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Size Dependence of the Fermi Energy of Spherical Metal Nanocluster

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In this paper, expression for the determination of the size-dependent Fermi energy of a metal nanocluster in the model of free electrons and spherical potential well of infinite depth is obtained. The calculations are performed for Al and Au clusters. The effect of the change of the system dimension on the evolution of size dependences is investigated.

Keywords: Metal cluster, Fermi energy, Oscillations, Size dependence.

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1. INTRODUCTION

A carrying neutral (nonabsorbing) medium with metal particles impregnated into it is used when producing composite materials [1]. Optical properties of such systems, first of all, are determined by the physical properties of their components [2, 3]. At that, effective characteristics of the composite can significantly differ from both the properties of metallic inclusions and dielectric matrix [4-6]. However, strong light absorption by metallic inclusions, which is impossible to get rid of without the use of laser medium, prevents the practical application of nanocomposite materials [7].

Thus, the study of the optical properties of an individual nanoparticle is the actual question. It is shown in the works [8-10] that the main contribution to the optical conductivity of metal nanosystems is determined by the Fermi energy, which for the specified systems has an oscillating behavior.

The aim of this work is to study the size dependence of the Fermi energy of a spherical metal nanocluster.

2. BASIC RELATIONS

It is reasonable to solve the problem of finding the wave functions and energy spectrum of electrons in a spherical metal nanoparticle in the spherical coordinate system. In this case, the Schrödinger equation with the Hamiltonian

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m_e}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}+U(r), \quad (1)$$

where m_e is the free electron mass; $U(r)$ is the potential energy, which for the case of a spherical well (of volume Ω and radius r_0) of infinite depth has the view

$$U(r)=\begin{cases}\infty, & r>r_0;\\ 0, & r<r_0,\end{cases}$$

allows separation of variables, and the wave function can be written as

$$\psi_{mnp}(r,\theta,\varphi)=R_{nl}(r)Y_{l,m}(\theta,\varphi), \quad (2)$$

$Y_{l,m}(\theta, \varphi)$ is the angular part of the wave function, and the radial dependence of the wave function is described by the Bessel functions of half-integer order

$$R_{nl}(r)=C_{nl}\frac{j_l(k_{nl}r)}{r}. \quad (3)$$

Here

$$C_{nl}=\left\{\int_0^{r_0} j_l^2(k_{nl}r)\,dr\right\}^{-\frac{1}{2}};$$

$k_{nl} = a_{nl}/r_0$ and a_{nl} are the positive zeros of the spherical Bessel function $j_l(\xi)$, $n = 1, 2, ...$

Equal energies are determined by the formula

$$\varepsilon_{nl}=\frac{\hbar^2}{2m_e}k_{nl}^2. \quad (4)$$

Let us now consider the question of finding the size dependence of the Fermi energy of metal 0*D*-systems. We assume that, as well as in the case of the 2*D*- [9] and 1*D*- [10] systems, the number of filled states in a spherical metal nanoparticle is equal to the number of conduction electrons, that is

$$N=\int_0^{\varepsilon_F} g(\varepsilon)d\varepsilon=2\int_0^{\varepsilon_F}\sum_{n,l}\delta(\varepsilon-\varepsilon_{nl})d\varepsilon=\bar{n}\Omega, \quad (5)$$

where $g(\varepsilon)=2\sum_{n,l}\delta(\varepsilon-\varepsilon_{nl})$ is the energy density of states of the 0*D*-system; $\bar{n}$ is the concentration of conduction electrons in the 3*D*-metal; $\Omega=4\pi r_0^3/3$ is the volume of the sphere.

To calculate the integral in (5), we will use the expansion of the δ-function in a Fourier series in sines on a finite interval of $\varepsilon \in (0, \varepsilon_F)$ [11]:

$$\delta(\varepsilon-\varepsilon_{nl})=\frac{2}{\varepsilon_F}\sum_{m=1}^{\infty}\sin\frac{\pi m\varepsilon}{\varepsilon_F}\sin\frac{\pi m\varepsilon_{nl}}{\varepsilon_F}. \quad (6)$$

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Substituting (6) into (5) and calculating the obtained integrals, we find

$$\bar{n}\Omega = \begin{cases} \frac{8}{\pi}\sum_{\kappa=1}^{\infty}\frac{1}{2\kappa-1}\sum_{n,l}\sin\frac{\pi(2\kappa-1)\varepsilon_{nl}}{\varepsilon_F}, & m=2\kappa-1; \\ 0, & m=2\kappa. \end{cases} \quad (7)$$

Expression (7) is a transcendental equation for the determination of the size-dependent Fermi energy.

3. RESULTS AND DISCUSSION

The calculations were carried out for the values of electron concentration of $\bar{n} = \left(4\pi r_s^3/3\right)^{-1}$, $r_s = 3.01a_0$ and $2.07a_0$ for Au and Al, respectively (a_0 is the Bohr radius; r_s is the average distance between electrons).

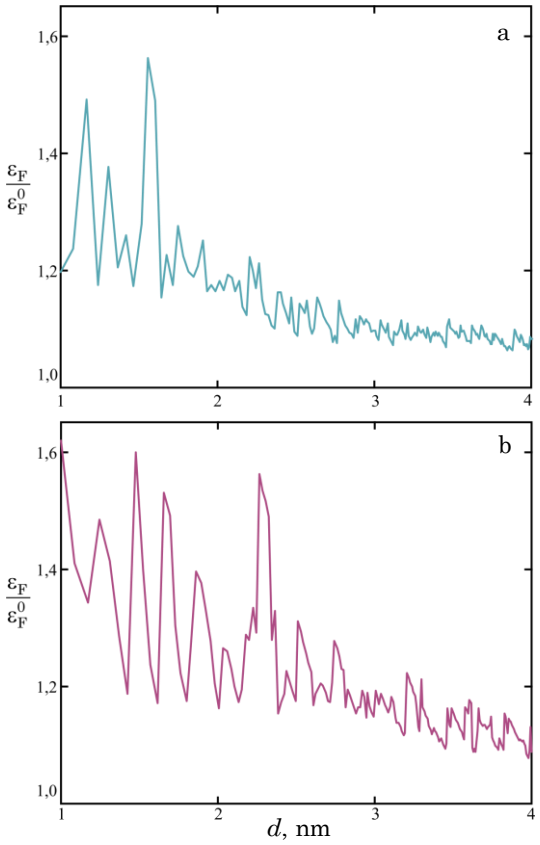

Fig. 1 – Size dependence of the Fermi energy of nanoclusters of different metals: a – Al; b – Au

The calculation results shown in Fig. 1 demonstrate the significant role of the size quantization effects in the dependence of the Fermi energy on the cluster diameter. Oscillations have the greatest amplitude for the values of $d \approx 1.4 \div 1.6$ nm and 2.4 nm (for Au clusters). This is explained by the fact that a spherical nanocluster contains a magic number of atoms for these values of the diameter. At values of $d > 2.4$ nm, oscillation amplitude decreases and tends to zero.

As in the case of nanowires (Fig. 2), size dependence of ε_F seems to be chaotic. However, "chaotic" oscillations of the Fermi energy of nanowires are small-scale, while for Al and Au clusters oscillation amplitude reaches values from 0.4 to $0.45\varepsilon_F/\varepsilon_F^0$.

On the size dependence of the Fermi energy of the cluster, as well as for the nanowire, maximum appears, whenever radius r_0, which increases, reaches the value, at which condition $a_{nl} < k_F r_0$ begins to hold for one more pair of numbers (n', l'). The distance between the neighboring maximums

$$\Delta d_{cl} \approx 2\left(a_{n'l'} - a_{nl}\right)/k_F^0$$

is obtained with imposing roots of the spherical Bessel functions of different orders.

Differences in size dependences of the Fermi energy of Al and Au clusters are conditioned by different values of the electron density $\bar{n}$ of these metals. For Al clusters, as well as for wires, scale of oscillations Δd_{cl} is smaller, since distribution density of roots a_{nl} is larger.

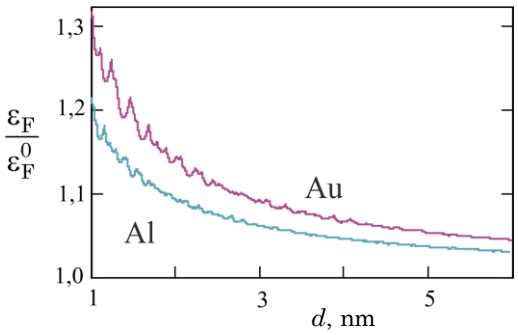

Fig. 2 – Size dependence of the Fermi energy of gold and aluminum nanowires [10]

4. CONCLUSIONS

Procedure for the determination of the Fermi energy of metal 0*D*-systems has been proposed for the first time. The calculated size dependence for the clusters of different metals has an "oscillating" behavior. Oscillation amplitude tends to zero and oscillation period – to infinity with increasing nanocluster diameter, as well as in the case of a nanowire.

It is established that the change in the dimension of metal systems leads to differences in the size dependences of the Fermi energy. Thus, oscillations are small-scale in the 1*D*-systems, and during the transition to the 0*D*-system their amplitude significantly increases. This is associated with an additional restriction of the charge carrier motion in the 0*D*-systems and substantial difference in the density of electron states in these systems.

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