Effects of broadening and electron overheating in tunnel structures based on metallic clusters

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We study the influence of energy levels broadening and electron subsystem overheating in island electrode (cluster) on current-voltage characteristics of three-electrode structure. A calculation scheme for broadening effect in one-dimensional case is suggested. Estimation of broadening is performed for electron levels in disc-like and spherical gold clusters. Within the two-temperature model of metallic cluster and by using a size dependence of the Debye frequency the effective electron temperature as a function of bias voltage is found approximately. We suggest that the effects of broadening and electron overheating are responsible for the strong smoothing of current-voltage curves, which is observed experimentally at low temperatures in structures based on clusters consisting of accountable number of atoms.

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I. INTRODUCTION

The nanodispersed metallic systems are prospective objects of nanotechnology. Therefore understanding of their physical properties is of scientific and hopefully of practical interest.

Transport of electrical charge across a nanoscale tunnel junction is accompanied by many effects, such as the Coulomb blockade of the average current, transfer of energy between electrons and ions, and consequently heating of the junction. In nanometer scale devices electron transport can occur through well-resolved quantum states. If the temperature is increased, the Coulomb and quantum staircases of current are gradually smeared out by thermal fluctuations (see, for example [1, 2]).

Simple tunnel construction can be schematically represented by the distinctive “sandwich”: thick film / dielectric nanofilm / isolated Au(111) electrode (cluster) on current-voltage characteristics of three-electrode structure. A calculation scheme for broadening effect in one-dimensional case is suggested. Estimation of broadening is performed for electron levels in disc-like and spherical gold clusters. Within the two-temperature model of metallic cluster and by using a size dependence of the Debye frequency the effective electron temperature as a function of bias voltage is found approximately. We suggest that the effects of broadening and electron overheating are responsible for the strong smoothing of current-voltage curves, which is observed experimentally at low temperatures in structures based on clusters consisting of accountable number of atoms.

Predicted earlier size dependence of the Debye temperature is experimentally confirmed in Ref. [32] and then it is precised by temperature dependence in Ref. [34]. Suppression of the electron-phonon interactions in granules is a result of deformations of a phonon spectrum in these systems. This interaction can to be suppressed so that electron-electron interaction appears as a basic mechanism of dissipation affecting a particle energy. This leads to the overheating of electronic subsystem which can be described by Fermi statistics with some effective (raised) temperature while the ionic subsystem temperature varies only slightly.

It is supposed that the relaxation of the non-equilibrium electrons in small metal particles, films...
and wires \(^{33,36}\) occurs owing to excitation of the Rayleigh waves or surface acoustic phonons. However, the obtained expressions in the cited works contain no asymptotic transition to infinite systems.

According to the Weyl's theorem (see Ref. \(^{37}\)), it is possible to separate the bulk and surface acoustical phonons only for the large metal sample. For small-sized samples the modes are mixed, a sound velocity becomes indefinite and, as a rule, in practice it is used as a fitting parameter. On the other hand, measurements of an electron-ion power exchange in the free clusters \(^{38}\) have demonstrated that, for reasonable estimations, it is quite possible to use the conception of bulk phonons, but with the account of the size dependence of the Debye frequency. Such an approach for the metallic nanoclusters, films and wires can be considered as an extrapolation.

II. BROADENING OF LEVELS

The scattering matrix relates the initial state and the final state for an interaction of particles. The free electronic states of the cluster do not decay so that they are stationary. For free clusters the poles of the scattering matrix \(S(k)\), located on the real axis at the plane of complex values of waving numbers \(k\), correspond to the stationary states.

If a cluster is placed between electrodes, its electronic states become quasi-stationary. Broadening occurs due to a tunneling effect by analogy with the formation of states become quasi-stationary. Broadening occurs due to the increase of the bias voltage applied between electrodes. Both tunnel barriers are three-dimensional. Therefore, the problem of calculation of broadening, in general case, is far from being trivial. An analytical solution of resonance tunneling problem is possible only for one-dimensional geometry and rectangular barriers (see \(^{38}\)).

According to the indeterminacy principle broadening effects are related to the finite life time. Energies of the quasi-stationary states become complex and their imaginary parts describe levels broadening. The poles of the \(S\)-matrix corresponding to these states are located in the lower half of the complex plane wave number \(k\). The state with well defined energy is accordingly replaced by the Lorentz distribution with the scale parameter which specifies the half-width at half-maximum \(\gamma_p\):

\[
L_p(\varepsilon) = \frac{1}{2\pi} \frac{\gamma_p}{(\varepsilon - \varepsilon_p)^2 + \gamma_p^2/4},
\]

Here an index \(p\) denotes the set of quantum numbers (except for a spin) which correspond to the single-electron state with energy \(\varepsilon_p\) (Fig. 1). \(L_p(\varepsilon) \rightarrow \delta(\varepsilon - \varepsilon_p)\) as \(\gamma_p \rightarrow 0\) where \(\delta(x)\) is the Dirac \(\delta\)-function.

Taking into account the broadening function, the electron density of states can be expressed as

\[
\overline{\rho}(\varepsilon) = 2 \sum_p L_p(\varepsilon),
\]

where the factor 2 takes into account a spin degeneracy.

Current flowing through a quantum granule (with limitation on its Coulomb instability \(^{7}\)) is determined by the equality condition between the emitter and collector currents \((I^e = I^c \equiv I)\) or

\[
-e \sum_{n_{\min}}^{n_{\max}} P_n \left(\overline{w}^e_n - \overline{w}^c_n\right) = -e \sum_{n_{\min}}^{n_{\max}} P_n \left(\overline{w}^c_n - \overline{w}^e_n\right).
\]

The probability \(P_n\) of finding of \(n\) “surplus” \((n > 0)\) or failing \((n < 0)\) electrons at central electrode is defined by the master equation in the stationary limit. In reality, one calculates the reduced current \(I \equiv I/(eP_0\Gamma^e)\) where \(\Gamma^{e,c}\) are tunnel rates, \((-e)\) is the electron charge. In order to find \(P_n \neq 0/P_0\) the recurrent relation is used:

\[
P_{n+1} = P_n \frac{w^{in}_n}{w^{out}_{n+1}}
\]

where \(w^{in}_n = \overline{w}^e_n + \overline{w}^c_n\) and \(w^{out}_n = \overline{w}^e_n + \overline{w}^c_n\) are the total electron streams from/to leads into/out the cluster, and \(\overline{w}^{e,c}_n\) are the partial tunneling streams, accordingly. Here the upper/under arrows and indexes “\(e,c\)” denote the emitter-granule and collector-granule and back transitions in accordance with arrows direction.

Taking into account the broadening of levels for \(V > 0\), we have

\[
\overline{w}^e_n = \frac{1}{\pi} \Gamma^e \sum_p \int_{\mu^e_p}^{\infty} \frac{\gamma(\varepsilon^e_p)}{(\varepsilon^e - \varepsilon^e) + (\gamma(\varepsilon^e)/2)^2} \times f(\varepsilon^e - \mu^e_p; T) \left[1 - f(\varepsilon^e - \mu^c_p; T_c)\right] d\varepsilon^e,
\]

Figure 1: The energy diagram for tunnel structure based on the non-magic granule before application of voltage.
\[
\overline{w}_n^c = \frac{1}{\pi R} \sum_p \int_{U_0+U}^{+\infty} \frac{\gamma(\overline{\epsilon})}{(\epsilon' - \overline{\epsilon})^2 + (\gamma(\overline{\epsilon})/2)^2} \times \left[ f(\epsilon' - \mu_\Psi^c; T) [1 - f(\epsilon' - \overline{\mu}_C^c; T_e)] \right] \, d\epsilon',
\]
(6)

\[
\overline{w}_n^e = \frac{1}{\pi R} \sum_p \int_{U_0+U}^{+\infty} \frac{\gamma(\overline{\epsilon})}{(\epsilon' - \overline{\epsilon})^2 + (\gamma(\overline{\epsilon})/2)^2} \times \left[ 1 - f(\epsilon' - \mu_\Psi^c; T) f(\epsilon' - \overline{\mu}_C^c; T_e) \right] \, d\epsilon',
\]
(7)

\[
\overline{w}_n^e = \frac{1}{\pi R} \sum_p \int_{U_0+U}^{+\infty} \frac{\gamma(\overline{\epsilon})}{(\epsilon' - \overline{\epsilon})^2 + (\gamma(\overline{\epsilon})/2)^2} \times \left[ 1 - f(\epsilon' - \mu_\Psi^c; T) f(\epsilon' - \overline{\mu}_C^c; T_e) \right] \, d\epsilon',
\]
(8)

where \( f(\epsilon - \mu; T) = 1 + \exp[(\epsilon - \mu)/k_b T] \) is the Fermi-Dirac distribution.

Because of the applied voltage and charging of a granule \( W^c \), the spectrums and the chemical potentials are shifted:

\[
\overline{\epsilon}^c = \epsilon_p + \overline{E}_c(n \pm 1/2) - e\eta^+ V,
\]
\( \overline{\epsilon}^c = \epsilon_p + \overline{E}_c(n \mp 1/2) + e(1 - \eta^+) V, \)
\( \overline{U}^c = -e\delta\phi + \overline{E}_C(n \mp 1/2) - \eta^+ V, \)
\( \overline{U}^e = -e\delta\phi + \overline{E}_C(n \pm 1/2) + e(1 - \eta^+) V, \)
\( -\mu_\Psi^c \equiv W^c_0, \quad \overline{\mu}_C^c = \mu^c + U^\overline{c}, \quad \overline{\mu}_C^c = \mu^c_0 - eV. \)

Here the upper/under arrows at the left correspond to the following signs at the right. \( \epsilon_p \) is electron spectrum in a cluster in absence of both the voltage and charging, \( W^c_0 \equiv -\mu^c_0 \) is a work function of semi-infinity metal, \( \mu^c \) is an electron chemical potential of granule, \( \delta\phi = (\mu^c - \mu^c_0) \) is a contact potential difference between cluster and electrodes.

For \( V > 0 \) the fraction of voltage reads

\[
\eta^+ = \frac{C}{e(d_e + L) + d_e}
\]
(9)

where \( L = 2R \) and \( H \) for a sphere and disk, accordingly, \( \epsilon \) is a dielectric constant of film which covers the left electrode. \( \eta^+ V \) is the potential in a coordinate \( z = d_e + L/2 \) in the case of absence of cluster (it is assumed that the electric field in the cluster is screened completely).

For \( V < 0 \) the voltage fraction \( \eta^- \) equals \( 1 - \eta^+ \).

As an approximation, the profile of the one-electron effective potential in the cluster can be represented as a potential well of the depth \( U_0 < 0 \). The three-dimensional Schrödinger equation for a quantum box can be separated into one-dimensional equations. The spectrum of wave numbers in a spherical and cylindrical potential wells are determined from the continuity condition of a logarithmic derivative of the wave function on the boundaries.

Neglecting the area near near cylinder edges, the energy spectrum in metal nanodisk is found by a simple way as follows

\[
\epsilon_p = U_0 + \frac{\hbar^2}{2m_e} (k_n^2 + k_{n_\perp}^2)
\]
(10)

where \( U_0 < 0 \) is the position of conductivity band of a semi-infinite metal \( \epsilon^0 \). \( k_{n_\perp} \) is a solution of wave equation for radial direction. Quantization of the wave number \( k_n \) along the cylinder axis is determined by the solution of the equation:

\[
k_n H = n_z \pi - 2 \arcsin(k_n/z_0)
\]
(11)

where \( n_z \) is the integer number, \( \hbar k_0 \equiv \sqrt{2m_e |U_0|} \). Since the tunneling takes place mainly in \( z \)-direction, “partial” broadening of \( k_n \) spectrum corresponds to general spectrum \( \epsilon_p \).

In order to calculate the electron levels broadening in quantum metal disk, let us consider the decay of cluster’s states due to the tunneling. For simplest potential profile which corresponds to Fig. 1, we use the solution of the Schrödinger equation in the form:

\[
\psi(z) = \begin{cases} 
  e^{ik_n z} + B_1 e^{-ik_n z}, & z < 0, \\
  A_1 e^{ik_n z} + B_2 e^{-k_n z}, & 0 < z < d_e, \\
  A_2 e^{ik_n z} + B_3 e^{-k_n z}, & d_e < z < d_e + H, \\
  A_3 e^{ik_n z} + B_4 e^{-k_n z}, & d_e + H < z < d_e + H + d_e, \\
  A_4 e^{ik_n z}, & z > d_e + H + d_e 
\end{cases}

(12)

for the electrons stream falling from the left to the right and

\[
\psi(z) = \begin{cases} 
  e^{-ik_n z} + B_5 e^{ik_n z}, & z > d_e + H + d_e, \\
  A_5 e^{ik_n z} + B_6 e^{-k_n z}, & d_e + H < z < d_e + H + d_e, \\
  A_6 e^{ik_n z} + B_7 e^{-k_n z}, & d_e < z < d_e + H, \\
  A_7 e^{-k_n z} + B_8 e^{ik_n z}, & 0 < z < d_e, \\
  A_8 e^{-ik_n z}, & z < 0 
\end{cases}

(13)

for the stream falling from right to left, accordingly. According to \( 12 \) and \( 13 \), \( \hbar k_n \) is equal to \( \sqrt{2m_e |U_0| - \hbar^2 k_{n_\perp}^2} \).

Using the continuity condition of the wave functions on the boundaries \( z = 0, d_e, d_e + H \) and \( d_e + H + d_e \), we obtain the system of equations for the determination of
the coefficients $A$ and $B$ which we then solve numerically by the LU-expansion method.

A total wave function can be written using the $S-$matrix as

$$\psi(z) \sim \{ \psi(z) - S\psi(z) \}.$$  

For any coordinates inside the electron reservoirs (left and right electrodes), $z = z^* \leq 0$ or $z^* \geq d_c + H + d_c$ (Fig. 1), one can calculate the matrix

$$S = \left( \psi / \bar{\psi} \right)_{z = z^*}. \quad (14)$$

By the Muller's method we calculate the pole of $S-$matrix at the lower half-plane of the complex wave numbers $k$, in the vicinity of point $k_{n_s}$. The imaginary part of the energy $\hbar^2 k^2_{n_s}/2m_e$ gives the energy broadening.

It is easy to generalize a method on $V \neq 0$ regime. In this case underbarrier wave functions will be expressed through the Airy functions.

For estimation of the broadening in a spherical cluster, it is possible to use the solution of the well-known problem for open dot – spherically symmetric potential in depth $U_0$, of radius $R$ and barrier thickness $d_c$. We define broadening by analogy with the book \[38\] as

$$\gamma_p \approx 8e^{-4\kappa_p d_c} \frac{\hbar^2 k_p^4}{m_e k_0^4(1 + \kappa_p d_c)}. \quad (15)$$

### III. BALANCE EQUATION

The two-temperature model describes a system of electrons and ions, which is out of equilibrium between electronic and ionic subsystems. For a metallic sample, this condition can be fulfilled, provided one applies an electric field.

In a two-temperature model a balance equation in a cluster in presence of voltage has the simplest form

$$\Omega \frac{\partial (c_e T_e)}{\partial t} = P(T_e, T_i) - Q(T_e, T_i),$$

$$\Omega \frac{\partial (c_i T_i)}{\partial t} = Q(T_e, T_i) \quad (16)$$

where $c_{e,i}$ is specific heat capacity of electronic and ionic subsystems (with temperatures $T_e$ and $T_i$, respectively) of cluster with the volume $\Omega$, $P$ is a input power, $Q$ is the exchange energy between electrons and ions per second.

Since the specific heat of the electronic subsystem is much smaller than that of phonons, the electron-electron and the phonon-phonon processes are much faster than the electron-phonon processes, i.e. the characteristic relaxation time for the electron subsystem temperature is much shorter than that for the phonon subsystem. The result is that when injecting power into the metal cluster, the electron temperature grows very rapidly until the energy flux from electrons to phonons becomes equal to the absorbed power so that the local equilibrium in the electron subsystem is achieved ($dT_e/dt = 0$),

$$P(T_e, T_i) - Q(T_e, T_i) = 0. \quad (17)$$

For $Q$ we use the result of Ref. \[10\], obtained for the case of a massive metal, on the basis of the kinetic equation:

$$Q(T_e, T_i) = \frac{2}{(2\pi)^3} \frac{m_e^2 U^2_{e-ph} k_B^5 T_0^5}{\hbar^4 \rho s^4} \times$$

$$\left\{ \frac{T_e}{T_0}^{5/2} \langle T_D/ T_0 \rangle \left. \int_0^L \frac{x^4 dx}{c^4(x^4 - 1)^2} \right|_{c^4 - 1} \left. \int_0^L \frac{x^4 dx}{c^4 - 1} \right|_{c^4 - 1} \right\}. \quad (18)$$

Here $U_{e-ph}$ is the electron-phonon interaction constant, $T_0$ is the Debye temperature in a massive metal, $\rho$ is the density of Au, and $s$ is the “average” sound speed \[54\]. In literature, it is accepted to use the following expression for $T_e, T_i \gg T_0$ in the Eq. \[18\]

$$Q(T_e, T_i) = \Omega c (T_e - T_i).$$

For low-dimensional object of a volume $\Omega$ and surface area $S$ the size dependence of the Debye temperature in quasi-classical approximation is given by \[32\):

$$T_D = T_0 \left[ 1 + \frac{\xi}{8} / \left[ 1 + \frac{\xi}{4} + \left( \frac{\xi}{3} \right)^2 \right] \right], \quad \xi = \frac{1}{2} \frac{S}{k_{WS} \Omega} \quad (19)$$

where $k_{WS} = (6\pi^2/v) ^{1/3}$ is the maximum wave number in a massive metal, $v = 4\pi r_0^3/3$, and $r_0$ is the atom density parameter ($r_0 = 3 d_0$ for Au). Reasonable accuracy of the expression \[19\] was demonstrated in experiment \[32\] where x-ray scattering was studied on gold clusters with diameters ranging from 1.5 to 4.3 nm.

The feeding power can be counted up in the form $P^\pm = I^\pm V^\pm$ using the experimental $I(V)$ dependence. After that, the expression \[13\], in which a replacement $T_0 = T_D \quad (19)$ is performed, is substituted in \[17\]. Under the assumption of the equality between the temperatures of the ionic subsystem $T_i$ (constant throughout the tunnel structure) and thermostat, and from the solution of \[17\], one can find an electronic temperature $T_e$, which characterizes the Fermi distribution, (see \[5\] and \[8\]).

### IV. RESULTS AND DISCUSSION

We consider Au disks of monoatomic thickness whose radii vary in the range $2R \simeq \{1, 8.5\}$ nm and which contain $\simeq \{14, 10^3\}$ atoms. Similarly, the spherical clusters with $2R \simeq \{1, 4, 2.8\}$ nm contain $\simeq \{100, 600\}$ atoms. (In Refs. \[3, 4\] cluster sizes are given in terms of mono-layer numbers; therefore, we used normalized curve from Fig. 1 of Ref. \[40\] in order to express these sizes in terms of nanometers.)
The characteristic Coulomb energy of charging is $e^2/C$ where $C$ is self-capacitance of a single granule in vacuum. The calculations of Ref. [7] demonstrated that these $C$ values are too small for the width of the current gap to be explained. Therefore we determine the characteristic energy of clusters charging as $\bar{E}_C = e^2/C_{\text{eff}}$. Effective capacitance $C_{\text{eff}} = (R + \delta)$ is used in order to explain experimental results for spherical clusters. The additional small quantity $\delta$ is caused by an increase of radius of the charging electron “cloud”. For gold $\delta$ is equal approximately to 1.8 $a_0$. The most obvious example is the case of a disc, since almost half of the disc surface contacts to the dielectric film with $\epsilon = 3$. In this case $C_{\text{eff}}$ is estimated as a capacitance of the spheroid with minor axis of length $H$. A major axis $a$ is obtained from a condition $\pi R^2 H = 4\pi a(H/2)^2/3$. Thus, we have

$$C_{\text{eff}} = \frac{1 + \epsilon \sqrt{a^2 - (H/2)^2}}{2 \arccos(H/2a)}.$$ 

We note that the value of the capacitance is sensitive to the shape of the granule surface so that even small deviation from the spherical shape can change significantly the capacitance.

In this work calculations are performed for structures based on clusters, for which $I - V$ curves were measured at different temperatures, namely, for a disk with a diameter $2R = (4 \pm 0.5)$ nm and thickness $H \approx 0.3$ nm [3] and for spheres with $2R = (2 \pm 0.35)$ nm [3, 4, 5]. Because of the uncertainly of sizes and number of atoms, we used the jellium model and found that disc and sphere contain 240 and 248 atoms, accordingly. Then $\bar{E}_C = 0.44$ and 1.31 eV for the disc and sphere, respectively. In spite of the fact that volumes of these two clusters are nearly the same, a difference between their shapes produces a significant mismatch in $\bar{E}_C$.

Clusters under consideration are non-magic. The Fermi level $E_F$ and levels of lowest unoccupied $\varepsilon_{LU}$ and occupied $\varepsilon_{LO}$ electron states in the clusters are in line. Spectra were calculated and reported in our earlier works [3, 8].

Taking into consideration the conditions of experiments [3, 6, 8, 9, 10] and the symmetry of measured $I - V$ curves, the following numbers have been chosen as input parameters in our calculations: $d_e = 10$ Å, $d_s = 2$ Å (Fig. 1), and $\beta = 2/\sqrt{3}$ for structures based on a disk and sphere, accordingly.

Calculated $I - V$ curves for different magnitudes of a parameter $\beta$ were analyzed in Ref. [7] where the effects of broadening and overheating were neglected. As follows from the expression

$$\Delta V_g = \frac{\bar{E}_C}{2e}(\frac{1}{2 - \eta^+} + \frac{1}{2 - \eta^-}),$$

the current gap is independent on $\beta$. However, the current jumps are very sensitive to the value of $\beta$ which, in its turn, has no influence on threshold voltages. With the growth of $\beta$, the steepness of $I - V$ curves parts which correspond to $V > 0/V < 0$, decreases/increases, respectively. For granular films a theory of Ref. [11] gives a similar result, however, measurements of Ref. [11] demonstrate the influence of tunneling resistances (in other words, of parameter $\beta$) on the current gap width.

We perform calculations for gold clusters with the electron-phonon interaction constant $U_{e-ph} = 1$ eV [22], the Debye temperature $T_D = 150$ K, the density of Au $\rho = 19.3 \times 10^3$ kg/m$^3$, and the “average” sound speed $s = 1500$ m/s [34].

The size dependences of the Debye temperature $T_D(R)$ were analyzed taking into account Eq. (19). The actual forms $T_D(R)$ in a wide range of sizes are plotted in Fig. 2. Different asymptotic behaviors of these two curves is due to the fact that in Eq. (19) at $R \rightarrow \infty$, one has $S/\Omega \rightarrow 0$ for spheres and $2/H$ for discs.

The feeding power leads to the overheating of the electron subsystem. With the increase of the bias voltage $V$ the number of electrons relaxing in the granule increases significantly. Among them are all the electrons with energies in the interval $\gamma V$ below the Fermi level of the granule, since the flow of tunneling electrons increases from below lying levels, thereby, involving large number of conductivity electrons to the relaxation process. The granule does not fragmentize during the significant overheating of the electron subsystem, because the $I - V$ curves are reproduced during the cyclic changes of the bias voltage [3, 4, 5, 6].

The dependences $T_c(V)$ for two structures based on sphere and disk (temperature of ions 5 K and 30 K, ac-
Figure 3: Size dependences of the electronic kinetic temperature $T_e(N)$ in spheres (continuous line) and discs (dotted line) for different values of injected power $P = 10^a P_0$, $P_0 = 10^{-12}$ W. $N$ is the number of atoms.

One of the conclusions of recent article [13] is the fact of the increase of the kinetic electron temperature with the decrease of cluster size for $P = \text{const}$. The results of our calculations, which are presented in Fig. 3, confirm this conclusion.

The calculated $I - V$ characteristics for structures, based on spherical and disk clusters, are plotted in the Figs. 4 and 5. At low temperatures, the calculated values of gap width $\Delta V_g$ are in accordance with the experimental data for a structure on disc-like cluster (Fig. 5). A difference (approximately in 1.5 times) for a structure on a spherical cluster (Fig. 4) can be possibly attributed to the fact that we have neglected the mutual capacities effect.

The broadening of the levels mimics a quasi-continuous spectrum in a cluster. The calculation of broadening is performed for disk in absence bias of a voltage. This approximation has to be considered as an estimate of a minimum broadening for the whole $I(V)$ curve. In the disc-shaped dot, the electron states are realized only with “subbands” $n_z = 1$ and 2. States with $n_z = 1$ almost do not decay. The broadening of the levels with $n_z = 2$ is approximately 0.7 eV. Estimation of broadening in spheres is rather rough, since it does not take into account obvious three-dimensionality of the problem.

Width $\Delta V_g$ for non-magic clusters is determined only by charging energy $E_C$. An overheating in current gap is not substantial, because feeding energy is minimal. At $T = 300$ K our calculation gives $\Delta V_g$, in satisfactory agreement with experiment for structure based on the disc. The result for a disk however is quite sensitive to
In this work the semi-empirc estimations of two mechanisms are performed: (i) broadening of electronic levels due to a tunnel effect, (ii) heating of electronic gas in the isolated metal clusters in presence of bias voltage. The calculations are carried out for two gold clusters of close volume and different shapes (cylindrical and spherical).

A calculation scheme of $S$-matrix poles for the broadening effect in simplest model of rectangular barriers of three-electrode structure is suggested. For monoatomic disc, containing approximately 250 atoms, the broadening of “work subband” $\gamma$ is 0.7 eV, provided that the difference between discrete levels is close to 0.2 eV in the vicinity of the granule Fermi level $\Delta\varepsilon_F$.

In the framework of two-temperature model of metal cluster, and by using a size dependence of the Debye frequency, the effective electron temperature vs. bias voltage is found approximately. The strong dependence of electronic kinetic temperature vs. voltage is found. For helium temperature of ion subsystem, the heating temperature of electrons in a quantum disk is almost one order of magnitude higher than that in a sphere; it achieves thousands of Kelvins.

We suggest an explanation for the effect of strong smoothing of current-voltage curves in structures based on clusters consisting of accountable number of atoms which was observed experimentally at low temperatures. We believe that this effect can be attributed to the level broadening and electron subsystem overheating, with the influence of broadening being much more important.

The indicated mechanisms can violate the basic inequalities, which have to be fulfilled for single-electronic devices to be able to work

$$\tilde{E}_C, \Delta\varepsilon_F \gg k_B T,$$

because, in these conditions, it is necessary to replace $\Delta\varepsilon_F$ by $\Delta\varepsilon_F - \gamma_F$ and $T$ by $T_e$. ($\gamma_F$ is the “average” broadening of discrete levels in the vicinity of the granule’s Fermi level).

Fabrication of stable in sizes and shapes elements is one of the key problems of nanoelectronics. Structures created on metallic clusters is not while succeeded. This problem, possibly, can be realized on the clusters by sort Zn@C$_{28}$ [42]. They convenient to those that tunneling transitions can be exactly enough organized as dielectric shell round the atom of metal steady. It turns out to be a difficult task to describe a device based on such a cluster by using simple models: in particular, because it is not possible to use a charging energy $\tilde{E}_C$ as an informative parameter. For this purpose it is necessary to know an electron affinity and ionization potential of metal atom in the shell of carbon atoms. Moreover effect of overheating will be absent owing to lack of an electron gas.

A thermoemission current depends exponentially on the ratio of granule electron work function and the kinetic temperature. Change of current is substantial, provided
that the temperature is changed in tens of times. We suppose that the broadening of the levels must be also taken into account for the proper description of thermooptical and photoemission in similar structures.

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