Coulomb energy of excitations in a discrete electronic system

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The nature of the Coulomb energy of excitations in small tunnel junctions is discussed. The conventional electrostatic definition of this energy is physically meaningless.

An important characteristic of a small tunnel junction is its Coulomb energy W_c in the charged state, which, in the combination $\gamma = W_c/T$, where T is the temperature, determines the scale of Coulomb-blockade effects in systems of this sort. The numerous studies of the particular features of the Coulomb blockade in the steady state and in dynamic situations have usually employed the assumption that the Coulomb energy W_c can be written in the form $W_c = n^2e^2/(2C)$, where the phenomenological constant C represents the electrical capacitance of the blocking unit, and $n = 1,2,3,...$ (see the original papers[1-5] and, as a recent review, Ref. 6). In those cases in which authors have in principle calculated a value for W_c, the hypothesis that the energy W_c was of an electrostatic nature has been justified. However, the original equations were not fully studied in those papers (see the papers by Kulik and Shekhter,[5] Nazarov,[7] and Glazman and Matveev[8]).

In this letter we wish to discuss the properties of the energy W_c for a junction with a blocking unit (a grain) in a simple model which gives a qualitatively correct description of the properties of the Coulomb interaction in the Coulomb-blockade problem.

1. We consider a system of three plates, arranged in the $Y = 0$ plane as shown in Fig. 1. This simple configuration simulates the problem of a junction with a grain, whose role is played by the central plate, on the interval $-a \leqslant x \leqslant +a$, between two metal banks. This model is of course unsuitable for describing the actual discrete nature (or point nature) of the electron charge. However, for answering the qualita-

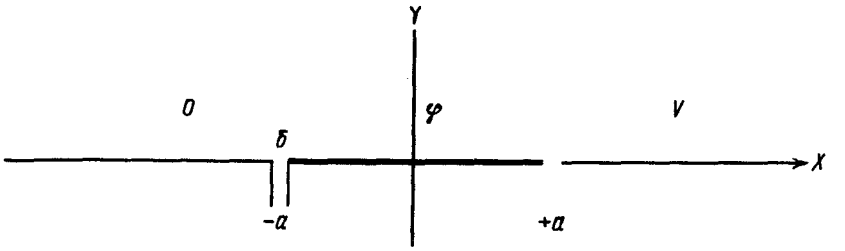

FIG. 1.

tive questions in which we are interested here it is sufficient to assume a quantized charge per unit length of the plates.

We assume that the potentials on the plates have the values 0, φ, V from left to right. What is the electrostatic energy of the junction as a function of φ at a fixed V?

A convenient feature of this geometry is that in this case we can use the known solution of the Dirichlet problem with a unit potential $u = 1$ on the line segment $b \leqslant x \leqslant c$ and a potential which vanishes elsewhere, i.e., on the lines $-\infty < x \leqslant b$ and $c < x < +\infty$:

$$u(x, y, b, c) = \frac{1}{\pi}\left(\arctan\frac{c-x}{y} - \arctan\frac{b-x}{y}\right). \tag{1}$$

Constructing the total potential $u(x,y)$ as the combination

$$u(x, y) = \varphi u(x, y, -a, +a) + V u(x, y, a, \infty), \tag{2}$$

we find a solution of $u(xy)$ which satisfies the necessary boundary conditions:

$$u(x, y)|_{y\to 0} = \begin{cases} 0 & -\infty \leq x \leq -a \\ \varphi & -a < x < +a \\ V & +a \leq x < \infty \end{cases}. \tag{2a}$$

The corresponding distribution of the electron density along the electrodes, $n(x)$, is

$$n(x) = \frac{1}{4\pi e}\left(\frac{\partial u}{\partial y}\bigg|_{+0} - \frac{\partial u}{\partial y}\bigg|_{-0}\right) = \frac{a(V-2\varphi)+Vx}{2\pi^2 e(a^2-x^2)}. \tag{3}$$

With expression (3) for $n(x)$, we can easily calculate the Coulomb energy W_c per unit length for our system of three plates:

$$W_c(\varphi, V) = \frac{1}{2}Q_1\varphi + \frac{1}{2}Q_2 V, \quad Q_1 = e\int_{-a}^{+a} n(x)dx, \quad Q_2 = e\int_{a}^{\infty} n(x)dx. \tag{4}$$

The charges Q_1 and Q_2, with $n(x)$ from (3), have logarithmic divergences of obvious origin. To eliminate them, we must assume (for example) that the width of the central plate is smaller than $2a$ by an amount $\delta/a \ll 1$.

The energy $W_c(\varphi,V)$ has a minimum at $\varphi = V/2$. In this case the charge on the central plate, Q_1, is zero. In the region $\varphi \neq V/2$, the energy $\delta W_c = W_c(\varphi_1 V) - W_c(V/2,V)$ can be written

$$\delta W_c = \frac{1}{2}C\left(\varphi - \frac{V}{2}\right)^2, \quad C = \frac{1}{\pi^2}\ln\frac{a}{\delta}. \tag{5}$$

Expression (5) agrees with the phenomenological determination of W_c in the theory of the Coulomb blockade.[1-8] However, the net charge which arises at a grain under the conditions $\varphi \neq V/2$, reaches it from both banks of the system according to (3) and (4) [see the distribution of the corresponding density $n(x)$ in Fig. 2a]. This distribution of the charge density $en(x)$ qualitatively contradicts the distribution which we would expect for this charge density in the case of individual hops of an electron from a bank to the grain or vice versa, as represented in Fig. 2(b). We are left with the conclusion that, whatever is going on, the activation energy W_a observed in the low-temperature limit $\gamma = W_a/T \gg 1$ in a study of the temperature dependence of

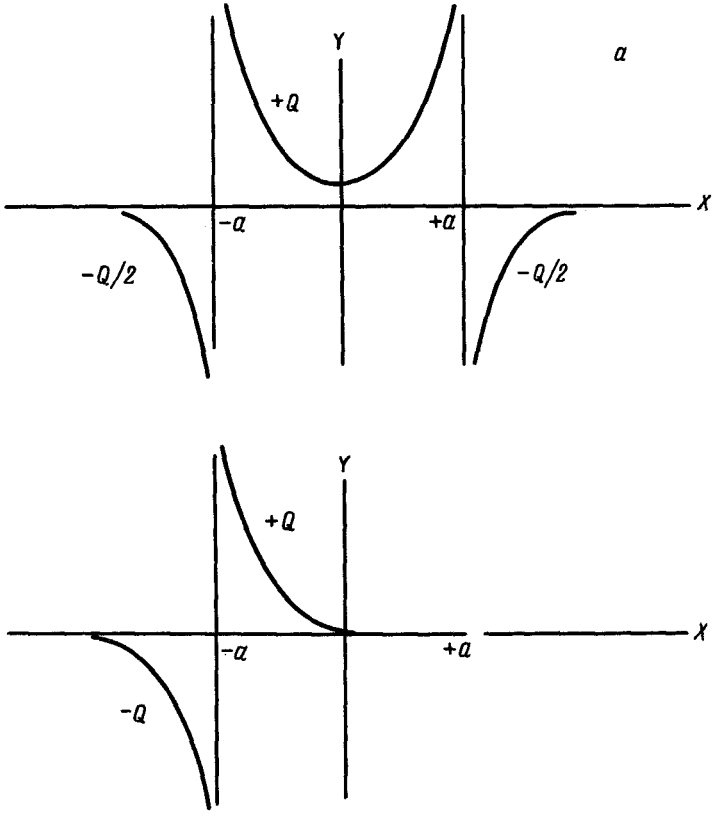

FIG. 2.

the conductance of a tunnel junction with a blocking grain cannot be defined in electrostatic terms; W_a is not equal to the quantity δW_c in (5).

2. It can thus be assumed that the energy W_a is formed near an individual tunnel junction. Let us assume for definiteness that we are dealing with a junction between a plane and a sphere of radius R, which are separated by a gap $d(r)$:

$$d(r) = d_0\left(1+\frac{1}{2}\frac{r^2}{R^2}\right), \quad r \ll R, \tag{6}$$

where r is the distance along the plane of the junction.

The proposal is to estimate W_a as the energy of a plane capacitor which has a unit charge e, in which the distance (D) between plates is $D = d_0 + 2r_d$ (where r_d is the Debye screening length inside the metal and is on the order of interatomic distances), and which has an area $S = \pi r_*^2$, where r_* is an effective radius. A tunneling occurs within this capacitor. The estimate of the energy is

$$W_a \simeq \frac{2e^2D}{\kappa r_*^2}, \tag{7}$$

where κ is the dielectric constant.

The quantity r_* arises as the radius of a path in a calculation of the total current through the tunnel junction. Competing factors here are (a) the tunneling probability, which falls off exponentially with an increase, as a function of r, in the thickness of the tunnel junction, $d(r)$ [see (6)], and (b) the Coulomb energy of an electron in the tunnel gap, written as in (7) with an arbitrary radius r and incorporated in the dispersion relation for the tunneling electrons. The latter step is legitimate in the Thomas–Fermi approximation. As a result, we find

$$r_*^4 = \frac{4\pi R^2\hbar e^2 D}{\kappa T d_0\sqrt{2m_*(V_0-\mu)}}. \tag{8}$$

Here V_0 is the barrier height, μ is the position of the Fermi level, and m_* is an effective mass.

Estimates (7) and (8) are valid if individual electron hops are predominant in the tunneling. A necessary condition for a current flow of this sort is the familiar requirement that the conductance G of the tunnel junction satisfy the limitation $G < e^2/h$. We are assuming here that this limitation is satisfied.

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