On the theory of the inelastic tunnel effect in normal metals

S. I. Shevchenko
Physico-technical Institute of Low Temperatures, Ukrainian Academy of Sciences
(Submitted July 10, 1972)
Zh. Eksp. Teor. Fiz. **64**, 1776-1785 (May 1973)

The problem of the tunnel effect in the presence of inelastic scattering of electrons by impurity centers imbedded in the barrier is solved. It is shown that the specific properties of the current-voltage characteristic due to the scattering significantly depend on the position of the impurity in the barrier. If the impurity centers are deeply located in the barrier then in the absence of impurity heating the correction to the current due to interaction with the impurity centers, is proportional to $(eV - \Omega)\theta(eV - \Omega)$ (eV is the applied voltage and Ω is the proper frequency of the impurity center). However if the impurity centers lie on the barrier surface or outside the surface, logarithmic singularities arise which change sign on change of polarity of the voltage. If the heat moving to the impurity centers is not removed to the external medium, the current correction will be proportional to $[(eV)^2 - \Omega^2]\theta(eV - \Omega)$, providing the impurities are located at a great depth and the impurity temperature will be a monotonic function of eV without saturation.

Following the work by Jaclevic and Lambe[1], who observed on tunnel-junction current-voltage characteristic (CVC) peaks connected with inelastic scattering of the tunneling electrons by impurities in the insulator, many experiments were reported in which the tunnel effect was used as a source of information on the energy spectrum of a substance introduced into the barrier. To determine the character of the singularities that appear on the CVC, they used initially[2] a method proposed in[3] (see also[4]). However, after it became clear[5] that this method can lead to unphysical results, a number of papers were published (see[5-8]), in which new schemes were proposed for calculating the inelastic tunnel current. These schemes, however, also contained assumptions that could not be rigorously justified. For example, Appelbaum and Brinkman[5] dispensed with the tunnel Hamiltonian, but calculated the current essentially in terms of the rate of change of the number of electrons on one of the sides of the insulating layer, whereas under stationary conditions this change is equal to zero. Davis[7] sought the wave function of the system in the form of a Slater determinant, and for convenience in calculation he added to each column of the determinant the same column multiplied by some small parameter. But since the number of columns is proportional to the number of electrons N in the system, the error incurred thereby is generally speaking of the order of N. In addition, Davis[7] used an approximation in which the electroneutrality condition was violated.

In the present paper, the density matrix formalism is used to solve the problem. This makes it possible to consider the case of nonzero temperatures and take into account effects due to heating of the impurity centers. It turns out that the current-voltage characteristic of the junction is essentially nonlinear when account is taken of the impurity-center heating.

1. FORMULATION OF PROBLEM

We regard the tunnel junction as two metallic half-spaces separated by an insulating layer. Among the atoms of the insulating layer we shall distinguish between the atoms of the dielectric liner and the impurity centers. The interaction with the liner atoms will be replaced by interaction with the external field—the barrier field. The interaction with the impurity centers will be taken into account separately. Instead of a real impurity center we shall consider here a harmonic oscillator, and assume that the interaction of the electron with the impurity center is proportional to the shift of the oscillator from the equilibrium position. In accord with the foregoing, we express the Hamiltonian of the entire system in the form

$$H = \sum_i -\frac{1}{2m}\frac{\partial^2}{\partial \mathbf{r}_i^2} + \sum_i U_0(\mathbf{r}_i) + \sum_i e\varphi(\mathbf{r}_i) + \sum_{in} U_1(\mathbf{r}_i - \mathbf{r}_{0n})\xi_n - \sum_n \frac{1}{2M_n}\frac{\partial^2}{\partial \xi_n^2} + \sum_n \frac{M_n}{2}\Omega_n^2\xi_n^2. \tag{1}$$

The second term describes the field of the barrier (insulating layer), the third the energy in the external field, the fourth the energy of interaction between the electrons and the impurity centers ($\mathbf{r}_{0n}$ is the coordinate of the n-th impurity center), and the last two describe the energy of the impurity centers.

If we denote by a_w and a_w^+ the operators for annihilation and creation of an electron in the state ψ_s, where

$$\left\{-\frac{1}{2m}\frac{\partial^2}{\partial \mathbf{r}^2} + U_0(\mathbf{r}) + e\varphi(\mathbf{r})\right\}\psi_s = \varepsilon_s\psi_s, \tag{2}$$

and by b_n and b_n^+ the operators of annihilation and production of the n-th boson, then the Hamiltonian H is expressed in terms of these operators in the form

$$H = \sum_s \varepsilon_s a_s^+ a_s + \sum_{spn} g_{spn} a_s^+ a_p (b_n^+ - b_n) + \sum_n \Omega_n (b_n^+ b_n + 1/2). \tag{3}$$

The matrix elements are

$$g_{spn} = -\frac{i}{(2M_n\Omega_n)^{1/2}}\int_{-\infty}^{\infty} \psi_s^*(\mathbf{r}) U_1(\mathbf{r} - \mathbf{r}_{0n})\psi_p(\mathbf{r})\, d\mathbf{r}. \tag{4}$$

We are interested in the current flowing in the system when an external voltage is applied to the junction. We calculate the current with the aid of the usual expression

$$I = \int_S \mathrm{Sp}\{j\rho\} dS = \int_S \langle j\rangle dS, \tag{5}$$

where j is the current-density operator, S is the area of the tunnel junction, and the statistical operator ρ satisfies the Liouville equation

$$i\dot{\rho} = [H, \rho]. \tag{6}$$

The problem consists of solving Eq. (6), which will be done in the sections that follow; we make at present one remark concerning the notation.

The subscript s in (2) stands for the aggregate of quantum numbers characterizing the eigenstate. It is convenient to separate from this aggregate the index σ, which indicates from which direction the given electron is incident on the insulating layer. We replace σ by a minus sign in the case of incidence from the left, and by a plus sign in the case of incidence from the right. We shall thus replace, when the need arises, s by $k\sigma$ (k is not the modulus of the wave vector, $k = \{k_x, k_y, k_z\}$), and in order not to clutter up the formulas we shall use the following symbols:

$$\varepsilon_s = \varepsilon_{k\sigma} = \varepsilon_\sigma(k), \quad g_{spn} = g_{k\sigma, k'\sigma', n} = g_{\sigma\sigma'}(k, k', n) \tag{7}$$

etc.

2. SOLUTION OF THE LIOUVILLE EQUATION

We consider first the case when there is no interaction with the oscillators. It is then necessary to solve Eq. (6) with the Hamiltonian

$$H_0 = \sum_s \varepsilon_s a_s^+ a_s. \tag{8}$$

The Hamiltonian H_0 is diagonal in the representation of the operators a, The numbers of particles on the right (N_+) and on the left (N_-) of the insulating layer are not diagonal in this representation. For example, the number of electrons in the left-hand metal is

$$N_- = \int \psi^+(\mathbf{r})\psi(\mathbf{r})\theta(-z)\,d\mathbf{r} = \sum_{\substack{k,k'\\ \sigma\sigma'}} C_{\sigma\sigma'}(k, k')a_\sigma^+(k)a_{\sigma'}(k'), \tag{9}$$

$$C_{\sigma\sigma'}(k, k') = \int \psi_{k\sigma}^*(\mathbf{r})\psi_{k'\sigma'}(\mathbf{r})\theta(-z)\,d\mathbf{r}. \tag{10}$$

The wave functions that enter in this formula satisfy the conditions

$$\psi_+ \sim O(T) \text{ if } z<0, \quad \psi_- \sim O(T) \text{ if } z>0. \tag{11}$$

Here T^2 is the transparency of the barrier. These relations do not hold only for states whose energy is commensurate with or larger than the height of the potential barrier U_0. But if the difference between U_0 and the Fermi energy ϵ_F is much larger than the electron temperature T_e, then the probability of excitation of such states will be exponentially small ($\sim \exp\{-(U_0 - \epsilon_F)/T_e\}$). We shall consider precisely this case, and will neglect such states.

With the aid of (11) it is easy to establish that the coefficients C_{ps} have the following properties:

$$\begin{gathered} C_{--}(k, k') = \delta_{kk'} + O(T^2), \quad C_{++}(k, k') \sim O(T^2), \\ C_{+-}(k, k'), \quad C_{-+}(k, k') \sim O(T). \end{gathered} \tag{12}$$

Consequently, the number of particles to the left of the barrier can be written, with accuracy linear in O(T), in the form

$$N_- = \sum_k a_-^+(k)a_-(k) + \sum_{k,k'} C_{-+}(k, k')a_-^+(k)a_+(k') + \text{h.c.} \tag{13}$$

An analogous expression holds also for the number of particles to the right of the insulating layer (the minus signs in the subscripts should be replaced by plus, the plus by minus, and a minus sign should be placed before C).

We can, however, go over to a new representation in which the particle numbers N_- and $N_+ = N - N_-$ (N is the total number of particles in the system) are diagonal and the Hamiltonian H_0 is no longer diagonal (cf.[9,10]). We introduce to this end the operators

$$\begin{aligned} \alpha_-(k) &= a_-(k) + \sum_{k,k'} C_{-+}(k, k')a_+(k'), \\ \alpha_+(k) &= a_+(k) - \sum_{k,k'} C_{+-}(k, k')a_-(k'). \end{aligned} \tag{14}$$

With the aid of Eq. (13) and an analogous expression for N_+ we obtain, with accuracy linear in O(T),

$$N_- = \sum_k \alpha_-^+(k)\alpha_-(k), \quad N_+ = \sum_k \alpha_+^+(k)\alpha_+(k). \tag{15}$$

By direct calculation of the commutators we obtain with the same accuracy

$$\alpha_s\alpha_{s'} + \alpha_{s'}\alpha_s = 0, \quad \alpha_s^+\alpha_{s'} + \alpha_{s'}\alpha_s^+ = \delta_{ss'}. \tag{16}$$

Substituting (14) in (8) we find that the Hamiltonian H_0 expressed in terms of the operators α takes the form

$$\begin{aligned} H_0 = &\sum_k \varepsilon_-(k)\alpha_-^+(k)\alpha_-(k) + \sum_k \varepsilon_+(k)\alpha_+^+(k)\alpha_+(k) \\ &+ \sum_{k,k'} T_{+-}(k, k')\alpha_+^+(k)\alpha_-(k') + \text{h.c.} \end{aligned} \tag{17}$$

The matrix elements are here

$$T_{+-}(k, k') = [\varepsilon_+(k) - \varepsilon_-(k')]C_{+-}(k, k'). \tag{18}$$

Expression (17), as expected, coincides with the tunnel Hamiltonian proposed in[3].

The advantage of the new representation is that now Eq. (6) is easy to solve. To this end, the operator ρ_0, satisfying the equation

$$i\dot{\rho}_0 = [H_0, \rho_0], \tag{19}$$

must be represented as a series in powers of T:

$$\rho_0 = \rho_{00} + \rho_{01} + \ldots \tag{20}$$

Gathering in (19) terms of the same order in T, we easily obtain the corresponding equations for ρ_{0i} and find that

$$\begin{aligned} \rho_{00} = Q_e^{-1}\exp\Big\{-\beta_e\Big[&\sum_k (\xi_+(k) + eV)\alpha_+^+(k)\alpha_+(k) \\ &+ \sum_k \xi_-(k)\alpha_-^+(k)\alpha_-(k)\Big]\Big\}, \end{aligned} \tag{21}$$

$$\begin{aligned} Q_e = \mathrm{Sp}\exp\Big\{-\beta_e\Big[&\sum_k (\xi_+(k) + eV)\alpha_+^+(k)\alpha_+(k) \\ &+ \sum_k \xi_-(k)\alpha_-^+(k)\alpha_-(k)\Big]\Big\}; \end{aligned} \tag{22}$$

$$eV = e[\varphi(-\infty) - \varphi(\infty)], \quad \xi_\sigma(k) = \varepsilon_\sigma(k) - \varepsilon_F. \tag{23}$$

where $\beta_e = 1/T_e$. The matrix ρ_{01} is equal to

$$\rho_{01} = \Big[\sum_{k,k'} \frac{T_{+-}(k, k')\alpha_+^+(k)\alpha_-(k')}{\xi_-(k') - \xi_+(k) + i\delta} - \text{h.c.}, \rho_{00}\Big]. \tag{24}$$

There is no need to expand the commutator in this formula, for it is convenient to have ρ_{00} in pure form when averaging with ρ_{01}.

In the presence of interaction with the oscillators, it is necessary to solve Eq. (6) with the total Hamiltonian (3), after first expressing H in terms of the operators[1)] α. If it is assumed that the interaction with the oscillators is weak, then the Hamiltonian terms containing g

can be regarded as perturbations. Representing ρ as a series in powers of g:

$$\rho = \rho_0 + \rho_1 + \rho_2 + \ldots, \tag{25}$$

we can find, in analogy with the above, the matrices ρ_i:

$$\rho_0 = (\rho_{00} + \rho_{01} + \ldots) Q_V^{-1} \exp\left\{-\beta_V \sum_n \Omega_n (b_n^+ b_n + 1/2)\right\}; \tag{26}$$

$$Q_V = \mathrm{Sp} \exp\left\{-\beta_V \sum_n \Omega_n (b_n^+ b_n + 1/2)\right\}, \tag{27}$$

where $\beta_V = 1/T_V$ and T_V is the temperature of the oscillators. We note that ρ_0 in (26) does not coincide with ρ_0 in (20). We shall take ρ_0 to mean from now on the quantity defined by (26).

The matrix ρ_1 will not be needed in what follows, since it is linear in the boson operators, and averaging b or b^+ with ρ_0 yields zero. The matrix ρ_2 is given by

$$\rho_2 = -\int_{-\infty}^{0} \Big[\sum_{s'p'n'} g_{s'p'n'} \alpha_{s'}^+(t) \alpha_{p'}(t) b_{n'}^+(t) + \text{h.c.}, \Big[\sum_{spn} \frac{g_{spn} \alpha_s^+(t) \alpha_p(t) b_n^+(t)}{i(\xi_s - \xi_p + \Omega_n - i\delta)} + \text{h.c.}, \rho_0 \Big] \Big] dt. \tag{28}$$

3. CALCULATION OF THE CURRENT

We are interested only in the current due to the interaction of the electrons with the oscillators. We shall denote it by I_g. To calculate it we average the current density operator, which is equal to

$$\hat{j} = \frac{ie}{2m} \sum (\psi_p \nabla \psi_s^* - \psi_s^* \nabla \psi_p) a_s^+ a_p \equiv \sum j_{sp} a_s^+ a_p, \tag{29}$$

with ρ_2 from (28). After substituting (28) and (29) in (5) and making some simple algebraic transformations, we obtain

$$I_g = \int \sum dS\, A_{psp's'n} \langle [\alpha_p^+ \alpha_s \alpha_{p'}^+ \alpha_{s'}] b_n^+ b_n + \alpha_p^+ \alpha_s \alpha_{p'}^+ \alpha_{s'} \rangle_0 + \text{c.c.} \tag{30}$$

Here $A_{\ldots}$ are coefficients whose explicit form is of no interest at present, and the subscript 0 at the angle brackets shows that the averaging is carried out with ρ_0.

We assume in this section that the oscillator temperature is $T_V = 0$, and then $\langle b_n^+ b_n \rangle_0 = 0$. The remaining mean value of the four operators can be expressed in terms of the mean value of two operators, since

$$\rho_0 \sim \rho_{00} + \rho_{01}(\rho_{00}) + \ldots,$$

and Wick's theorem can be used when averaging with ρ_{00}. Neglecting the terms obtained by averaging with ρ_{01} (see footnote 2 below), we obtain from (30)

$$I_g = \int \sum_{s,p} dS \frac{n_p(1-n_s) g_{spn}^*}{\xi_s - \xi_p + \Omega_n + i\delta} \Big(\sum_{s'} \frac{1}{\xi_{s'} - \xi_s - i\delta} j_{ss'} g_{s'pn} - \sum_{p'} \frac{1}{\xi_p - \xi_{p'} - i\delta} g_{sp'n} j_{p'p} \Big) + \text{c.c.}, \tag{31}$$

where the occupation numbers $n \equiv \langle \alpha^+ \alpha \rangle_{00}$ are equal to

$$n_-(k) = \Big[\exp\Big(\frac{\xi_-(k)}{T}\Big) + 1\Big]^{-1}; \quad n_+(k) = \Big[\exp\Big(\frac{\xi_+(k) + eV}{T}\Big) + 1\Big]^{-1}. \tag{32}$$

The current I_g does not depend on z. It will be convenient for us to calculate it as $z \to -\infty$. If the electrons are specularly reflected from the insulating layer, the wave functions at the point with coordinates z, ρ are equal to

$$\psi_- = \exp(ik_z z + i\mathbf{k}_\rho \rho) + R_k \exp(-ik_z z + i\mathbf{k}_\rho \rho), \quad \psi_+ = T_k \exp(-ik_z z + i\mathbf{k}_\rho \rho). \tag{33}$$

The coefficients T and R in these formulas are determined by the explicit form of the potential barrier separating the two metals, and we always have $|R_k|^2 + |T_k|^2 = 1$.

With the aid of (33) and (29) we obtain the matrix elements of the current operator

$$j_{--}(k,k') = i\frac{e}{m} 2k_z \sin(k_z' - k_z) z \exp(i(\mathbf{k}_\rho' - \mathbf{k}_\rho)\rho), \tag{34}$$

$$j_{-+}(k,k') = j_{+-}^*(k',k) = -\frac{e}{m} k_z T_k R_k^* \exp[i(k_z' - k_z) z + i(\mathbf{k}_\rho' - \mathbf{k}_\rho)\rho]. \tag{35}$$

Since the matrix elements $j_{--} \sim 1$ and j_{+-}, $j_{-+} \sim O(T)$, it would seem that it suffices to retain in (31) only the terms with j_{--}. Actually, this is not quite so. A distinction must be made between the case when the oscillators lie deep in the insulating layer, and the case when they are on the surface or are even outside the insulating layer. We consider first the case when the impurity centers lie deep in the layer. All the matrix elements are then $g \sim U_1 \cdot O(T)$ and we can indeed retain in (31) only the terms with j_{--}. Substituting (34) in (31) and integrating, we obtain

$$I_g = 2\pi e \sum_m \iint |g_{+-}(k,k',m)|^2 \{n_-(k')[1-n_+(k)]\delta(\xi_+ - \xi_- + \Omega_m) - n_+(k)[1-n_-(k')]\delta(\xi_-(k') - \xi_+(k) + \Omega_m)\} N(\xi_k) N(\xi_{k'})\, d\xi_k\, d\xi_{k'}. \tag{36}$$

Here $N(\xi)$ is the density of states with energy ξ. The presence of δ functions in (36) shows that in the case when the impurity centers are deep in the barrier the contribution to the current is made only by transitions with energy conservation. As a result, the dependence of the conductivity (equal by definition to the derivative dI_g/deV) on the voltage has a steplike form. Near $eV = \pm\Omega_m$ we have

$$dI_g/deV = 2\pi e \sum_m |g_{+-}(k_F, k_F, m)|^2 N^2(0)\, \theta(|eV| - \Omega_m). \tag{37}$$

In view of the dependence of g on the potential difference (see (4) and (2)) we can conclude that the current-voltage characteristic, generally speaking is not symmetrical with respect to replacement of V by $-V$. The asymmetry of the CVC about the $V = 0$ axis was experimentally observed in[11], where a perfectly clear interpretation of the result is given, so that we shall not dwell on this any longer.

Let now the oscillators be located outside the insulating layer or on its surface, we assume, for concreteness, that they lie in the left-hand metal. In this case the matrix elements g_{--} and g_{-+} are already of different order:

$$g_{--} \sim U_1, \quad g_{+-} \sim U_1 \cdot O(T).$$

Therefore it suffices to retain in (31), at the terms with g_{+-}, only the matrix elements j_{--}, and at the terms with g_{--} it is necessary to take also j_{+-} (and j_{-+}) into account[2]. Substituting (35) in (31), we find that it is necessary to add to the current (36) another current, whose value at $T_e \ll \Omega_n$ is

$$I_{g1} = e \sum_m \iint \Big\{ \frac{n_-(k')[1-n_+(k)] g_{-+}(k',k,m) g_{--}(k,k',m) i T_k^* R_k}{\xi_+(k) - \xi_-(k') + \Omega_m + i\delta} - \frac{n_+(k)[1-n_-(k')] g_{+-}(k,k',m) g_{--}(k',k,m) i T_k R_k^*}{\xi_-(k') - \xi_+(k) + \Omega_m + i\delta} + \text{c.c.} \Big\} N(\xi) N(\xi')\, d\xi\, d\xi'. \tag{38}$$

Unlike the case when the impurities are deep in the barrier, the contribution to the current is made here also by virtual transitions with energy nonconservation in the intermediate states, since the principal-value integrals no longer cancel out in this case. The terms with the δ-functions, as in (36), lead to a stepwise dependence on the voltage, and the terms with the integrals in the sense of the principal value lead to logarithmic singularities at $eV = \pm\Omega_m$:

$$\frac{dI_{g1}}{deV} = \sum_m \pi \operatorname{Re} B_m(0)\,\theta(|eV|-\Omega_m) + \operatorname{sign}(eV)\operatorname{Im} B_m(0)\ln\frac{|eV|-\Omega_m}{E_c}; \tag{39}$$

$$B_m(0) = 2eg_{-+}(k_F, k_F, m)\,g_{--}(k_F, k_F, m)\,T_k{}^2R_kN^2(0), \tag{40}$$

where E_c is a certain cutoff energy. The need for cutoff arises in connection with the neglect of the dependence of B on the energy in the integration in (38).

For the case $T_e = 0$, the current I_{g1} was first calculated by an exceptionally cumbersome method by Davis[7]. From (39) follows the interesting result that the sign at the singularity is reversed when the polarity of the voltage is reversed, in the case when the impurity lies outside the insulating layer. Expressions (37) and (39) yield the solution of the problem of the character of the CVC singularities in the inelastic tunnel effect.

4. EFFECT OF HEATING

Starting with formula (31) of the preceding section, we have assumed that the oscillator temperature is equal to zero. Actually this temperature is not an independent parameter. The temperature T_V should be determined from the energy-balance equation and in the general case is a function of the potential difference eV. To write down the balance equation, it is necessary to take into account the interaction of the oscillators with the thermostat. In a consistent approach, it is necessary to take this into account also in the Hamiltonian H, but if the interaction with the thermostat is small enough, then the presence of the temperature can be accounted for only in the balance equation. We shall take the heating effects into account only for the case of impurity centers lying deep in the barrier.

Thus, let $T_V \neq 0$. Introducing the notation

$$N_m = \langle b_m{}^+ b_m\rangle_0 = \left[\exp\left(\frac{\Omega_m}{T_V}\right) - 1\right]^{-1}, \tag{41}$$

we find with the aid of (30) that the current I_g acquires a new term

$$I_{g2} = -2\pi e\sum_m \iint |g_{+-}(k,k',m)|^2 N(\xi_k)N(\xi_{k'})N_m\{n_+(k)[1-n_-(k')]$$
$$\times[\delta(\xi_-(k')-\xi_+(k)-\Omega_m)+\delta(\xi_-(k')-\xi_+(k)+\Omega_m)] - n_-(k')[1-n_+(k)]$$
$$\times[\delta(\xi_+(k)-\xi_-(k')-\Omega_m)+\delta(\xi_+(k)-\xi_-(k')+\Omega_m)]\}d\xi\,d\xi'. \tag{42}$$

This expression differs from (36) in that it contains terms describing transitions from the region + to − and from − to +, in which the electrons acquire an energy Ω_m from the oscillators. This circumstance is perfectly natural, since such processes are not forbidden at nonzero oscillator temperature.

To assess the character of the voltage dependence of the current $I_g + I_{g2}$, we must find the oscillator temperature T_V. We perform the corresponding calculations under the assumption that all the oscillators have the same natural frequency Ω and that the interaction of the oscillators with the thermostat (crystal lattice) tends to zero[3]. We assume also (this is a situation most frequently encountered in experiment) that $\epsilon_F \gg \Omega \gg T_e$ and $\epsilon_F \gg eV$. The factors preceding the curly brackets in the integrands of (39) and (42) can then be expressed in terms of their values on the Fermi surface. Introducing the notation

$$\frac{1}{R} = 2\pi e\sum_m |g_{+-}(k_F, k_F, m)|^2N^2(0) \tag{43}$$

and integrating with respect to ξ in (39) and (42), we obtain

$$R[I_g + I_{g2}] = (N+1)[F(\Omega-eV) - F(\Omega+eV)] + N[F(-\Omega-eV) - F(-\Omega+eV)]. \tag{44}$$

Here F(x) stands for

$$F(x) = x[\exp(x/T_e) - 1]^{-1}, \tag{45}$$

and N is the value of N_m from (41) at $\Omega_m = \Omega$.

The first term in (44) describes transitions in which the electrons give up energy to the oscillator, and the second transitions in which the electrons themselves acquire energy. Taking this circumstance into account, we can easily see that the balance equation, which determines the oscillator temperature, takes the following form[4]:

$$(N+1)[F(\Omega-eV) + F(\Omega+eV)] = N[F(-\Omega-eV) + F(-\Omega+eV)]. \tag{46}$$

A simple analysis of this equation yields the oscillator temperature as a function of eV:

$$T_V = \begin{cases} T_e & \text{if } T_e \gg eV > 0 \quad (47a)\\ T_e(1 + eV/(\Omega-eV)) & \text{if } \Omega - eV,\ eV \gg T_e \quad (47b)\\ \Omega/\ln(2\Omega/T_e) & \text{if } T_e \gg |\Omega - eV| \quad (47c)\\ eV/2 & \text{if } eV \gg \Omega \quad (47d)\end{cases}$$

Similar results hold also for the case $eV < 0$.

It appears that attention should be called to two results, namely (47b) and (47d). The first shows that even in the region where $\Omega - eV \gg T_e$ and the current flowing through the junction is exponentially small ($\sim \exp[-(\Omega - eV)/T_e]$) the temperature T_V can exceed appreciably the electron temperature T_e. It follows from (47d) that the oscillator temperature does not saturate with increasing eV, as might be assumed because the oscillators give up energy to the tunneling electrons at an ever increasing intensity with increasing T_V.

Substituting (47) in (44) we can obtain the dependence of the current on the voltage eV. In the general case this results in rather cumbersome expressions. It is possible, however, to obtain very simple results by taking the following circumstance into account: In experiment one usually measures not the current $I_g + I_{g2}$ itself, but the second derivative of the current with respect to the voltage. The reason is that the second derivative has singularities at $|eV| = \Omega$. These singularities are quite sharp only if eV experiences only large scale changes, for which $|\Delta eV| \gg T_e$. If it is assumed that eV in (44) and (46) is just such a quantity, the N is equal to (it is assumed that $eV > 0$)

$$N = \frac{eV-\Omega}{2\Omega}\theta(eV-\Omega), \tag{48}$$

and (44) takes the following form:

$$[I_g + I_{g2}]R = \frac{(eV)^2-\Omega^2}{\Omega}\theta(eV-\Omega). \tag{49}$$

It follows therefore that heating of the oscillators leads at $eV \gg \Omega$ to a quadratic voltage dependence of the

current due to the interaction of the electrons with the oscillators. It is also easy to see (see (44) and (48)) that in the presence of heating the second derivative of (49) at the point $eV = \Omega$ is twice as large as at $T_V = 0$.

The results (47), (48), and (49) were obtained under the assumption that the oscillators do not radiate into the surrounding medium the energy acquired from the tunneling electrons. In the presence of such radiation, the temperature of the oscillators will obviously be lower than in (47), so that these formulas give the upper bound of T_V.

I take the opportunity to thank I. O. Kulik, who called my attention to the group of problems considered in the paper, and L. A. Pastur for numerous useful discussions.

[1)]After going over to the operators α, the matrix elements g_{sp} go over to certain new matrix elements $\tilde{g}_{sp}$. Since $\tilde{g}_{sp}$ is of the same order as the corresponding g_{sp}, and we do not need the exact values of the matrix elements, we shall write g_{sp} in lieu of $\tilde{g}_{sp}$, as before.

[2)]In this case, when calculating the mean value, $\langle \alpha_p + \alpha_s \alpha_{p'} \alpha_{s'} \rangle_0$, it is generally impossible to neglect the terms obtained from the averaging with ρ_{01}. Calculation shows, however, that the contribution to the current from these terms is small in comparison with (36) and (38).

[3)]The simplest justification of this assumption is provided by the experiments of Klein and Zeger [12], who observed strong heating of the impurity centers in the barrier, thus indicating weak heat conduction from the impurities to the lattice.

[4)]It may seem strange at first glance that the balance equation, meaning also T_V, does not depend on the electron-oscillator interaction constant g. This circumstance, however, is simply due to the fact that the interaction of the oscillators with the lattice is customarily assumed equal to zero. In this case, even an infinitesimally weak interaction between the oscillators and the electrons can lead to strong heating of the oscillators. This approximation is valid if the average lifetime τ of the molecular excitation is much larger than the average time τ_{em} between two successive inelastic collisions between the electrons and the molecule. With increasing current, τ_{em} decreases so that at large currents we have $\tau \gg \tau_{em}$. Numerical estimates for τ and τ_{em} are given, e.g., in [11].

[1] R. C. Jaklevic and I. Lambe, Phys. Rev. Lett., 17, 1139 (1966).
[2] D. I. Scalapino, Electron Tunneling as a Probe of Barrier Excitations, Preprint, 1968.
[3] M. H. Cohen, L. M. Falikov, and I. C. Phillips, Phys. Rev. Lett., 8, 31 (1962).
[4] I. O. Kulik and I. K. Yanson, Effekt Dzhozefsona v sverkhprovodyashchikh tunnel'nykh strukturakh (Josephson Effect in Superconducting Tunnel Structures) Nauka (1970).
[5] I. A. Appelbaum and W. F. Brinkman, Phys. Rev., 183, 553 (1969).
[6] I. A. Appelbaum and W. F. Brinkman, Phys. Rev., 186, 464 (1969).
[7] L. C. Davis, Phys. Rev., B2, 1714 (1970).
[8] G. K. Birkner and W. Shatthe, Phys. Lett. 36A, 3 (1971).
[9] Yu. M. Ivanchenko, K. teorii mnogochastichnogo tunnelirovaniya (On the Theory of Multiparticle Tunneling) Preprint, Donetsk (1965).
[10] A. V. Svidzinskiĭ and V. A. Slyusarev, Teoriya tunnelirovaniya v sverkhprovodnikakh (Theory of Tunneling in Superconductors), Preprint, Khar'kov (1970).
[11] I. K. Yanson, N. I. Bogatina, B. I. Verkin, and O. I. Shklyarevskiĭ, Zh. Eksp. Teor. Fiz. 62, 1023 (1972) [Sov. Phys.-JETP 35, 540 (1972)].
[12] I. Klein and A. Zeger, Phys. Lett., 30A, 96 (1969).

Translated by J. G. Adashko
191