UDK 535.3

ABSORPTION OF ELECTROMAGNETIC RADIATION MULTILAYER GLOBULAR PARTICLES

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Definitely polarizability multi-balls. To construct solutions of the problem of electrostatics applied translational matrix. Examples of test calculations.

Polarizability, laminated balls translational matrix.

Determination of polarizability of small particles of arbitrary shape and structure is one of the most important stages in the study of the optical properties of individual particles or aggregates, and matrix-dispersed systems with inclusions [1,3,5,9]. It is known [1] that the applied field induces in him a particle is proportional to the dipole moment. For an ideal dipole potential, which is located at the origin, we have the expression:

$$\Phi = \frac{p\cos\theta}{4\pi\varepsilon_m r^2},$$

where p - the dipole moment, Debye; r - the distance to the observation point, m; θ -meridional angle in a spherical coordinate system degree ε_m - permittivity of the medium, dimensionless.

Dipole moment by definition is of

$$p = \varepsilon_m \alpha \mathbf{E}_0,$$

where $\mathbf{E}_0$ - the intensity of electrostatic field, V / m; α - polarizability, dimensionless.

For continuous homogeneous dielectric-Ball Φ_p waste the potential thatoccurs in a uniform field acting along the axis defined by the well-known formula:

$$\Phi_p = a^3 E_0 r\cos\theta \frac{\varepsilon_1 - \varepsilon_m}{\varepsilon_1 + 2\varepsilon_m}\frac{1}{r^3},$$

and the dipole moment of ball radius a is:

$$p = 4\pi\varepsilon_m a^3 \frac{\varepsilon_1 - \varepsilon_m}{\varepsilon_1 + 2\varepsilon_m} E_0.$$

Comparing the above equations gives the formula for calculating the polarizability balls α :

$$\alpha = 4\pi a^3 \frac{\varepsilon_1 - \varepsilon_m}{\varepsilon_1 + 2\varepsilon_m}.$$

Thus, the spherical particle polarizability of arbitrary structure is defined as the coefficient of the perturbation potential multiplied by 4π . Therefore the problem is to find an explicit expression for the potential in each case.

The purpose of research - development of methods of calculating the structural and polarizability uniform spherical particles.

Materials and methods research. This article presents one of the possible approaches to determining the polarizability spherical particles with an arbitrary number of layers with the use of so-called translational matrices [2,4,6-13]. Translational matrix can transfer boundary conditions on the layer in the layer, and to calculate the perturbed potential reservoir of particles they are very comfortable. In particular, the electrostatic approximation considered multilayer (concentric) balls.

Studies. Closed formulas for calculating the polarizability coated bullets (bullet-layer) is well known [1], but the problem for multi-ball is much more complicated due to the increasing number of equations in the boundary conditions. For balls of arbitrary law changes the dielectric function of the radial coordinate analytical solutions can be obtained only for particular cases. We suggest rather general algorithm for constructing numerical solution taking into account the singularity at the beginning of a spherical coordinate system.

Earlier [4,6] the problem was solved for the electrostatic layered ellipsoid in a uniform field. From the solution of this problem can be obtained solution of the problem for the world. But because of the importance of the case it makes sense to get a bullet solution to the problem for multi-balls directly. In addition, the synthesis of solutions to the ball permittivity layers having transversal anisotropy requires separate consideration.

Consider a spherical particle (Fig. 1), which consists of concentric n layers of complex dielectric permittivity ε_j and outer radii layers r_j ($j = 1, 2, \ldots, n$ - number of layers).The ball is in an external electric field E_0. The external radius of the layer suppose $r_n = a$.

Numbered layers starting from the center, ie the core bullets $j = 1$,and for the environment - $j = n+1$.Dielectric constant of the environment is denoted by $\varepsilon_{n+1} = \varepsilon_m$.

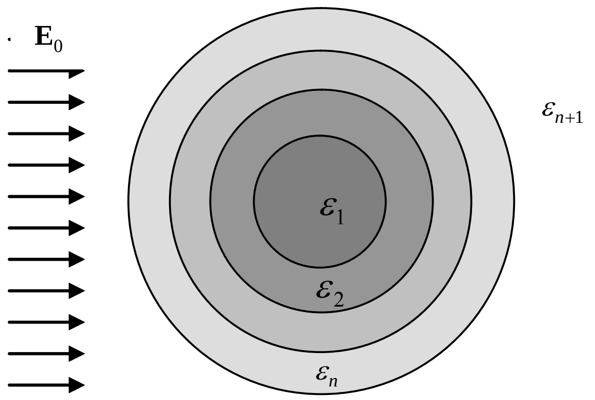

Figure 1. Multilayered ball in an electric field

The problem we solve in spherical coordinates r, θ, φ, associated with the center of the world.Electrostatic field potentials in layers denoted by $u_j = u_j(r, \theta, \varphi)$, potential of the external field – through $u_0 = u_0(r, \theta, \varphi)$, азбуренийпотенціал, якийвноситькуля, через $u_p = u_p(r, \theta, \varphi)$.

All potentials are the solutions of the Laplace equation

$$\frac{\partial}{\partial r}\left(r^2 \frac{\partial u_j}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial u_j}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 u_j}{\partial\phi^2} = 0, \quad (1)$$

and the layers within $r = r_j$, ($j = 1, 2, \ldots, n-1$)be rebutted if coupling

$$u_j = u_{j+1}, \ \varepsilon_j \frac{\partial u_j}{\partial r} = \varepsilon_{j+1}\frac{\partial u_{j+1}}{\partial r}. \quad (2)$$

На поверхні кулі, тобто у випадку, коли $j = n$, conditions will have ($u_{n+1} = u_0 + u_p$):

$$u_n = u_0 + u_p, \ \varepsilon_n \frac{\partial u_n}{\partial r} = \varepsilon_m\left(\frac{\partial u_0}{\partial r} + \frac{\partial u_p}{\partial r}\right). \quad (3)$$

By conditions (2) - (3) are limited solutions are added at the origin and at infinity, ie

$$u_1 < \infty \text{ at } r \to 0 \text{ i } u_p \to 0 \text{ at } r \to \infty . \qquad (4)$$

Solutions of equations for each layer and the expression for the perturbed potential is served in the form of expansions by spherical harmonics $Y_{lm}(\theta,\varphi)$ at $j = 2,3,...,n$

$$u_j(r,\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{m=l}\left[A_{lm}^{(j)}\left(\frac{r}{a}\right)^l + B_{lm}^{(j)}\left(\frac{a}{r}\right)^{l+1}\right]Y_{lm}(\theta,\varphi);$$

$$u_1(r,\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}^{(1)}\left(\frac{r}{a}\right)^l Y_{lm}(\theta,\varphi), u_p(r,\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} B_{lm}^{(n+1)}\left(\frac{a}{r}\right)^{l+1} Y_{lm}(\theta,\varphi), \qquad (5)$$

where, as usual, $Y_{lm}(\theta,\varphi) = \sum_{m=-l}^{l} P_l^{|m|}(\cos\theta)e^{im\varphi}$, and $P_l^{|m|}(\cos\theta)$ –attached Legendre functions.With such a choice of solutions to the conditions (4) are met, because the potential in the core bullets made $B_{lm}^{(1)} = 0$, and for the perturbed potential - $A_{lm}^{(n+1)} = 0$.

On the surface of a sphere, ie, $r = a$ external potential $u_0(r,\theta,\varphi)$ and its partial derivatives $\partial u_0(r,\theta,\varphi)/\partial r$ will set some functions $F(\theta,\varphi) = u_0(a,\theta,\varphi)$, $G(\theta,\varphi) = \partial u_0(a,\theta,\varphi)/\partial r$, which in very general terms can be expanded in a series in spherical harmonics

$$F(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-1}^{m=l} f_{lm}P_l^{|m|}(\cos\theta)e^{im\varphi}, G(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-1}^{m=l} g_{lm}P_l^{|m|}(\cos\theta)e^{im\varphi}, \qquad (6)$$

where the expansion coefficients are calculated by the formula

$$f_{lm} = \frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\int_0^{2\pi} e^{im\varphi}d\varphi\int_0^{\pi} F(\theta,\phi)P_l^{|m|}(\cos\theta)\sin\theta d\theta;$$

$$g_{lm} = \frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\int_0^{2\pi} e^{im\varphi}d\varphi\int_0^{\pi} G(\theta,\phi)P_l^{|m|}(\cos\theta)\sin\theta d\theta.$$

Substituting the expansions (5) - (6) in terms of interface for each pair of indices l,m resulting in $j = 1,2,...,n-1$ to systems of algebraic equations of the form:

$$A_{lm}^{(j)}\left(\frac{r_j}{a}\right)^l + B_{lm}^{(j)}\left(\frac{a}{r_j}\right)^{l+1} = A_{lm}^{(j+1)}\left(\frac{r_j}{a}\right)^l + B_{lm}^{(j+1)}\left(\frac{a}{r_j}\right)^{l+1};$$

$$A_{lm}^{(j)}\varepsilon_j l\left(\frac{r_j}{a}\right)^{l-1} + B_{lm}^{(j)}\varepsilon_j(l+1)\left(\frac{a}{r_j}\right)^{l+2} = A_{lm}^{(j+1)}\varepsilon_{j+1}l\left(\frac{r_j}{a}\right)^{l-1} + B_{lm}^{(j+1)}\varepsilon_{j+1}(l+1)\left(\frac{a}{r_j}\right)^{l+2}; \qquad (7)$$

and for $j = n$ system will have

$$A_{lm}^{(n)} + B_{lm}^{(n)} = f_{lm} + B_{lm}^{(n+1)},\ \varepsilon_n (A_{lm}^{(n)} + B_{lm}^{(n)}) = \varepsilon_m (g_{mn} - (l+1) B_{lm}^{(n+1)}). \qquad (8)$$

However, as indicated $A_{lm}^{(n+1)} = 0, B_{lm}^{(1)} = 0.$

To find the perturbed potential must have only the constant $B_{lm}^{(n+1)}$.Extra steel expelled from the system through translational matrices. As in [4,6,7] after some transformations we obtain an expression for the transition matrix from j до $(j+1)$ layer

$$T_j^{(l)} = \frac{1}{\Delta_j^{(l)}} \begin{bmatrix} t_{11,j}^{(l)} & t_{12,j}^{(l)} \\ t_{21,j}^{(l)} & t_{22,j}^{(l)} \end{bmatrix}, \qquad (9)$$

where $\Delta_j^{(l)} = -\varepsilon_{j+1}(2l+1)(a/r_j)^2$ uptoafactor ε_{j+1} Vronsky is the determinant corresponding solutions computed at the interface layer and the matrix elements are defined by the formulas:

$$t_{11,j}^{(l)} = -\varepsilon_{j+1}(l+1)\left(\frac{a}{r_j}\right)^2 - \varepsilon_j l \left(\frac{a}{r_j}\right)^2;$$

$$t_{12,j}^{(l)} = -\varepsilon_{j+1}(l+1)\left(\frac{a}{r_j}\right)^{2l+3} - \varepsilon_j (l+1) \left(\frac{a}{r_j}\right)^{2l+3};$$

$$t_{21,j}^{(l)} = -\varepsilon_{j+1} l \left(\frac{r_j}{a}\right)^{2l-1} + \varepsilon_j l \left(\frac{r_j}{a}\right)^{2l-1};$$

$$t_{22,j}^{(l)} = -\varepsilon_{j+1} l \left(\frac{r_j}{a}\right)^2 + \varepsilon_j (l+1) \left(\frac{r_j}{a}\right)^2.$$

Translational matrix determined by the product of matrices of transition layers

$$T_l(r_1, r_n) = \begin{bmatrix} t_{11}^{(l)} & t_{12}^{(l)} \\ t_{21}^{(l)} & t_{22}^{(l)} \end{bmatrix} = \prod_{j=1}^{n-1} T_{n-j}^{(l)}. \qquad (10)$$

With the use of translation matrix will have

$$\begin{bmatrix} A_{lm}^{(n)} \\ B_{lm}^{(n)} \end{bmatrix} = \begin{bmatrix} t_{11}^{(l)} & t_{12}^{(l)} \\ t_{21}^{(l)} & t_{22}^{(l)} \end{bmatrix} \cdot \begin{bmatrix} A_{lm}^{(l)} \\ 0 \end{bmatrix} = \begin{bmatrix} t_{11}^{(l)} & t_{12}^{(l)} \\ t_{21}^{(l)} & A_{lm}^{(l)} \end{bmatrix},$$

potential and then the last layer will be determined by the formula

$$U_n^{(l)} = t_{11}^{(l)} A_{lm}^{(l)} \left(\frac{r}{a}\right)^l + t_{21}^{(l)} A_{lm}^{(l)} \left(\frac{a}{r}\right)^{l+1}, \quad (11)$$

and the boundary condition (2) takes the form:

$$(t_{11}^{(l)} + t_{21}^{(l)}) A_{lm}^{(l)} - B_{lm}^{(n+1)} = f_{lm}; \varepsilon_n \left[t_{11}^{(l)} l - t_{21}^{(l)} (l+1) \right] A_{lm}^{(l)} + \varepsilon_m (l+1) B_{lm}^{(n+1)} = \varepsilon_m a g_{lm}. \quad (12)$$

After finding the coefficients for the perturbed potential we obtain the expression:

$$u_p(r,\theta,\varphi) = \sum_{l=1}^{\infty} \frac{\varepsilon_m a g_{lm} \left[t_{11}^{(l)} + t_{21}^{(l)} \right] - \varepsilon_n f_{lm} \left[t_{11}^{(l)} l - t_{21}^{(l)} (l+1) \right]}{\varepsilon_m (l+1) \left[t_{11}^{(l)} + t_{21}^{(l)} \right] - \varepsilon_n \left[t_{11}^{(l)} l - t_{21}^{(l)} (l+1) \right]} \left(\frac{a}{r}\right)^{l+1} Y_l(\theta,\varphi). \quad (13)$$

Let us consider a homogeneous field with potential $u_0 = -E_0 z = -E_0 \cos\theta,$ acting along the axis z . In this case, the expansion potential of the external field, only one member $(\cos\theta = P_1(\cos\theta), l = 1, m = 0),$ a $f_{10} = -E_0 a, g_{10} = -E_0 a$. Accordingly, for the case in indexes $l = 1, m = 0$ All other potential expansion coefficients rotate to zero. The expression for the perturbed potential takes the form (index "lm" drop, and also denote $t_{11}^{(1)} = t_{11}, t_{21}^{(1)} = t_{21}$):

$$u_p(r,\theta,\varphi) = \frac{\varepsilon_n \left[t_{11} - 2t_{21} \right] - \varepsilon_m \left[t_{11} + t_{21} \right]}{2\varepsilon_m \left[t_{11} + t_{21} \right] - \varepsilon_n \left[t_{11} - 2t_{21} \right]} \left(\frac{a}{r}\right)^3 E_0 r \cos\theta. \quad (14)$$

Hence we find an expression for calculating the polarizability layered balls

$$\alpha = 4\pi a^3 \frac{\varepsilon_n [t_{11} + 2t_{21}] - \varepsilon_m [t_{11} + t_{21}]}{2\varepsilon_m [t_{11} + t_{21}] + \varepsilon_n [t_{11} - 2t_{21}]}. \quad (15)$$

For a solid ball ($n = 1$)should take $t_{11} = 1$, $t_{21} = 0$ and then obtain the expression above.For balls in the shell ($n = 2$) After some transformations we have

$$\alpha = 4\pi a^3 \frac{(\varepsilon_2 - \varepsilon_m)(\varepsilon_1 + 2\varepsilon_m) r_2^3 + (\varepsilon_1 - \varepsilon_2)(\varepsilon_m + 2\varepsilon_2) r_1^3}{(\varepsilon_2 + 2\varepsilon_m)(\varepsilon_1 + 2\varepsilon_m) r_2^3 + 2(\varepsilon_2 - \varepsilon_m)(\varepsilon_1 - \varepsilon_2) r_1^3}. \quad (16)$$

This expression coincides with the formula given in [1].

Here are some results of numerical calculations. Consider a single bimetallic spherical particle consisting of a silver core and gold shell. To describe the dielectric constant of silver and gold using Drude model:

$$\varepsilon = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + i\gamma_p)}, \quad (17)$$

where ω_p – plasma frequency for solid material; γ_p – frequency absorption. The calculations assumed that for silver $\varepsilon_\infty = 4,5$, $\gamma_p = 0,24 \cdot 10^{14}\ c^{-1}$, and for gold $\varepsilon_\infty = 10,0$, $\gamma_p = 0,34 \cdot 10^{14}\ c^{-1}$ (i – imaginary unit) [1,5,9]. Figure 2 shows the spectral dependence of the imaginary part of the dimensionless polarizability $\alpha^* = \alpha/(4\pi a^3)$ spherical particles of silver core and a gold shell for some values of volumetric filling $f = (r_1/r_2)^3$ (outer radius of the particle $a = r_2$ remained unchanged). For environmental values taken permittivity $\varepsilon_m = 1,7$ .This spectral dependence of the imaginary part of the effective dielectric constant is calculated by the formula Maxwell-Garnett:

$$\frac{\tilde{\varepsilon} - \varepsilon_m}{\tilde{\varepsilon} + 2\varepsilon_m} = f\alpha / a^3;\ \tilde{\varepsilon} = \frac{1 + 2f\alpha^*}{1 - f\alpha^*}\varepsilon_m;\ \alpha^* = \alpha / a^3 \qquad (18)$$

when substituted for it polarizability values found for the bimetallic spherical particles (silver core gold shell).

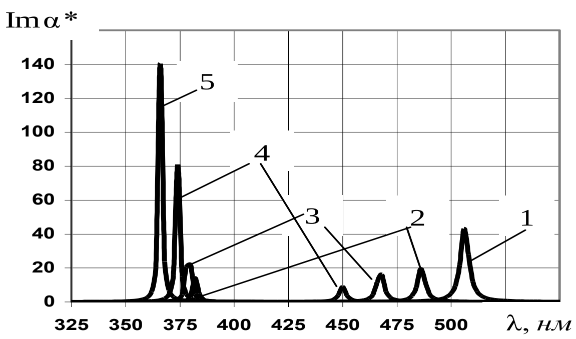

Fig.2. The spectral dependence of the imaginary part of the dimensionless polarizability $\alpha^* = \alpha/(4\pi a^3)$ spherical particles of silver core and a gold shell for different values of volumetric filling $\nu = (r_1/r_2)^3$:
$1 - \nu = 0$ **(<u>solid gold particle</u>)**; $2 - \nu = 0,25$; $3 - \nu = 0,5$; $4 - \nu = 0,75$;
$5 - \nu = 1$ **(<u>solid silver particle</u>)**

From the graph (Fig. 2) that the presence of membranes leads to the splitting values wavelength surface plasmons. Thus, in the range of wavelengths between λ_{Ar}=366 нм (wavelength surface plasmons solid silver particles) i λ_{Au}=506 нм (wavelength surface plasmons solid gold particles) there are two peaks located between these boundary values. In this case, the absolute values of the maxima significantly reduced. Since the absorption in the electrostatic approximation proprotsiyne $\mathrm{Im}\,\alpha$, a maximum absorption at a particular particle will repeat dependencies, shown in Figure 2.

Conclusions

The paper presents and practically implemented method of calculating the polarizability structurally inhomogeneous spherical particles. Examples of test calculations confirm its high efficiency. This opens up the possibility of theoretical studies (numerical experiments) to determine how the characteristics of the interaction of electromagnetic radiation with individual particles or ensembles, and dielectric function matrix-dispersed systems with inclusions. This fact is particularly significant in the study of biological objects (cells, bacteria) or the optical dielectric spectroscopy models which may be structurally heterogeneous world with regard to the dielectric anisotropy**.**

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