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ONE-ELECTRON OPTICAL PROPERTIES OF ELLIPSOID METAL NANOSHELLS

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We investigate optical properties of nanoshells (small composite clusters composed of a dielectric core and a metal shell; contribution of the shell dominates in the optical properties of the whole cluster) in the frequency range far from plasmon resonance. In particular, nanoshells with the shape of a stretched rotation ellipsoid are considered. For such shell-type particle the electron wavefunction, the electron energy, the wavenumber spectrum, and the matrix elements of corresponding optical transitions were found. Using these quantities, the classical optical conductivity of such shells (the quantum effects are not considered) and the quantum optical conductivity (relevant addendums for the classical conductivity that are caused by the quantum effects like the electron spectrum discreteness) were found. Oscillating nature of the dependence of these addendums on the incident light frequency is established.
Keywords: nanoshells, optical conductivity, small clusters, spectrum quantization.

INTRODUCTION

Nanotechnologies that use metal nanoparticles become popular recently. As a further development of these technologies, new technologies that use so-called nanoshells [1-4] have become possible after this type of nanoparticles have been obtained. A nanoshell is a composite nanoparticle that consists of a dielectric core and a thin metal shell.

Technical applications of metal nanoparticles in common are mostly based on their unique optical properties. For instance, these particles can effectively absorb light on a given wavelength. Composite nanoparticles of this type represent a special practical interest because they allow widening of the operating range of work wavelengths in comparison to traditional solid metal nanoparticles. Also, nanoshells turn out to be rather promising for a number of technological applications (especially in medicine and biology, see, for example, [4]) because their optical properties can be regulated more flexibly than in traditional systems. This flexibility appears because the internal and the external radii of the metal shell (that dominates in the optical response of the whole particle) can be changed independently.

It should be mentioned that such shell-type particles have become of particular interest quite recently. They have been studied intensively both theoretically [5-11] (using classical and quantum approach) and experimentally [3,5,12,13]. However, their optical properties have been studied near plasmon resonance for the most part. The articles that investigate contribution of individual transitions into the light absorption (the infrared spectrum mostly; experimental studies of thin metal films and small metal particles in the infrared spectrum are represented, for example, by [14]) usually consider one of two

opposite limiting cases. The first case corresponds to the situation when distances between electron quantum levels are small as compared to the light quantum energy, and the sum over electron states is replaced with an integral. The second limiting case corresponds to the situation when distances between energy levels are of the same order with the light quantum energy, and only two or three levels are to be taken into account. However, a typical shell has much more of actual electron energy levels. On the other hand, in this study we demonstrate that the quantum effects related to the electron energy quantization within the shells cannot be neglected. The reason is that the energy states for a thin shell are quasi-one-dimensional, so the distance between them becomes greater as the shell becomes thinner. Related theoretical studies for thin metal films [15] show that such effects make an essential contribution to the film optical properties in the infrared spectrum that we consider.

Note that an oscillating dependence of electrical and optical properties of a metal nanowire on its thickness, similar to the dependence obtained in the current article, was observed experimentally in [16]. Such a dependence for a solid metal nanowire indicates that similar quantum effects in shell-type systems are much stronger. Theoretical studies of thin metal films [15] also show this quantum size effect.

Furthermore, studies on the subject mainly focused on the magnetic absorption (see, e.g., [17-19]), which represents only one component of the total light absorption (this component is related to the magnetic vector of electromagnetic wave). However, in small metal particles the prevalence of the magnetic absorption or the electric absorption is determined by the particle size, particle shape, and the electromagnetic wave frequency [20].

It is important to note that optical properties of small metal particles depend strongly on their shape (see, for example, [20]). This makes necessary separate studies of nanoshells of different shapes, too. Most theoretical studies focused on the cases of spherical and cylindrical shell (see, e.g., [21]). This makes an investigation of the single-electron optical properties of an ellipsoid nanoshell with consideration of above-mentioned quantum effects especially important.

In this work, we perform a theoretical study of the optical properties of ellipsoid nanoshells. We obtain the wavefunctions, the wave number spectrum and the energy spectrum for an electron in a nanoshell with the shape of a stretched rotation ellipsoid. Using them, we obtain the matrix elements of the optical transitions (electric absorption) in single-electron approximation for frequencies far from plasmon resonance and, finally, the optical conductivity of above-mentioned shells.

1. SETTING OF THE PROBLEM. GENERAL EXPRESSION FOR THE OPTICAL CONDUCTIVITY OF A SMALL METAL PARTICLE

Let us consider a nanoshell with the shape of a rotation ellipsoid and an electromagnetic wave that falls on it. We consider single-electron light absorption in such particle. As we mentioned before, the metal shell dominates in the optical response of the whole composite nanoshell. So, we can model our composite nanoshell with just an ellipsoid metal shell.

Size of the particle is considered small comparing to the incident light wavelength, so the field of the electromagnetic wave can be considered uniform on the distances of the order of the particle size. Also, the nanoshell is considered thin enough so the local field inside the shell is approximately uniform (see the chapter "Local field in an ellipsoid nanoshell"). (Local fields in spherical nanoshells were studied theoretically, for instance, in [3] with references on [22-24].)

Considering the symmetry of our system, it is convenient to use the spheroidal coordinates (ξ,η,φ) with the constant parameter a (see the Appendix). Let's consider a shell limited by two rotation ellipsoids. The ellipsoids are described by the equations $\xi=\xi_1$, $\xi=\xi_2$. Their semiaxes have the lengths

$$R_{\parallel}^{(1)} = a\xi_1, \quad R_{\perp}^{(1)} = a\sqrt{\xi_1^2 - 1}, \tag{1}$$

for the internal ellipsoid and

$$R_{\parallel}^{(2)} = a\xi_2, \quad R_{\perp}^{(2)} = a\sqrt{\xi_2^2 - 1} \tag{2}$$

for the external one. The parameter a of the coordinate system can be considered as a characteristic size of the shell.

Our task is to obtain the electron wavefunctions in such shells, the electron energy spectrum, the matrix elements of the optical transitions and finally, using these quantities, to find the optical conductivity (an electric component) of such ellipsoid shell. We will use the following expression (see, for example, [25, 26]) for optical conductivity components for a small metal particle in general case

$$\sigma_j = \frac{\pi e^2 \omega}{V_s} \sum_{i,f} \left| < i \mid x_j \mid f > \right|^2 f_e(E_i)(1 - f_e(E_f))\delta\left(E_f - E_i - \hbar\omega\right), \tag{3}$$

here the optical conductivity tensor $\hat{\sigma}$ written in the diagonal form. The expression is obtained for the case of a spatially uniform electrical field inside the particle.

In our case, it is convenient to introduce two components of the absorbed energy and, consequently, two components of the optical conductivity. If we direct x_3 axis along the rotation axis of the shell ellipsoid, absorbed energy components that correspond to x_1 and x_2 axes are equal because of the system symmetry. Also, because of the system symmetry, the matrix elements that correspond to x_1 and x_2 axes are equal, too. So, we can introduce orthogonal ($\sigma_\perp=\sigma_1=\sigma_2$) and parallel ($\sigma_\parallel=\sigma_3$) optical conductivity components.

In this work, we perform theoretical study of optical properties of ellipsoid nanoshells. We obtain the wavefunctions, the wave number spectrum and the energy spectrum for an electron in a nanoshell with the shape of a stretched rotation ellipsoid. Using them, we obtain the matrix elements of the optical transitions (electric absorption) in single-electron approximation for frequencies far from plasmon resonance and, finally, the optical conductivity of above-mentioned shells. Note that optical conductivity of such shell becomes an essentially tensor quantity, and its optical properties become anisotropic.

2. LOCAL FIELD IN AN ELLIPSOID SHELL

As we mentioned in the previous chapter, the expression (3) is obtained for the case of spatially uniform local field inside the particle – in our case, inside the ellipsoid shell.

So, in order to use this expression, we have to find an expression for this local field and to show that it can be considered approximately uniform.

We consider an ellipsoid shell described in the previous chapter. (The rotation axis of the ellipsoid coincides with the Oz axis in the corresponding Cartesian coordinates.) The shell is placed in an external electric field $\boldsymbol{\mathcal{E}}_0$ that can be described with a potential V_0. (The field $\boldsymbol{\mathcal{E}}_0$ can be considered uniform because the shell size is much smaller than an incident light wavelength. Time-dependent oscillating factor $\cos(\omega t)$ doesn't influence our results and can be omitted.)

According to the superposition principle considering two orientations of $\boldsymbol{\mathcal{E}}_0$ – along Oz axis, so

$$V_0 = V_{0X} = -\boldsymbol{\mathcal{E}}_0 x = -\boldsymbol{\mathcal{E}}_0 a\sqrt{\left(\xi^2-1\right)\left(1-\eta^2\right)}\cos\varphi, \tag{4}$$

and along one of two axes Ox or Oy, say Ox, so

$$V_0 = V_{0Z} = -\boldsymbol{\mathcal{E}}_0 z = -\boldsymbol{\mathcal{E}}_0 a\xi\eta. \tag{5}$$

is enough for a description of an arbitrary oriented field. Using reasons analogous to given in [27] we can seek the potential in the form

$$V = V_0 + V_0 F(\xi), \quad \xi \in (\xi_2, +\infty), \tag{6}$$

where $F(\xi)$ is a certain admissible function of ξ. After solving the Laplace equation in the spheroidal coordinates for a potential given by (6) and using sewing conditions on the shell boundary, we obtain the following expression for a potential inside the shell:

$$V = AV_0 + CV_0 \cdot Df(\xi), \quad \xi \in [\xi_1, \xi_2), \tag{7}$$

here the function $f(\xi)$

$$f(\xi) = f_{\perp}(\xi) = \frac{\xi}{\xi^2-1} + \frac{1}{2}\ln\frac{\xi-1}{\xi+1} \tag{8}$$

for an orthogonal (to the ellipsoid rotation axis) orientation of the electric vector, and

$$f(\xi) = f_{\parallel}(\xi) = \frac{1}{\xi} + \frac{1}{2}\ln\frac{\xi-1}{\xi+1} \tag{9}$$

for a parallel orientation. The coefficient A

$$A = \frac{\dfrac{\varepsilon}{\varepsilon-1}\dfrac{1}{\xi_1\left(\xi_1^2-1\right)} - f(\xi_1)}{f(\xi_2)\xi_2\left(\xi_2^2-1\right)\left((\varepsilon-1)\left(f(\xi_2)-f(\xi_1)\right)+\dfrac{\varepsilon}{\xi_1\left(\xi_1^2-1\right)}\right)-(\varepsilon-1)f(\xi_2)-f(\xi_1)+\dfrac{\varepsilon}{\varepsilon-1}\dfrac{1}{\xi_1\left(\xi_1^2-1\right)}}, \tag{10}$$

and the product of the coefficients C and D

$$CD = \frac{1}{f(\xi_2)\xi_2\left(\xi_2^2-1\right)\left((\varepsilon-1)\left(f(\xi_2)-f(\xi_1)\right)+\dfrac{\varepsilon}{\xi_1\left(\xi_1^2-1\right)}\right)-(\varepsilon-1)f(\xi_2)-f(\xi_1)+\dfrac{\varepsilon}{\varepsilon-1}\dfrac{1}{\xi_1\left(\xi_1^2-1\right)}} \tag{11}$$

for both orientations of the incident light electric vector. So, an electric field inside the shell for the orthogonal orientation can be written in the form

$$\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}_o\left(A + CDf_{\perp}(\xi)\right) - \boldsymbol{\mathcal{E}}_o \boldsymbol{e}_{\xi} \frac{CD}{\xi^2 - 1}\sqrt{\frac{1-\eta^2}{\xi^2 - \eta^2}}\cos\varphi, \tag{12}$$

here $\vec{e}_{\xi}$ is a unit vector for the coordinate ξ, and for the parallel orientation

$$\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{E}}_o\left(A + CDf_{\parallel}(\xi)\right) - \boldsymbol{\mathcal{E}}_o \boldsymbol{e}_{\xi} \frac{CD\eta}{\xi\sqrt{\left(\xi^2 - 1\right)\left(\xi^2 - \eta^2\right)}}. \tag{13}$$

After performing a limiting process to a solid metal ellipsoidal particle and an spherical metal shell the expressions we obtain (for the potential and the field, correspondingly) transform into known expressions (from [27] and [3], correspondingly), thus validating the results we obtained.

Analysis of the expressions (12) and (13) shows that the field inside a thin (ξ_2-ξ_1<<ξ_2) ellipsoid shell can be considered approximately uniform if the following relation fulfils:

$$\left|\frac{\varepsilon - 1}{\varepsilon}\xi_1\left(\xi_1^2 - 1\right)\left(f(\xi_1) - f(\xi_2)\right)\right| << 1. \tag{14}$$

This relation has similar form for the both orientations of the incident light electric field, but we should note that the function $f(\xi)$ that enters (14) is given by (9) for the longitudinal field orientation and by (8) for the orthogonal orientation.

So, we can conclude that if the relation (14) fulfils, a field in an ellipsoidal nanoshell can be considered uniform with enough precision. This allows us to use (3) for a calculation of an optical conductivity of the shell.

3. THE ELECTRON WAVEFUNCTIONS AND THE ENERGY SPECTRUM

To calculate the optical conductivity of the shell we consider, we need, first, to obtain the wavefunctions and the energy spectrum for an electron in the shell, and second, use them to find the matrix elements that enter into (3). This chapter is dedicated to the wavefunctions and the energy spectrum calculations.

Let us consider the shell as an orthogonal potential well for an electron (by the coordinate ξ). The potential energy $V_e(\xi)$ of an electron in such shell can be written

$$V_e = V_e(\xi) = \begin{cases} 0, & \xi \in (\xi_1, \xi_2] \\ V_{0e}, & \xi \notin (\xi_1, \xi_2] \end{cases}, \tag{15}$$

where V_{0e} is the potential well depth. Here the dielectric inside and outside the shell is considered similar (this simplification doesn't influence our result as long as we can use the infinite potential well model).

The eigenfunctions of an electron in such potential well can be written in the form

$$\psi(\xi, \eta, \varphi) = R(\xi)S(\eta)\frac{\exp(im\varphi)}{\sqrt{2\pi}}, \tag{16}$$

the functions $R(\xi)$ and $S(\eta)$ are the radial and the angular wavefunction, correspondingly. After substituting a function of such type into the Schrödinger equation and variables separation we obtain for $R(\xi)$ and $S(\eta)$ inside the shell ($\xi\in[\xi_1,\xi_2]$)

$$\frac{d}{d\xi}\left(\left(\xi^2-1\right)\frac{dR}{d\xi}\right)+\left(-\lambda+(ka)^2\left(\xi^2-1\right)-\frac{m^2}{\xi^2-1}\right)R=0, \tag{17}$$

$$\frac{d}{d\eta}\left(\left(1-\eta^2\right)\frac{dS}{d\eta}\right)+\left(\lambda+(ka)^2\left(1-\eta^2\right)-\frac{m^2}{1-\eta^2}\right)S=0 \tag{18}$$

here k is the electron wave number, λ is the constant of the variables separation. For an electron outside the shell, we must replace k^2 with $k^2+\frac{2mV_{0e}}{\hbar^2}$ in these equations.

To solve the equations (17) and (18), we apply the theory of a spheroidal functions, see, for instance, [28]. First, we note that for typical nanoshells the condition $ka>>1$ fulfils. (If we take, say, $k=k_F=1{,}15\cdot10^{10}\ m^{-1}$ – the Fermi wave number of gold and $a=20$ *nm* – the typical nanoshell size, we obtain for the product $ka=230>>1$.) This, according to [28], allows us to expand the variables separation constant λ in series:

$$\lambda=\lambda_{lm}=-(ka)^2+ka(2l-2m+1)-\frac{1}{8}\left((2l-2m+1)^2+5-8m^2\right)+O\left(\frac{1}{ka}\right), \tag{19}$$

here l is an orbital quantum number. This representation allows us to solve (17) in the quasiclassical approximation. After applying certain transformations that we omit, the solution of (17) can be written in the form

$$R(\xi)\sim\frac{\exp\left(\pm i\int p_1(\xi)d\xi\right)}{\sqrt{\left(\xi^2-1\right)p_1(\xi)}} \tag{20}$$

with the function $p_1(\xi)$

$$p_1(\xi)=\sqrt{\frac{\xi^2}{\xi^2-1}(ka)^2-\frac{2l-2m+1}{\xi^2-1}ka-\frac{m^2}{\left(\xi^2-1\right)^2}}\approx\frac{\xi}{\sqrt{\xi^2-1}}ka. \tag{21}$$

After taking the integral using the quasiclassical approximation, we can rewrite the radial wavefunction in the form

$$R(\xi)\sim\frac{\sin\left(ka\sqrt{\xi^2-1}+\alpha\right)}{\sqrt{\xi\sqrt{\xi^2-1}}}, \tag{22}$$

where α is a certain initial phase.

The procedure of finding the angular wavefunction $S(\eta)$ is more complex. After applying the results from [28] for the quasi-classical approximation for spheroidal functions, the solution of (18) inside the shell can be written in the form

$$S(\eta)\sim\frac{1}{\sqrt{\left(1-\eta^2\right)p_2(\eta)}}\cos\left(\int_{-\eta_0}^{\eta}p_2(\eta)d\eta-\frac{\pi}{4}\right). \tag{23}$$

Here, in accordance with [28], we suppose that an electron in the shell is placed in the potential well $[-\eta_0, \eta_0]$; the function $p_2(\eta)$ can be written in the form

$$p_2^2(\eta) \approx (ka)^2\left(-\frac{\eta^2}{1-\eta^2}\right)+\frac{ka(2l-2m+1)}{1-\eta^2}-\frac{1}{8(1-\eta^2)}\left((2l-2m+1)^2+5\right)-\frac{m^2\eta^2}{(1-\eta^2)^2}, \tag{24}$$

and η_0 is the additional, lesser than 1 root of the equation $p_2(\eta)=0$:

$$\eta_0 = \sqrt{1+\frac{\lambda-\sqrt{\lambda^2+4m^2(ka)^2}}{2(ka)^2}}. \tag{25}$$

Taking into consideration the fact that outside the potential well the electron wavefunction decays exponentially and the fact that we can consider $\eta_0<<1$ (this relation, according to [28], implies from the relation $ka>>1$), we can, after certain transformations, rewrite $S(\eta)$ in the form

$$S(\tilde{\eta}) \sim \frac{1}{\sqrt[4]{1-\tilde{\eta}^2}}\cos\left(\left(q+\frac{1}{2}\right)\left(\tilde{\eta}\sqrt{1-\tilde{\eta}^2}+\arcsin\tilde{\eta}+\frac{\pi}{2}\right)-\frac{\pi}{4}\right), \tag{26}$$

where $\tilde{\eta}=\frac{\eta}{\eta_0}$, $q = l - m$.

So, we can write a quasi-classical electron wavefunction in the shell as follows:

$$\psi(\xi,\eta,\varphi) = \frac{A}{\sqrt[4]{\eta_0^2-\eta^2}}\cos\left(\left(\frac{\eta}{\eta_0}\sqrt{1-\left(\frac{\eta}{\eta_0}\right)^2}+\arcsin\frac{\eta}{\eta_0}+\frac{\pi}{2}\right)\left(q+\frac{1}{2}\right)-\frac{\pi}{4}\right)\times$$
$$\times\frac{\sin\left(ka\sqrt{\xi^2-1}+\alpha\right)}{\sqrt{\xi\sqrt{\xi^2-1}}}\frac{\exp(im\varphi)}{\sqrt{2\pi}} \tag{27}$$

where A is a normalization constant. Outside the shell ($\eta \notin [-\eta_0, \eta_0]$) we can consider $\psi=0$. The normalization integral for the constant A is

$$A^2\int_0^{2\pi}\frac{d\varphi}{2\pi}\int_{\xi_1}^{\xi_2}d\xi\frac{\sin^2\left(ka\sqrt{\xi^2-1}+\alpha\right)}{\xi\sqrt{\xi^2-1}}\int_{-1+\delta}^{1-\delta}\frac{\eta_0 d\tilde{\eta}}{\eta_0\sqrt{1-\tilde{\eta}^2}}\times$$
$$\times\cos^2\left(\left(\tilde{\eta}\sqrt{1-\tilde{\eta}^2}+\arcsin\tilde{\eta}+\frac{\pi}{2}\right)\left(q+\frac{1}{2}\right)-\frac{\pi}{4}\right)a^3\left(\xi^2-\tilde{\eta}^2\eta_0^2\right)=1, \tag{28}$$

where $a^3\left(\xi^2-\tilde{\eta}^2\eta_0^2\right)d\xi d\eta d\varphi = a^3\left(\xi^2-\eta^2\right)d\xi d\eta d\varphi$ is a small volume element in the spheroidal coordinates (see the Appendix). After rather complex transformations, the following form of the constant A implies from (28):

$$A = 2\sqrt{\frac{1}{\pi a^3\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)}}. \tag{29}$$

So, finally we can rewrite a quasi-classical electron wavefunction in the shell as follows:

$$\psi(\xi,\eta,\varphi) = \sqrt{\frac{2}{\pi}}\frac{\exp(im\varphi)}{\sqrt{2\pi}}\sqrt{\frac{2}{a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)}}\frac{\sin\left(ka\sqrt{\xi^2-1}+\alpha\right)}{a\sqrt{\xi\sqrt{\xi^2-1}}}\times$$
$$\times\frac{1}{\sqrt[4]{\eta_0^2-\eta^2}}\cos\left(\left(\frac{\eta}{\eta_0}\sqrt{1-\left(\frac{\eta}{\eta_0}\right)^2}+\arcsin\frac{\eta}{\eta_0}+\frac{\pi}{2}\right)\left(q+\frac{1}{2}\right)-\frac{\pi}{4}\right) \tag{30}$$

Now we have to find the wave number spectrum. First, we note that the interval $[\xi_1,\xi_2]$ should contain an integer number of the half-waves for the function $R(\xi)$:

$$ka\sqrt{\xi_2^2-1}-ka\sqrt{\xi_1^2-1}=\pi n. \tag{31}$$

So, we can write the wavenumber spectrum

$$ka=\frac{\pi n}{\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}} \tag{32}$$

and the corresponding electron energy spectrum

$$E=\frac{\hbar^2}{2m_e}\frac{\pi^2 n^2}{a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)}. \tag{33}$$

Note that the electron spectrum (32), (33) for the considered shell is quasi-one-dimensional, similar to the electron spectrum in an infinite rectangular potential well. This fact takes place because the shell we consider is thin.

In order to obtain the initial phase α, we use the fact that in our model the electron wavefunction is equal to zero on the extremities of the interval $[\xi_1,\xi_2]$. This condition can be written in the form

$$\begin{cases} ka\sqrt{\xi_1^2-1}+\alpha=0 \\ ka\sqrt{\xi_2^2-1}+\alpha=\pi n \end{cases}. \tag{34}$$

It is not necessary to solve this system because further we will only need α in the combinations that enter (34).

So, we obtained the wavefunctions and the wavenumber spectrum for an electron in an ellipsoid metal shell. As we can see, the expression we obtained for the radial wavefunction $R(\xi)$ tends to the known expression for a radial wavefunction of an electron in a spherical nanoshell [21] when our shell tends to spherical ($\xi\to\infty$). This validates the results we obtained.

4. THE MATRIX ELEMENTS OF THE OPTICAL TRANSITIONS. THE NANOSHELL OPTICAL CONDUCTIVITY IN THE FROM OF A SUM OVER ELECTRON STATES

Now, having the electron wavefunctions and the energy spectrum, we can calculate the matrix elements of the optical transitions that enter into (3). From the system symmetry the equality $<i|x_2|f>=<i|x_1|f>$ implies, so we have to calculate only $<i|x_3|f>$ and, for instance, $<i|x_1|f>$. For the matrix element $<i|x_1|f>$ we have

$$<i\,|\,x_1\,|\,f>\approx\frac{2a}{\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}}\,\frac{\delta_{m,m'+1}+\delta_{m,m'-1}}{2}\int\limits_{\xi_1}^{\xi_2}\sin\left(ka\sqrt{\xi^2-1}+\alpha\right)\frac{\sin\left(k'a\sqrt{\xi^2-1}+\alpha'\right)}{\xi\sqrt{\xi^2-1}}\times$$

$$\times\xi^2\sqrt{\xi^2-1}\cdot d\xi\cdot\frac{2}{\pi}\int\limits_{-\min(\eta_0,\eta_0')}^{\min(\eta_0,\eta_0')}\cos\left(\left(q+\frac{1}{2}\right)\left(\frac{\eta}{\eta_0}\sqrt{1-\left(\frac{\eta}{\eta_0}\right)^2}+\arcsin\frac{\eta}{\eta_0}+\frac{\pi}{2}\right)-\frac{\pi}{4}\right)\times \qquad (35)$$

$$\times\cos\left(\left(q'+\frac{1}{2}\right)\left(\frac{\eta}{\eta_0'}\sqrt{1-\left(\frac{\eta}{\eta_0'}\right)^2}+\arcsin\frac{\eta}{\eta_0'}+\frac{\pi}{2}\right)-\frac{\pi}{4}\right)\frac{d\eta}{\sqrt[4]{\left(\eta_0^2-\eta^2\right)\left((\eta_0')^2-\eta^2\right)}}$$

here we used the expression (27) for an electron wavefunction, the relation $|\eta|<\eta_0<<1$ (see the previous chapter) and the expression (A5) from the Appendix for a small volume element in the spheroidal coordinates. From here on non-primed quantities relate to the electron initial state, primed ones – to the final state.

Now we note that in this sum we can leave the addends with $q=q'$ only. Addends with $q\neq q'$ give the functions that quickly oscillate by η, so they will be negligibly small after the integration. Also, in typical cases the photon energy $\hbar\omega$ (for instance, 0,1 eV for a CO_2 laser) is much less than the Fermi energy of the shell metal E_F (3-5 eV for typical metals). So, we can introduce the quantity $\nu\equiv\frac{\hbar\omega}{E_F}$ and consider that it satisfies the relation $\nu<<1$. Using the fact that an electron distribution function for the shell metal is close to the Heavyside function, we, after rather complex transformations, can rewrite (35) in the form

$$<i\,|\,x_1\,|\,f>=\frac{\hbar^2}{m_e^2\omega^2 a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)}\left(1-(-1)^{n+n'}\right)\delta_{m,m'}\delta_{l,l'}\cdot kk'. \qquad (36)$$

The matrix element $<i|x_3|f>$ requires more complex transformations. The starting expression

$$< i \mid x_3 \mid f >= \frac{2a}{\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}}\delta_{m,m'}\int_{\xi_1}^{\xi_2}\xi^3 d\xi \frac{\sin\left(ka\sqrt{\xi^2-1}+\alpha\right)\sin\left(k'a\sqrt{\xi^2-1}+\alpha'\right)}{\xi\sqrt{\xi^2-1}}\times$$

$$\times\frac{2}{\pi}\int_{-\min(\eta_0,\eta_0')}^{\min(\eta_0,\eta_0')}\frac{\cos\left(\left(q+\frac{1}{2}\right)\left(\frac{\eta}{\eta_0}\sqrt{1-\left(\frac{\eta}{\eta_0}\right)^2}+\arcsin\frac{\eta}{\eta_0}+\frac{\pi}{2}\right)-\frac{\pi}{4}\right)}{\sqrt[4]{\left(\eta_0^2-\eta^2\right)\left((\eta_0')^2-\eta^2\right)}}\times$$

$$\times\cos\left(\left(q'+\frac{1}{2}\right)\left(\frac{\eta}{\eta_0'}\sqrt{1-\left(\frac{\eta}{\eta_0'}\right)^2}+\arcsin\frac{\eta}{\eta_0'}+\frac{\pi}{2}\right)-\frac{\pi}{4}\right)\cdot\eta d\eta \tag{37}$$

after applying the analogous considerations plus the method of a stationary phase (see, for example, [29]) for the integration by ξ and the numerical integration, can be transformed into the following:

$$< i \mid x_3 \mid f >= \frac{2\hbar^2\delta_{m,m'}\delta_{l,l'}}{m_e^2\omega^2 a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)}\left((-1)^{n+n'}\frac{\sqrt{\xi_2^2-1}}{\xi_2}-\frac{\sqrt{\xi_1^2-1}}{\xi_1}\right)kk'\cdot\frac{2}{\pi}\eta_0 . \tag{38}$$

To verify the results we obtained, let's compare them with the analogous expressions for a spherical shell. For the latter, the radial wavefunction in the spheroidal coordinates is written

$$R(r)\approx\left(\frac{2}{r_2-r_1}\right)^{\frac{1}{2}}\frac{1}{r}\sin\left(kr-(l+1)\frac{\pi}{2}+\alpha\right), \tag{39}$$

where $r_{1,2}$ are the internal and external shell radii, correspondingly. Then, after corresponding transformations the radial part of the matrix element (all three of them are equal because of the system symmetry) can be written

$$< i \mid x \mid f >_r = \frac{1}{r_2-r_1}\left((-1)^{n+n'}-1\right)\left(\frac{1}{k_+^2}-\frac{1}{k_-^2}\right), \tag{40}$$

where $k_\pm = k\pm k'$. For an ellipsoid nanoshell, an intermediate expression for the radial part of the matrix element, for example, by x_1 can be written

$$< i \mid x_1 \mid f >_\xi = \frac{a}{\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}}\left((-1)^{n+n'}-1\right)\left(\frac{1}{c_+^2}-\frac{1}{c_-^2}\right), \tag{41}$$

where $c_\pm = (k'\pm k)a$. This expression, really, tends to (39) if an ellipsoid shell is deformed into a spherical; similarly for the matrix element by x_3. So, such passage to the limit substantiates the results we obtained.

5. CALCULATIONS OF THE OPTICAL CONDUCTIVITY

Using matrix elements of the optical transitions we obtained in the previous chapter, we can obtain the optical conductivity of an ellipsoid metal shell. After substituting these matrix elements into (3) and certain simplifications we can write down

$$\sigma_{\perp}=\frac{\pi e^2\omega}{V_s}\frac{2\hbar^4}{m_e^4\omega^4a^2\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2}\sum_{i,f}\left(1-(-1)^{n+n'}\right)k^2(k')^2 f_e(E_i)(1-f_e(E_f))\delta\left(E_f-E_i-\hbar\omega\right) \tag{42}$$

$$\sigma_{\parallel}=\frac{\pi e^2\omega}{V_s}\frac{32\hbar^4}{\pi^2m_e^4\omega^4a^2\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2}\sum_{i,f}\frac{2l-2m+1}{ka}k^2(k')^2 f_e(E_i)(1-f_e(E_f))\times$$
$$\times\left(1-\frac{\xi_1^2+\xi_2^2}{2\xi_1^2\xi_2^2}-(-1)^{n+n'}\frac{\sqrt{\left(\xi_1^2-1\right)\left(\xi_2^2-1\right)}}{\xi_1\xi_2}\right)\delta\left(E_f-E_i-\hbar\omega\right) \tag{43}$$

First, we shall perform the summation over *l*, *m*, *l'* and *m'*. For the orthogonal conductivity component the summation can be easily performed, we obtain

$$\sigma_{\perp}=\frac{\pi e^2\omega}{V_s}\frac{8\hbar^4}{\pi^2m_e^4\omega^4}\sum_{n,n'}\left(1-(-1)^{n+n'}\right)k^4(k')^2 f_e(E_n)(1-f_e(E_{n'}))\delta\left(E_{n'}-E_n-\hbar\omega\right) \tag{44}$$

The sum that enters into (43) requires more complex transformations. After using the fact that the discrete function $\left(1-(-1)^{n-n'}\right)$ can be replaced with its average equal to 1 (in analogous way to the calculation accomplished in [30]), we can write down

$$\sigma_{\parallel}=\frac{\pi e^2\omega}{V_s}\frac{32\hbar^4}{\pi^4m_e^4\omega^4}\left(1-\frac{\xi_1^2+\xi_2^2}{2\xi_1^2\xi_2^2}\right)\frac{32}{3}\frac{\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}}{\pi}\times$$
$$\times\sum_{n,n'}\left(1-(-1)^{n+n'}\right)k^4(k')^2 f_e(E_n)(1-f_e(E_{n'}))\delta\left(E_{n'}-E_n-\hbar\omega\right) \tag{45}$$

The optical conductivity can be easily calculated if we neglect the discreteness of an electron energy levels and replace the sum that enters into (44) and (45) with the corresponding integral. This corresponds to the classical approximation – quantum effects related to the electron spectrum discreteness are not considered. We shall consider them later by calculating the correction to this classical expression.

So, after performing integration in analogous way to [25], we obtain the following classical expressions:

$$\sigma_{\perp}^0=\frac{32e^2}{\pi^3\hbar V_s}a^2\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2\frac{g(\nu)}{\nu^3}$$
$$\sigma_{\parallel}^0=\frac{32e^2}{\pi^3\hbar V_s}a^2\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2\frac{g(\nu)}{\nu^3}\frac{64}{3\pi^2}\left(1-\frac{\xi_1^2+\xi_2^2}{2\xi_1^2\xi_2^2}\right)\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right) \tag{46}$$

where

$$g(\nu)=\int\limits_{1-\nu}^{1}p^{3/2}\sqrt{p+\nu}dq=\left(\frac{(p(p+\nu))^{3/2}}{3}-\frac{\nu(2p+\nu)\sqrt{p(p+\nu)}}{8}+\frac{\nu^3}{8}\ln(\sqrt{p}+\sqrt{p+\nu})\right)\Bigg|_{1-\nu}^{1}. \quad (47)$$

After applying expressions for the shell volume (46) can be rewritten

$$\sigma_{\perp}^{0}=\frac{24e^2}{\pi^4\hbar a}\frac{\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2}{\left(\xi_2-\xi_1\right)\left(\xi_2^2+\xi_2\xi_1+\xi_1^2-1\right)}\frac{g(\nu)}{\nu^3}$$

$$\sigma_{\parallel}^{0}=\frac{24e^2}{\pi^4\hbar a}\frac{\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2}{\left(\xi_2-\xi_1\right)\left(\xi_2^2+\xi_2\xi_1+\xi_1^2-1\right)}\frac{g(\nu)}{\nu^3}\frac{64}{3\pi^2}\left(1-\frac{\xi_1^2+\xi_2^2}{2\xi_1^2\xi_2^2}\right)\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right) \quad (48)$$

The expressions obtained so far are classical (denoted by the index 0 in $\sigma_{\perp}^{0}$, $\sigma_{\parallel}^{0}$) – the quantum effects related with the electron energy quantization in the shell are not considered. As we mentioned before, such effects can become noticeable even in the case of small solid metal particles. And for thin metal shells these effects are much more essential.

Using of the Poisson formula allows us to obtain analytical expressions for the optical conductivity that take into consideration these quantum effects. The Poisson formula applies to an arbitrary function of a natural argument $y_1(n)$:

$$\sum_{n=1}^{\infty}y_1(n)=\int\limits_{0}^{\infty}dn\left(y_1(n)+2\sum_{s=1}^{\infty}y_1(n)\cos(2\pi sn)\right). \quad (49)$$

Before applying (49) to (44) and (45) we should note that δ-function of a discrete argument doesn't have mathematical sense. To give it necessary physical sense, we should use the fact that δ-function is a limit of a flock of classical functions. During a passage to the limit area under the graph of such classical function remains equal to 1 while the width of the peak (of graph figure, in general) tends to zero and height to infinity.

It is convenient for us in such situation to use the concept of the 'spread' δ-function:

$$\delta^*(x)=\begin{cases}0, & x<-\dfrac{\Delta E}{2}\\ \dfrac{1}{\Delta E}, & -\dfrac{\Delta E}{2}<x<\dfrac{\Delta E}{2}\\ 0, & x>\dfrac{\Delta E}{2}\end{cases} \quad (50)$$

when the case $\Delta E\to 0$ corresponds to the 'classical' δ-function.

Then, we notice that we can replace $E_{n'}\to E_n+\hbar\omega$ in (44) and (45). The possibility of such replacement implies from the look of the δ-function that expresses the energy conservation law in (44) and (45). After using such replacement, we can introduce the concept of the energy states density – the following function:

$$G(E)=\sum_{n'=1}^{\infty}\left(1-(-1)^{n-n'}\right)\delta\left(E_{n'}-E_n\right). \tag{51}$$

So, the expressions (44) and (45) contain $G(E+\hbar\omega)$. After introducing the δ-function in the above-described way, the energy states density

$$G^*(E)=\sum_{n'=1}^{\infty}\left(1-(-1)^{n-n'}\right)\delta^*\left(E_{n'}-E_n\right) \tag{52}$$

becomes a classical function and the Poisson formula can be applied to it. (During the process we replace the discrete function $\left(1-(-1)^{n-n'}\right)$ with its average equal to 1 in analogous way to the calculation accomplished in [30].) Using the electron energy spectrum (33), we obtain

$$\begin{aligned} G^*(E_\perp)&=\frac{a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)\sqrt{2m_e}}{\pi\hbar\sqrt{E}}\times \\ &\times\left(1+2\sum_{s'=1}^{\infty}\cos\left(\frac{2a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)}{\hbar}s'\sqrt{2m_eE}\right)\frac{\sin(s'X)}{s'X}\right)\end{aligned} \tag{53}$$

where

$$X=a\frac{\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}}{\hbar}\sqrt{\frac{2m_e}{E}}\Delta E\,. \tag{54}$$

As it is easily seen, the first addend in (53) gives the known expression for the one-dimensional energy states density. The addends of the series in (53) consider the oscillations of the states density caused by a spectrum quantization. After taking the limit $\Delta E\to 0$ we obtain relevant result for the function $G(E)$.

Now we can apply this summation method to (44) and (45). We apply it twice (summation over n and n'). Note that in this double sum we only keep the addends with $s=s'$; other addends are quickly oscillating and can be considered negligibly small after the integration. Taking into consideration the proximity of the electron energy to the Fermi energy and using the inequality $E_F>>\theta$ (here E_F is the Fermi energy of the shell metal and the quantity θ is the temperature in energy units), we obtain after complex transformations

$$\sigma_{\perp}(\omega)=\sigma_{\perp}^{0}(\omega)\left(1+\frac{2\pi\theta\left(1-e^{-\frac{\hbar\omega}{\theta}}\right)^{-1}\left(\Phi(E_F)-\Phi(E_F-\hbar\omega)\right)}{(\hbar\omega)^3 g(\nu)}\right)=\frac{24e^2}{\pi^4\hbar a}g(\nu)\times$$

$$\times\frac{\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2}{(\xi_2-\xi_1)(\xi_2^2+\xi_2\xi_1+\xi_1^2-1)}\left(1+\frac{2\pi\theta\left(1-e^{-\frac{\hbar\omega}{\theta}}\right)^{-1}\left(\Phi(E_F)-\Phi(E_F-\hbar\omega)\right)}{(\hbar\omega)^3 g(\nu)}\right), \quad (55)$$

$$\sigma_{\parallel}(\omega)=\sigma_{\parallel}^{0}(\omega)\left(1+\frac{2\pi\theta\left(1-e^{-\frac{\hbar\omega}{\theta}}\right)^{-1}\left(\Phi(E_F)-\Phi(E_F-\hbar\omega)\right)}{(\hbar\omega)^3 g(\nu)}\right)=\frac{24e^2}{\pi^5\hbar a}\times$$

$$\times\frac{\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)^2}{(\xi_2-\xi_1)(\xi_2^2+\xi_2\xi_1+\xi_1^2-1)}g(\nu)\cdot\frac{64}{3\pi^2}\left(1-\frac{\xi_1^2+\xi_2^2}{2\xi_1^2\xi_2^2}\right)\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)\times, \quad (56)$$

$$\times\left(1+\frac{2\pi\theta\left(1-e^{-\frac{\hbar\omega}{\theta}}\right)^{-1}\left(\Phi(E_F)-\Phi(E_F-\hbar\omega)\right)}{(\hbar\omega)^3 g(\nu)}\right)$$

here the function

$$\Phi(E_F)=E_F^{\frac{3}{2}}(E_F+\hbar\omega)^{\frac{1}{2}}\sum_{s=1}^{\infty}\frac{\sin\tilde{\varphi}_s(E_F)}{sh\left(\pi\theta\tilde{\varphi}_s'(E_F)\right)}, \quad (57)$$

and $\tilde{\varphi}_s$ is the following function of energy:

$$\tilde{\varphi}_s(E)\equiv s\frac{2a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)}{\hbar}\sqrt{2m_e}\left(\sqrt{E+\hbar\omega}-\sqrt{E}\right). \quad (58)$$

Numerical calculations show that the first five terms in the sum over *s* secure a sufficient accuracy for the quantum correction for typical shells and light frequencies.

As we can see, expressions for both conductivity components consist of two parts – classical conductivity, given by (48), and quantum corrections that consider quantum effects related with electronic spectrum quantization. Also, from the look of the expressions for electronic spectrum (32), (33) we can see that electronic spectrum for our shell becomes quasi-one-dimensional, similar to that of a one-dimensional potential well for electron. Really, if a shell is thin enough, a system becomes quasi-one-dimensional, so dependence of the optical conductivity components from ν should not depend from the shell shape. A shape of the shell is considered by a factor before this dependence. (See, for example, the expressions for a spherical shell [21].)

Graphical representation of the relative quantum correction $\frac{\Delta\sigma_{\perp}}{\sigma_{\perp}^{0}} = \frac{\Delta\sigma_{\parallel}}{\sigma_{\parallel}^{0}} \equiv \kappa$ as a function of the ratio ν for an ellipsoid nanoshell with parameters E_F=5.53 eV (the Fermi energy of Au), temperature Θ=300 K, longitudinal shell thickness $a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)$=100 nm (for a thick shell oscillations behaviour becomes clear) is given on Fig. 1.

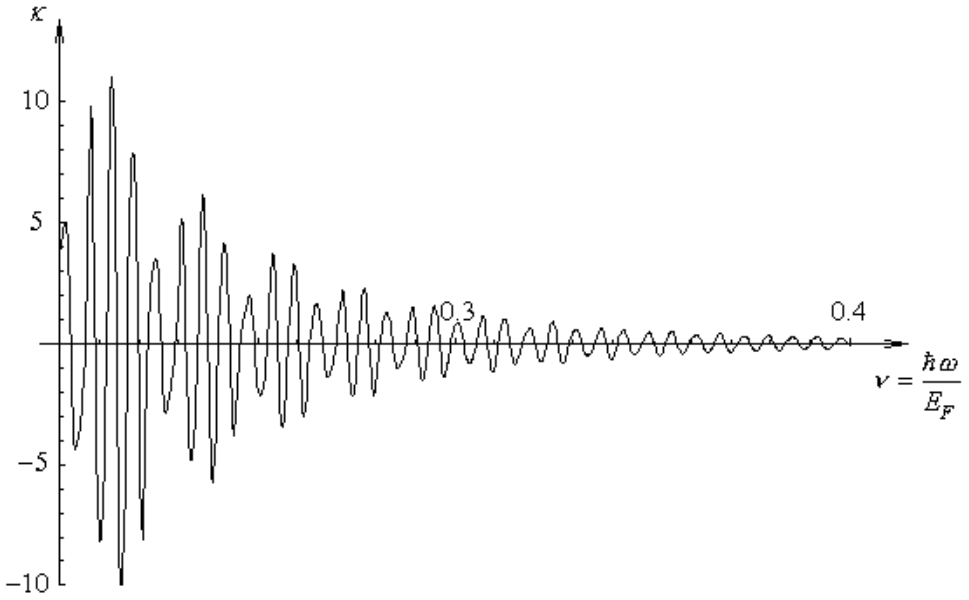

Fig. 1. Relative oscillatory quantum correction κ for an ellipsoid shell with E_F=5,53 eV (the Fermi energy of Au), temperature Θ=300 *K*, longitudinal shell thickness 100 *nm* as a function of the ratio ν of the photon energy to the Fermi energy of the shell metal.

We can see from the graph (and the numerical evaluation shows it, too) that these quantum corrections are essential and cannot be neglected, as in was predicted in introduction. For a thinner shell the contribution of these corrections is even more

essential. For example, for $a\left(\sqrt{\xi_2^2-1}-\sqrt{\xi_1^2-1}\right)$=10 nm (typical shell thickness) amplitude of the oscillations of the relation κ exceeds 200 in the vicinity of the point ν=0.2.

So, the graph shows that considering of an electron energy quantization leads to the appearance of an oscillating dependence of the optical conductivity components from the incident light frequency. Analysis shows that the oscillations frequency depends from the shell thickness. As we mentioned in introduction, such type of dependence was noticeable even for relatively thick nanowires [14]. So, when investigating one-electron light absorption by nanoshells for the energies much less than the Fermi energy of the shell metal one should consider the effects caused by the electron energy spectrum quantization.

Note that unlike the case of a spherical shell [21], optical conductivity of an ellipsoid shell is essentially a tensor quantity with two (for the considered case of a rotation ellipsoid) unequal, in general, components.

Note also that when $\hbar$ formally tends to 0 (the classical case), the optical conductivity oscillations frequency (determined from (55) or (56)) tends to the frequency of classical oscillations. These are the oscillations with an electron passage frequency from one shell wall to other [31]. This fact also validates the results we obtained.

RESULTS AND REMARKS

Thus, we obtained the quasi-classical wavefunctions and calculated the wave number spectrum and the energy spectrum for an electron in a nanoshell with the shape of a stretched rotation ellipsoid. The metal shell was considered as a thin shell. We showed that in this case the system is quasi-one-dimensional (similar to the one-dimensional potential well for electron). As a result, the distance between the energy levels increases, and the quantum effects related to the discreteness of the electron energy spectrum become essential.

Then, we found the matrix elements of the corresponding optical transitions and used them to represent the optical conductivity as the sum over electron states. This sum was used to derive the analytical expression for the optical conductivity of the considered shells.

Firstly, we found the analytical expressions for the classical (with electron spectrum quantization ignored) conductivity (the electric absorption) of these particles. From this classical expression we can already see that for an ellipsoid nanoshell the optical conductivity becomes an essentially tensor quantity (it cannot be reduced to one scalar).

Secondly, we considered the quantization effect and found the correction to these classical expressions. It was shown that this quantum correction makes an essential contribution into the total shell absorption. It was also shown that this correction depends on the incident light frequency in an oscillatory way. So, this oscillating effect should be taken into consideration when investigating light absorption of thin nanoshells for the energies much less than the Fermi energy of the shell metal as this quantum addend exceeds classical addend considerably. A dependence of the analogous nature was observed in the experiments with solid metal nanowires [14] and in the quantum theories

of thin metal films (see, e.g., [15]). Such an oscillatory dependence can be explained as follows. The light absorption is stronger when the energy $\hbar\omega$ is close to the difference between one of the electron energy levels and the Fermi energy. A smooth oscillating curve is observed instead of discrete peaks due to the thermal smearing of the electron distribution function by energy.

Note that a tensor nature of the optical conductivity and, consequently, the dependence of the conductivity from an incident light polarization (implies from the fact that the field that enters into our expressions is a local field) are essentially new properties of an ellipsoid nanoshell comparing to a spherical shell. Note also that both expressions obtained for the optical conductivity components consist of two factors – a factor that depends from the light frequency and a factor that considers the particle shape. Therefore, for a thin shell the problem becomes quasi-one-dimensional (an electron in a one-dimensional potential well) so the dependence of the shell absorption from the light frequency is not influenced by the particle shape. We can guess that an analogous effect should take place for a thin enough nanoshell of an arbitrary smooth shape.

APPENDIX. SHPEROIDAL COORDINATES

The spheroidal coordinates (ξ,η,φ) are linked to the rectangular coordinates through the following relations:

$$\begin{cases} x = a\sqrt{\left(\xi^2-1\right)\left(1-\eta^2\right)}\cos\varphi \\ y = a\sqrt{\left(\xi^2-1\right)\left(1-\eta^2\right)}\sin\varphi, \\ z = a\xi\eta \end{cases} \tag{A1}$$

here

$$\xi\in[1,+\infty),\quad \eta\in[-1,1],\quad \varphi\in[0,2\pi), \tag{A2}$$

a is a constant parameter.

The coordinate φ is equivalent to the polar angle in the spherical coordinates; the equation ξ=const describes a rotation ellipsoid with semiaxes $R_{\|}=a\xi,\quad R_{\perp}=a\sqrt{\xi^2-1}$ (where $R_{||}$ is a semiaxis directed along a rotation axis of the ellipsoid), so the parameter a satisfies the relation

$$a^2 = R_{\|}^2 - R_{\perp}^2. \tag{A3}$$

It is easily seen that

$$z^2 = a^2\eta^2 + \left(x^2+y^2\right)\frac{\eta^2}{1-\eta^2}, \tag{A4}$$

so the equation η=const describes a hyperboloid. We choose the upper hyperbola when $\eta>0$ and the lower hyperbola when $\eta<0$. Also, a differential of a volume for the spheroidal coordinates

$$dV = a^3\left(\xi^2-\eta^2\right)d\xi\,d\eta\,d\varphi \tag{A5}$$

will be used in our calculations, too.

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Кулиш В.В. Одноэлектронные оптические свойства эллипсоидальных металлических нанооболочек / Кулиш В.В., Томчук П.М. // Ученые записки Таврического национального университета имени В.И. Вернадского. Серия: Физико-математические науки. – 2010 – Т.23(62), №3. – С. 75-93.
Мы исследуем оптические свойства нанооболочек (малых композитных кластеров, состоящих из диэлектрического ядра и металлической оболочки; вклад металлической оболочки является доминирующим в оптических свойствах всего кластера) в области частот, далекой от плазмонного резонанса. Мы исследуем нанооболочки в форме вытянутого эллипсоида вращения. Для таких оболочечных частиц были найдены волновая функция электрона, спектр энергий и волновых чисел электрона, а также матричные элементы соответствующих оптических переходов. С использованием этих величин были найдены классическая оптическая проводимость (без учета квантовых эффектов) таких оболочек и квантовая оптическая проводимость (добавки к классической проводимости, квантовыми эффектами, такими как дискретность электронного спектра). Установлен осциллирующий вид зависимости этих слагаемых от частоты света, падающего на оболочку.
Ключевые слова: нанооболочки, оптическая проводимость, малые кластеры, квантование спектра.

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Ми досліджуємо оптичні властивості нанооболонок (малих композитних кластерів, що складаються з діелектричного ядра та металевої оболонки; внесок металевої оболонки є домінуючим у оптичних властивостях всього кластера) у області частот, далекій від плазмонного резонансу. Ми досліджуємо нанооболонки у формі витягнутого еліпсоїду обертання. Для таких оболонкових часток були знайдені хвильова функція електрона, спектр енергій і хвильових чисел електрона, а також матричні елементи відповідних оптичних переходів. З використанням цих величин були знайдені класична оптична провідність (без урахування квантових ефектів) таких оболонок та квантова оптична провідність (добавки до класичної провідності, квантовими ефектами, такими як дискретність електронного спектру). Встановлено осцилюючий вигляд залежності цих доданків від частоти світла, що падає на оболонку.
Ключові слова: нанооболонки, оптична провідність, малі кластери, квантування спектру.

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