary parts of the dipole moment vector density projection on the axis $Oz$ in the case of spherical nanoparticles are illustrated in Figs. 1 and 2. The angular arguments of those dependences are explained in Fig. 3. The knowledge of the dipole moment vector density makes it possible to calculate the vector of electric field strength outside the nanoparticle using formula (17). The result of corresponding calculations is depicted in Figs. 4 and 5.

Let us obtain approximate analytical formulas for integral (36) in two opposite limits:

$$|(\tilde{\nu} + i\mathbf{k}\,\mathbf{v})t_0| > 1 \tag{37a}$$

and

$$|(\tilde{\nu} + i\mathbf{k}\,\mathbf{v})t_0| < 1. \tag{37b}$$

Case (37a) corresponds to the dominating bulk scattering. Provided that it is satisfied, we obtain from

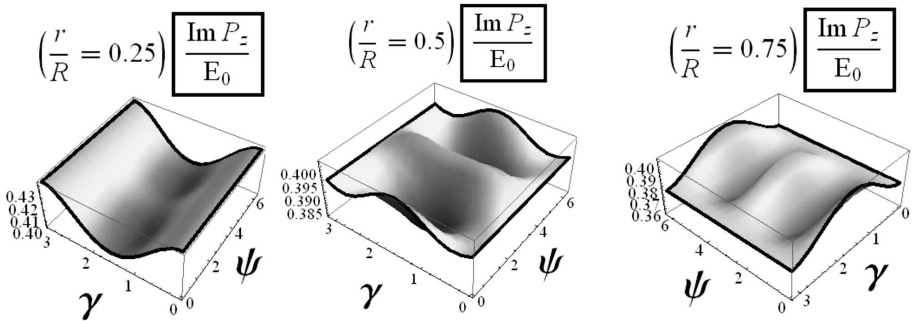


***Fig. 2.*** Imaginary part of the projection of the dipole moment density vector on the axis $Oz$

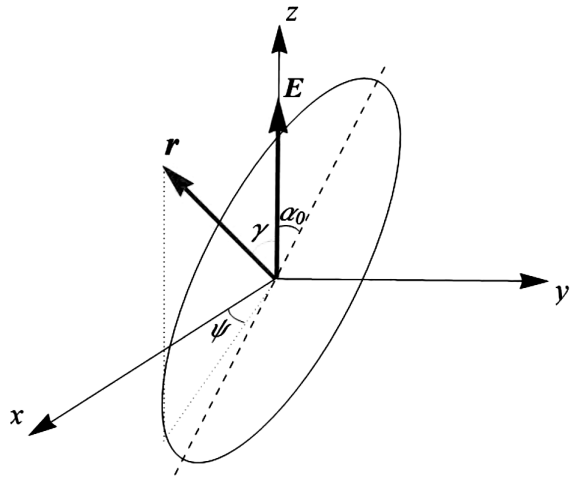


***Fig. 3.*** Orientations of the electric field strength vector and the radius vector with respect to the spheroid symmetry axis

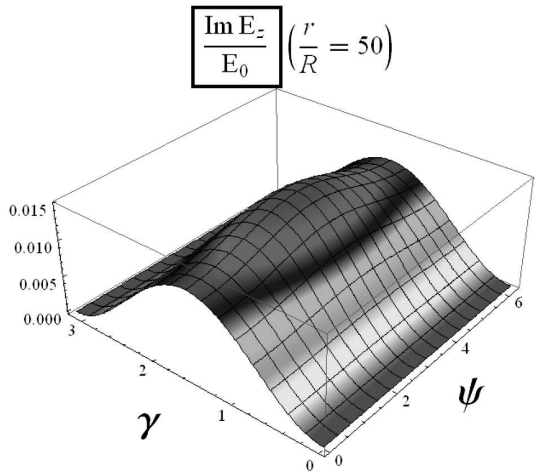


***Fig. 5.*** Imaginary part of the projection of the electric field strength vector on the axis $Oz$ outside the nanoparticle

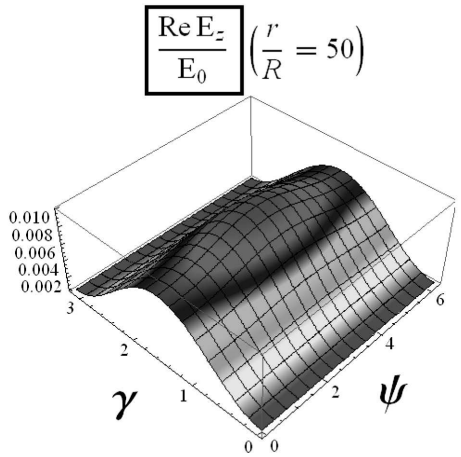


***Fig. 4.*** Real part of the projection of the electric field strength vector on the axis $Oz$ outside the nanoparticle

Eq. (36) that

$$P_\alpha(\mathbf{r},\omega)=\frac{i}{\omega}\sum\sigma_{\alpha\beta}E_\beta e^{i\mathbf{k}\,\mathbf{r}}, \tag{38}$$

where $\sigma_{\alpha\beta}$ are the components of the conductivity tensor,

$$\sigma_{\alpha\beta}(\mathbf{k},\omega)=-2\,e^2\left(\frac{m}{2\pi\hbar}\right)^3\times$$
$$\times\, e^{i\mathbf{k}\,\mathbf{r}}\int d^3v\,v_\alpha v_\beta\frac{f_0'(\varepsilon)}{\nu-i(\omega-\mathbf{k}\,\mathbf{v})}. \tag{39}$$

If the surface scattering dominates, i.e. in case (37b), we obtain from Eq. (36) that

$$\mathbf{P}(\mathbf{r},\omega)=-i\frac{2\,e^2}{\omega}\left(\frac{m}{2\pi\hbar}\right)^3 e^{i\mathbf{k}\,\mathbf{r}}\int d^3v\,\mathbf{v}(\mathbf{v}\mathbf{E}^{(0)})f_0'(\varepsilon)t_0. \tag{40}$$

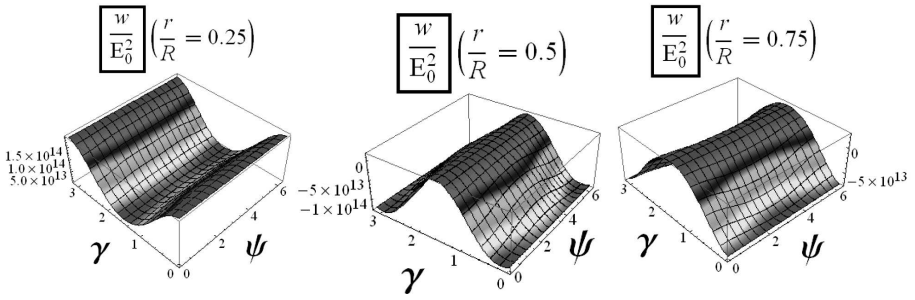


***Fig. 6.*** Angular and radial dependences of the absorbed energy density in the case of spherical nanoparticle (for the input parameters, see Appendix)

In what follows, we are interested in the absorbed energy density. It is equal to

$$w(\mathbf{r},\omega) \equiv \frac{1}{2}\,\mathrm{Re}\,\{\mathbf{j}(\mathbf{r},\omega)\mathbf{E}^*(\mathbf{r},\omega)\} =$$

$$= \frac{1}{2}\,\mathrm{Re}\,\{-i\omega\,\mathbf{P}(\mathbf{r},\omega)\mathbf{E}^*(\mathbf{r},\omega)\} =$$

$$= \frac{\omega}{2}\,\mathrm{Im}\,\{\mathbf{P}(\mathbf{r},\omega)\mathbf{E}^*(\mathbf{r},\omega)\}. \qquad (41)$$

Figure 6 illustrates the angular dependence of this quantity normalized to the incident wave intensity.

Formula (41) demonstrates that we have to know the projection of the vector $\mathbf{P}(\mathbf{r},\omega)$ on the field direction. Let the latter coincide with the direction of the axis $Oz$. Then, in the case of spherical nanoparticle, we obtain from Eq. (40) that

$$P_z(\mathbf{r},\omega) = i\,E^{(0)}\frac{3n_0\,e^2}{4m\omega}\frac{R}{v_\mathrm{F}}\times$$

$$\times\, e^{i\mathbf{k}\mathbf{r}}\left\{\left[1+\frac{1-\xi}{2\xi}\ln\left(\frac{1+\xi}{1-\xi}\right)\right]\sin^2\theta_0 +\right.$$

$$\left.+\,\frac{1}{2\xi}\left[\frac{1+\xi^2}{2\xi}-\left(\frac{1-\xi^2}{2\xi}\right)^2\ln\left(\frac{1+\xi}{1-\xi}\right)\left(3\cos^2\theta_0-1\right)\right]\right\}. \qquad (42)$$

Here, $\xi = r/R$, and $\theta_0$ is the angle between the directions of the field $\mathbf{E}$ and the vector $\mathbf{r}$. While obtaining Eq. (42), we took into account that $f_0'(\varepsilon) \approx \approx -\delta(\varepsilon-\varepsilon_\mathrm{F})$.

Now, let us substitute Eqs. (42) and (34) into formula (41) to obtain an expression for the density of the energy absorbed by a symmetric metal nanoparticle in the case where the surface scattering plays a dominating role:

$$w(\mathbf{r},\omega) = \frac{3n_0\,e^2}{8m}\frac{R}{v_\mathrm{F}}\frac{E_0^2}{\left|1+\frac{1}{3}\left(\frac{\epsilon_M(\omega)}{\epsilon(\omega)}-1\right)\right|^2}\times$$

$$\times\left\{\left[1+\frac{1-\xi}{2\xi}\ln\left(\frac{1+\xi}{1-\xi}\right)\right]\sin^2\theta_0 +\right.$$

$$\left.+\,\frac{1}{2\xi}\left[\frac{1+\xi^2}{2\xi}-\left(\frac{1-\xi^2}{2\xi}\right)^2\ln\left(\frac{1+\xi}{1-\xi}\right)\left(3\cos^2\theta_0-1\right)\right]\right\}. \qquad (43)$$

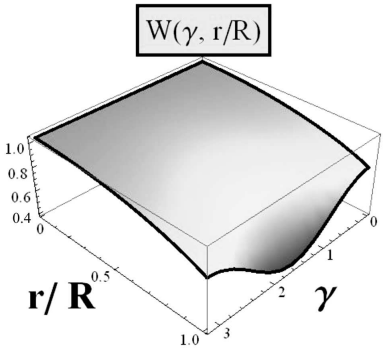


***Fig. 7.*** Dependence of the absorbed energy density (in rel. units) on the point position in a nanoparticle

From this formula and Fig. 7, one can see that the absorbed energy density at the surface scattering substantially depends on the position of the point in the nanoparticle (this position is fixed by the variables $r$ and $\theta_0$, and does not depend on $\varphi_0$).

In particular, the energy density has a strongly pronounced angular dependence near the particle surface. At the same time, the dependence on the wave incidence angle is absent at the particle center. The

total absorbed energy equals

$$w_0 = \int\limits_V d^3r\, w(\mathbf{r},\omega) = V\frac{3}{8}\frac{n_0\, e^2}{m}\frac{R}{v_{\rm F}} \times$$
$$\times \frac{\omega^4 E_0^2}{(\omega^2-\omega_s^2)^2 + \left(\frac{\pi}{3}\frac{\omega_p^2}{\epsilon(\omega)}\frac{v_{\rm F}}{R}\right)^2}. \qquad (44)$$

Here, $\omega_s = \frac{\omega_p}{\sqrt{3}}$ is the frequency of a plasma resonance in a spherical MNC.

It is important to emphasize that the result obtained for the total absorbed energy in the case of surface scattering turned out identical to that obtained in the dipole approximation [16], despite that now the absorbed energy density substantially depends on the coordinates.

The formula for $w_0$ in the case of bulk scattering can be obtained from expression (44) by formally substituting $\frac{3}{4}\frac{v_{\rm F}}{R} \to \nu$.

The total energy absorbed by an ellipsoidal metal nanoparticle per unit time can be obtained from Eqs. (40) and (41). If the particle has the ellipsoid-of-revolution shape, and if the surface scattering plays a dominating role, we have

$$w_0 = \frac{VE_0^2}{2}\left\{\frac{\sigma_\perp \omega^4 \sin^2\alpha}{(\omega^2-\omega_\perp^2)^2 + (L_\perp\frac{4\pi}{\omega}\sigma_\perp)^2} + \right.$$
$$\left. + \frac{\sigma_\parallel \omega^4 \cos^2\alpha}{(\omega^2-\omega_\parallel^2)^2 + (L_\parallel\frac{4\pi}{\omega}\sigma_\parallel)^2}\right\}. \qquad (45)$$

Here, $\omega_\perp$ and $\omega_\parallel$ are the frequencies of plasma oscillations across and along the ellipsoid symmetry axis, respectively; $L_\perp$ and $L_\parallel$ are the corresponding polarization coefficients; $\sigma_\perp$ and $\sigma_\parallel$ are the diagonal components of the conductivity tensor; and $\alpha$ is the angle between the field $\mathbf{E}_0$ and the ellipsoid rotation axis.

Expression (45) was obtained for an MNC in vacuum ($\epsilon(\omega) = 1$). In this case,

$$\omega_{\perp,\parallel} = \sqrt{L_{\perp,\parallel}}\,\omega_p. \qquad (46)$$

Expressions for the diagonal components of the conductivity tensor, $\sigma_{xx} = \sigma_{yy} \equiv \sigma_\perp$ and $\sigma_{zz} \equiv \sigma_\parallel$, can be found in work [16] for both the low- ($\omega < v_{\rm F}/R$) and high-frequency ($\omega > v_{\rm F}/R$) cases. In particular, for a prolate ellipsoid in the low-frequency interval, we have [16]

$$\sigma_\perp = \frac{9}{8}\frac{n_0\, e^2}{m}\frac{R_\perp}{v_{\rm F}}\left\{\frac{1}{2e_p^2}\sqrt{1-e_p^2} + \right.$$
$$\left. + \frac{1}{e_p}\left(1-\frac{1}{2e_p^2}\right)\arcsin e_p\right\}, \qquad (47)$$

$$\sigma_\parallel = \frac{9}{8}\frac{n_0\, e^2}{m}\frac{R_\perp}{v_{\rm F}}\left\{-\frac{1}{e_p^2}\sqrt{1-e_p^2} + \frac{1}{e_p^3}\arcsin e_p\right\}, \qquad (48)$$

where

$$e_p = R_\perp/R_\parallel.$$

Hence, for both ellipsoidal- and spherical-like nanoparticles, if the surface scattering plays a dominating role, the total energy absorbed per unit time considered as a function of the electric field at the particle center has the same form as in the case of dipole approximation. Only a redistribution of absorbed energy over the nanoparticle volume takes place, by leaving the total absorbed energy invariable. It is not so, if the bulk scattering dominates. As one can see from Eq. (39), the absorbed energy is determined by the conductivity, which is a function of $\mathbf{k}$.

## 6. Conclusions

1. The relation between the vectors of current density in a metal nanoparticle and electric field that induces this current was obtained in works [16,17] in the most general form of an integral equation, which is interpreted as Ohm's law for small clusters in the operator form.

2. The problem of studying the optical properties of metal clusters has been presented by a mathematical model with the singular integral equation (23) for the complex vector of electric field strength inside a nanoparticle.

3. As a first variant of the solution of the integral equation (23), we have selected an approach where the dipole approximation is chosen as the initial one for the electric field inside a nanoparticle. This way allowed us to obtain rather compact expressions for the vector of electric field strength in the first approximation and for the polarization density vector in the cases of ellipsoidal and spherical nanoparticles.

4. The approximate analytical expression obtained for the dipole moment density vector in two opposite limits – if only the bulk or surface scattering dominates – is studied in detail.

5. The expression obtained for the energy density absorbed by a symmetric metal nanoparticle, in which the surface scattering dominates, allows a conclusion to be drawn that this parameter substantially

depends on the position in the nanoparticle. An important result is obtained that if the surface scattering plays a dominating role, the total energy absorbed per unit time considered as a function of the electric field at the particle center has the same form as in the dipole approximation for both ellipsoidal and spherical nanoparticles. Only a redistribution of the absorbed energy over the nanoparticle volume takes place, by leaving the total absorbed energy invariant.

6. The results of computing experiments testify to the acceptable consistency of the proposed initial approximation for the electric field inside spherical nanoparticles with the results available for the optical and emission properties of metal nanoclusters [11–14]. The substantive content of the computing experiment consists, in particular, in the visualization of the real and imaginary parts of the polarization vector projection on the direction of the field inside the particle, as well as the corresponding projection of the vector of the electric field strength outside it.

## APPENDIX
### Results of computing experiments

The aim of computing experiments was to demonstrate the capability of the mathematical model to describe the light absorption and scattering by metal nanoclusters with the use of the integral equations (17), (22), or (23). To achieve this purpose, it was necessary to solve some tasks, the main of which can be formulated as follows.

• ***Choice of a method for the solution of the integral equation (23).*** The difficulty consists in that the central characteristic of this equation is a singularity of the integral operator in the region occupied by the nanoparticle. Currently, there is no general mathematical theory for the calculation of a multidimensional singular integral (an analog of the principal value of a one-dimensional singular integral). In the region outside the nanoparticle, Eq. (23) is a Fredholm equation of the second kind in the vector form. Actually, the numerical realization of its solution is reduced to the solution of a system of six integral equations for the real and imaginary coordinate projections of the electric field strength vector $\mathbf{E}(\mathbf{r},\omega)$. This fact allows us to draw a conclusion that there is no exact analytical method for the solution of Eq. (23). The choice has to be made among one of the approximate methods of the numerical-analytical character. This choice gives rise to the appearance of an error inherent in the solution method, which can be rather large by value.

• ***Construction of an algorithm that implements the method proposed for the solution of integral equations in the general theory of light absorption and scattering by metal nanoclusters.*** The principal feature of the required algorithm is the necessity to calculate multidimensional (two- and three-dimensional) integrals of rapidly oscillating functions (see, e.g., formula (12) and Fig. 13). As a basic integration tool, the cubature formulas on the basis of bicubic approximating splines [21] can be used.

• ***Software implementation of the algorithm of the solution of integral equations.*** The aim of the software algorithm implementation consists in the minimization of the calculation time provided the acceptable level of the total error of a result. This means, first of all, the choice of the optimum number of mesh nodes in the integration interval.

• ***Interpretation of the results of computing experiment.*** This is a comparison of the obtained results with available concepts of theoretical and experimental character, as well as with the results of available variants of analytical calculations.

To solve the integral equation (23), we have selected an approach, in which approximation (30) is accepted as the initial one for the electric field in a spherical nanoparticle. In this case, representation (34) can be taken as the first approximation for the vector of electric field strength $\mathbf{E}^{(1)}(\mathbf{r},\omega)$, which can be rewritten in the form

$$\mathbf{E}^{(1)}(\mathbf{r},\omega)=\frac{3\mathbf{E}_0\exp(-i\mathbf{kr})}{2+\frac{\varepsilon_M(\omega)}{\varepsilon(\omega)}},$$

provided that the spatial dependence of the external field vector $\mathbf{E}_0(\mathbf{r},\omega)$ is described by Eq. (33), in which $\mathbf{E}_0$ is a constant vector directed along the axis $Oz$; and the ratio of dielectric permittivities $\varepsilon_M(\omega)/\varepsilon(\omega)$ is determined by the expression

$$\frac{\varepsilon_M(\omega)}{\varepsilon(\omega)}=1-\frac{\omega_p^2}{\omega^2+\upsilon^2}+i\frac{\omega_p^2}{\omega^2+\upsilon^2}\frac{\upsilon}{\omega},$$

where $\omega_p^2=4\,\pi\,n_0e^2/m$ is the plasma frequency, and $\upsilon$ is a phenomenological parameter that characterizes the frequency of electron collisions in the nanoparticle bulk.

Using the expression for the electric field strength vector $\mathbf{E}^{(1)}(\mathbf{r},\omega)$ in formula (36), we obtain the following formula for the polarization vector in the first approximation:

$$\mathbf{P}(\mathbf{r},\omega)=i\frac{9\omega_p^2}{16\pi^2\,\omega}\frac{\exp(-i\,\mathbf{kr})}{[2+\varepsilon_M(\omega)/\varepsilon(\omega)]}\times$$

$$\times\int\limits_0^{2\pi}d\varphi\int\limits_0^{\pi}d\theta\,\sin\theta\,\mathbf{u}_0(\mathbf{u}_0\mathbf{E}_0)\frac{1-\exp[-(\tilde{\upsilon}+i\mathbf{k}\,\mathbf{v}_{\rm F})\,t_0]}{\tilde{\upsilon}+i\mathbf{k}\,\mathbf{v}_{\rm F}}.$$

In this formula,

$$\mathbf{u}_0=\mathbf{v}_{\rm F}/v_{\rm F}=\sin\theta\cos\varphi\;\mathbf{i}+\sin\theta\sin\varphi\;\mathbf{j}+\cos\theta\;\mathbf{k}$$

is a unit vector; $\mathbf{k}$ is a vector with the absolute value $k=|\mathbf{k}|=\omega/c$, which is directed along the axis $Ox$, so that $\mathbf{k}\,\mathbf{v}_{\rm F}=k\,v_{\rm F}\sin\theta\cos\varphi$; $\theta$ is the angle between the vectors $\mathbf{v}_{\rm F}$ and $\mathbf{E}_0$ ($\theta\in[0,\pi]$); $\varphi$ is the angle between the vector $\mathbf{k}$ and the projection of the vector $\mathbf{v}_{\rm F}$ on the plane $xOy$ ($\varphi\in[0,2\,\pi]$); $\tilde{\upsilon}=\upsilon-i\,\omega$;

$$t_0=\frac{a}{v_{\rm F}}\left(\frac{r}{a}\cos\alpha+\sqrt{1-\left(\frac{r}{a}\sin\alpha\right)^2}\right);$$

$\alpha$ is the angle between the vectors $\mathbf{r}$ and $\mathbf{v}_{\rm F}$ ($\alpha \in [0,\pi]$), so that $\cos\alpha = \mathbf{r}\,\mathbf{v}_{\rm F}/r\,v_{\rm F}$; $a$ is the nanoparticle radius;

$$\mathbf{r} = r\,(\sin\gamma\cos\psi\;\mathbf{i} + \sin\gamma\sin\psi\;\mathbf{j} + \cos\gamma\;\mathbf{k})$$

is the radius vector of the point; $\gamma$ is the angle between the vectors $\mathbf{r}$ and $\mathbf{E}_0$ ($\gamma \in [0,\pi]$); and $\psi$ is the angle between the vector $\mathbf{k}$ and the projection of the vector $\mathbf{r}$ on the plane $xOy$ ($\psi \in [0,2\pi]$).

If the vector $\mathbf{E}_0$ is directed along the axis $Oz$, the projection $\mathrm{P}_z^{(1)}(\mathbf{r},\omega)$ of the polarization vector can be written in the form

$$\mathrm{P}_z^{(1)}(\mathbf{r},\omega) = i\frac{9\omega_p^2 E_0}{16\pi^2\,\omega}[2+\varepsilon_M(\omega)/\varepsilon(\omega)]^{-1}\exp(-i\mathbf{kr})\times$$

$$\times\int\limits_0^{2\pi} d\varphi \int\limits_0^{\pi} d\theta\,\sin\theta\,\cos^2\theta\frac{1-\exp[-(\tilde{\upsilon}+i\mathbf{k}\,\mathbf{v}_{\rm F})\,t_0]}{\tilde{\upsilon}+i\mathbf{k}\,\mathbf{v}_{\rm F}}.$$

For the preparation of the computation program, we quote a specific formula for each multiplier in this expression in what follows.

**1**. $zne(\omega_p,\omega,\upsilon) = [2+\varepsilon_M(\omega)/\varepsilon(\omega)]^{-1} =$

$$= \left[\left(3-\frac{\omega_p^2}{\omega^2+\upsilon^2}\right)^2 + \left(\frac{\omega_p^2}{\omega^2+\upsilon^2}\frac{\upsilon}{\omega}\right)^2\right]^{-1}\times$$

$$\times\left[\left(3-\frac{\omega_p^2}{\omega^2+\upsilon^2}\right) - i\left(\frac{\omega_p^2}{\omega^2+\upsilon^2}\frac{\upsilon}{\omega}\right)\right];$$

**2**. $rezne(\omega_p,\omega,\upsilon) = \left[\left(3-\frac{\omega_p^2}{\omega^2+\upsilon^2}\right)^2 + \right.$

$$\left. + \left(\frac{\omega_p^2}{\omega^2+\upsilon^2}\frac{\upsilon}{\omega}\right)^2\right]^{-1}\left(3-\frac{\omega_p^2}{\omega^2+\upsilon^2}\right);$$

**3**. $imzne(\omega_p,\omega,\upsilon) = \left[\left(3-\frac{\omega_p^2}{\omega^2+\upsilon^2}\right)^2 + \right.$

$$\left. + \left(\frac{\omega_p^2}{\omega^2+\upsilon^2}\frac{\upsilon}{\omega}\right)^2\right]^{-1}\left(\frac{-\omega_p^2}{\omega^2+\upsilon^2}\frac{\upsilon}{\omega}\right);$$

**4**. $\exp(-i\,\mathbf{kr}) = \cos(\omega\,r\sin\gamma\cos\psi/c) -$

$$-\,i\sin(\omega\,r\sin\gamma\cos\psi/c);$$

**5**. $t_0(x,\gamma,\psi,\varphi,\theta) = \frac{a}{v_{\rm F}}\times$

$$\times\left(\begin{array}{l}x(\cos\gamma\cos\theta+\cos(\psi-\varphi)\sin\gamma\sin\theta)+\\ +\sqrt{1-x^2(1-(\cos\gamma\cos\theta+\cos(\psi-\varphi)\sin\gamma\sin\theta)^2}\end{array}\right);$$

**6**. $x = r/a$;

**7**. $\dfrac{1}{\tilde{\upsilon}+i\mathbf{k}\,\mathbf{v}_{\rm F}} =$

$$= z_0(\omega,\varphi,\theta)\,[\upsilon + i\omega\,(1-c^{-1}\,v_{\rm F}\sin\theta\cos\varphi)];$$

**8**. $z_0(\omega,\varphi,\theta) = [\upsilon^2+\omega^2\,(1-c^{-1}\,v_{\rm F}\sin\theta\cos\varphi)^2]^{-1};$

**9**. $s_0(x,\gamma,\psi,\varphi,\theta) = t_0(x,\gamma,\psi,\varphi,\theta)\,x_0(\varphi,\theta);$

**10**. $x_0(\varphi,\theta) = (1-c^{-1}\,v_{\rm F}\sin\theta\cos\varphi);$

**11**. $pr_0(x,\omega,\gamma,\psi) =$

$$= \int\limits_0^{2\pi}\int\limits_0^{\pi}\Big\{d\varphi\,d\theta\,\sin\theta\,\cos^2\theta\times z_0(\omega,\varphi,\theta)\times$$

$$\times[\upsilon-\upsilon\exp(-\upsilon\,t_0(x,\gamma,\psi,\varphi,\theta))\times$$

$$\times\cos\{\omega\,s_0(x,\gamma,\psi,\varphi,\theta)\}+\omega\,x_0(\varphi,\theta)\times$$

$$\times\exp(-\upsilon\,t_0(x,\gamma,\psi,\varphi,\theta))\sin\{\omega\,s_0(x,\gamma,\psi,\varphi,\theta)\}]\Big\};$$

**12**. $omvpr_0(x,\omega,\gamma,\psi,\varphi,\theta) = \omega\sin\theta\,\cos^2\theta\times$

$$\times z_0(\omega,\varphi,\theta)\times[\upsilon-\upsilon\exp(-\upsilon\,t_0(x,\gamma,\psi,\varphi,\theta))\times$$

$$\times\cos\{\omega\,s_0(x,\gamma,\psi,\varphi,\theta)\}+\omega\,x_0(\varphi,\theta)\times$$

$$\times\exp(-\upsilon\,t_0(x,\gamma,\psi,\varphi,\theta))\sin\{\omega\,s_0(x,\gamma,\psi,\varphi,\theta)\}];$$

**13**.

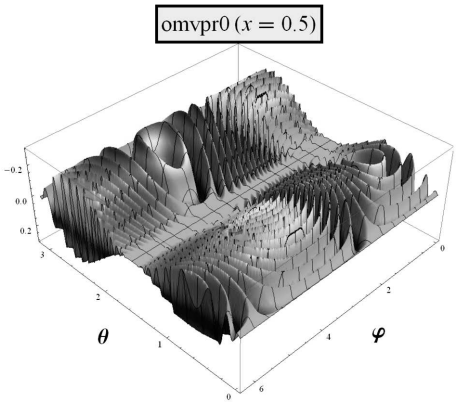


***Fig. 8.*** Plot of a rapidly oscillating function of a general form $omvpr_0(x,\omega,\gamma,\psi,\varphi,\theta)$ with $x \equiv r/a = 0.5$, $\omega = 10^{16}$ s$^{-1}$, $\gamma = \pi/4$, and $\psi = \pi/4$

Formula (12) is an integrand for the determination of the real-valued function $pr_0(x,\omega,\gamma,\psi)$. This formula is presented to demonstrate the complexity level at the calculation of multidimensional (two- and three-dimensional) integrals of rapidly oscillating functions (see, e.g., Fig. 8).

**14**. $pi_0(x,\omega,\gamma,\psi) =$

$$= \int\limits_0^{2\pi}\int\limits_0^{\pi}\Big\{d\varphi\,d\theta\,\sin\theta\,\cos^2\theta\times z_0(\omega,\varphi,\theta)[\omega\,x_0(\varphi,\theta) -$$

$$-\,\upsilon\exp(-\upsilon\,t_0(x,\gamma,\psi,\varphi,\theta))\times\sin\{\omega\,s_0(x,\gamma,\psi,\varphi,\theta)\} -$$

$$-\,\omega\,x_0(\varphi,\theta)\exp(-\upsilon\,t_0(x,\gamma,\psi,\varphi,\theta))\times$$

$$\times\cos\{\omega\,s_0(x,\gamma,\psi,\varphi,\theta)\}]\Big\}.$$

**15**. $rre\,\mathrm{P}_z(\mathbf{r},\omega) = -\dfrac{3\omega_p^2}{16\pi^2\,\omega}\,pi_0(x,\omega,\gamma,\psi).$

**16**. $iim\,\mathrm{P}_z(\mathbf{r},\omega) = \dfrac{3\omega_p^2}{16\pi^2\,\omega}pr_0(x,\omega,\gamma,\psi).$

**17**. The initial data:

$$\omega = 10^{16}\ \mathrm{s}^{-1},\quad \omega_p = 1.37\times10^{16}\ \mathrm{s}^{-1},$$

$$v_{\rm F} = 1.39\times10^{8}\ \mathrm{cm/s},\quad c = 3\times10^{10}\ \mathrm{cm/s},$$

$$\upsilon = 3.39\times10^{13}\ \mathrm{s}^{-1},\quad a = 2\times10^{-6}\ \mathrm{cm}.$$

**18**. $\mathrm{P}_z^{(1)}(\mathbf{r},\omega)/E_0 = 3[rezne(\omega_p,\omega,\upsilon) +$
$+\, i\, imzne(\omega_p,\omega,\upsilon)] \times$
$\times\, [\cos(\omega\, r \sin\gamma \cos\psi/c) - i \sin(\omega\, r \sin\gamma \cos\psi/c)] \times$
$\times\, [rre\, \mathrm{P}_z(\mathbf{r},\omega) + i\, iim\, \mathrm{P}_z(\mathbf{r},\omega)]$.

**19**. $re\mathrm{P}_z^{(1)}(\mathbf{r},\omega)/E_0 =$
$= 3\{[rre\, \mathrm{P}_z(\mathbf{r},\omega)\, rezne(\omega_p,\omega,\upsilon) - iim\, \mathrm{P}_z(\mathbf{r},\omega) \times$
$\times\, imzne(\omega_p,\omega,\upsilon)] \cos(\omega\, r \sin\gamma \cos\psi/c) +$
$+\, [rre\, \mathrm{P}_z(\mathbf{r},\omega)\, imzne(\omega_p,\omega,\upsilon) + iim\, \mathrm{P}_z(\mathbf{r},\omega) \times$
$\times\, rezne(\omega_p,\omega,\upsilon)] \sin(\omega\, r \sin\gamma \cos\psi/c)\}$.

**20**. $im\mathrm{P}_z^{(1)}(\mathbf{r},\omega)/E_0 =$
$= 3\{-[rre\, \mathrm{P}_z(\mathbf{r},\omega)\, rezne(\omega_p,\omega,\upsilon) -$
$-\, iim\, \mathrm{P}_z(\mathbf{r},\omega)\, imzne(\omega_p,\omega,\upsilon)] \sin(\omega\, r \sin\gamma \cos\psi/c) +$
$+\, [rre\, \mathrm{P}_z(\mathbf{r},\omega)\, imzne(\omega_p,\omega,\upsilon) +$
$+\, iim\, \mathrm{P}_z(\mathbf{r},\omega)\, rezne(\omega_p,\omega,\upsilon)] \cos(\omega\, r \sin\gamma \cos\psi/c)\}$.

**21**. $E_z 1\,(\mathbf{r},\omega) = E_0(\mathbf{r},\omega) +$
$+\, \dfrac{3\, E_0(\mathbf{r},\omega)}{\varepsilon(\omega)} [rezne(\omega_p,\omega,\upsilon) +$
$+\, i\, imzne(\omega_p,\omega,\upsilon)] \int \{\hat{S}_0(\mathbf{r},\mathbf{r}',\omega)\}_{z\,z}\, [rre\, \mathrm{P}_z(\mathbf{r},\omega) +$
$+\, i\, iim\, \mathrm{P}_z(\mathbf{r},\omega)]\, \exp(-i\mathbf{k}\,\mathbf{r})\, d\mathbf{r}' = E_0(\mathbf{r},\omega) +$
$+\, \dfrac{3\, E_0(\mathbf{r},\omega)}{\varepsilon(\omega)} [rezne(\omega_p,\omega,\upsilon) + i\, imzne(\omega_p,\omega,\upsilon)] \times$
$\times \int \left[ -k^2 \dfrac{R_z^2 - R^2}{R^3} - ik \dfrac{3R_z^2 - R^2}{R^4} + \dfrac{3R_z^2 - R^2}{R^5} \right] \times$
$\times\, [rre\, \mathrm{P}_z(\mathbf{r},\omega) + i\, iim\, \mathrm{P}_z(\mathbf{r},\omega)]\, \exp[i\,(kR - \mathbf{k}\,\mathbf{r})] d\mathbf{r}'$.

**22**. $re\, E_z in1\,(\mathbf{r},\omega) =$
$= \int\limits_0^a \rho'^2 d\rho' \int\limits_0^{2\pi} d\psi' \int\limits_0^{\pi} d\gamma' \sin\gamma' \Bigg\{ \Bigg[ \Bigg( -\, k^2 \dfrac{R_z^2 - R^2}{R^3} +$
$+\, \dfrac{3R_z^2 - R^2}{R^5} \Bigg) rre\, \mathrm{P}_z(\mathbf{r},\omega) + \left( k \dfrac{3R_z^2 - R^2}{R^4} \right) iim\, \mathrm{P}_z(\mathbf{r},\omega) \Bigg] \times$
$\times\, \cos[k\,(R - \rho'\, \sin\gamma' \cos\psi')] - \Bigg[ -\, rre\, \mathrm{P}_z(\mathbf{r},\omega) \times$
$\times\, k \dfrac{3R_z^2 - R^2}{R^4} + \left( -\, k^2 \dfrac{R_z^2 - R^2}{R^3} + \dfrac{3R_z^2 - R^2}{R^5} \right) \times$
$\times\, iim\, \mathrm{P}_z(\mathbf{r},\omega) \Bigg] \sin[k\,(R - \rho'\, \sin\gamma' \cos\psi')] \Bigg\}$.

**23**. $imE_z in1\,(\mathbf{r},\omega) =$
$\int\limits_0^a \rho'^2 d\rho' \int\limits_0^{2\pi} d\psi' \int\limits_0^{\pi} d\gamma' \sin\gamma' \Bigg\{ \Bigg[ -\, rre\, \mathrm{P}_z(\mathbf{r},\omega) \times$
$\times\, k \dfrac{3R_z^2 - R^2}{R^4} - \left( k^2 \dfrac{R_z^2 - R^2}{R^3} - \dfrac{3R_z^2 - R^2}{R^5} \right) \times$
$\times\, iim\, \mathrm{P}_z(\mathbf{r},\omega) \Bigg] \cos[k\,(R - \rho'\, \sin\gamma' \cos\psi')] +$
$+\, \Bigg[ \left( -\, k^2 \dfrac{R_z^2 - R^2}{R^3} + \dfrac{3R_z^2 - R^2}{R^5} \right) rre\, \mathrm{P}_z(\mathbf{r},\omega) +$
$+\, \left( k \dfrac{3R_z^2 - R^2}{R^4} \right) iim\, \mathrm{P}_z(\mathbf{r},\omega) \Bigg] \times$
$\times\, \sin[k\,(R - \rho'\, \sin\gamma' \cos\psi')] \Bigg\}$.

**24**. $re\, \dfrac{E_z 1\,(\mathbf{r},\omega)}{E_0\,(\mathbf{r},\omega)} = 1 + \dfrac{3}{\varepsilon(\omega)} \Bigg\{ \Bigg[ \left( 3 - \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \right)^2 +$
$+\, \left( \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \dfrac{\upsilon}{\omega} \right)^2 \Bigg]^{-1} \left( 3 - \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \right) re\, E_z in1\,(\mathbf{r},\omega) -$
$-\, \left[ \left( 3 - \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \right)^2 + \left( \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \dfrac{\upsilon}{\omega} \right)^2 \right]^{-1} \left( \dfrac{-\omega_p^2}{\omega^2 + \upsilon^2} \dfrac{\upsilon}{\omega} \right) \times$
$\times im\, E_z in1\,(\mathbf{r},\omega) \Bigg\}$.

**25**. $im\, \dfrac{E_z 1\,(\mathbf{r},\omega)}{E_0\,(\mathbf{r},\omega)} = \dfrac{3}{\varepsilon(\omega)} \Bigg\{ \Bigg[ \left( 3 - \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \right)^2 +$
$+\, \left( \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \dfrac{\upsilon}{\omega} \right)^2 \Bigg]^{-1} \left( 3 - \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \right) im\, E_z in1\,(\mathbf{r},\omega) +$
$+\, \left[ \left( 3 - \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \right)^2 + \left( \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \dfrac{\upsilon}{\omega} \right)^2 \right]^{-1} \times$
$\times\, \left( \dfrac{-\omega_p^2}{\omega^2 + \upsilon^2} \dfrac{\upsilon}{\omega} \right) re\, E_z in1\,(\mathbf{r},\omega) \Bigg\}$.

The relative energy density absorbed by the particle equals

**26**. $w(\mathbf{r},\omega)/|E_0|^2 = \dfrac{9\omega}{2}\, iim\, \mathrm{P}_z(\mathbf{r},\omega) \left[ \left( 3 - \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \right)^2 + \left( \dfrac{\omega_p^2}{\omega^2 + \upsilon^2} \dfrac{\upsilon}{\omega} \right)^2 \right]^{-1}$.


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ІНТЕГРАЛЬНІ РІВНЯННЯ
В ЗАГАЛЬНІЙ ТЕОРІЇ ПОГЛИНАННЯ І РОЗСІЯННЯ
СВІТЛА МЕТАЛЕВИМИ НАНОКЛАСТЕРАМИ

Р е з ю м е

У роботі проблема поглинання і розсіяння світла металевими нанокластерами зводиться до розв'язку сингулярного інтегрального рівняння усередині наночастинки відносно комплексного вектора напруженості електричного поля. В якості першого варіанту розв'язання інтегрального рівняння вибрано підхід, коли за початкове наближення прийняте дипольне наближення. Обчислювальний експеримент вказує на прийнятну узгодженість запропонованого наближення для електричного поля всередині сферичної наночастинки з відомими результатами для оптичних і емісійних властивостей металевих нанокластерів.