Quantum fluctuations of the charge of a metal particle under the Coulomb blockade conditions

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(Submitted 26 September 1990)
Zh. Eksp. Teor. Fiz. **99**, 1598–1611 (May 1991)

An investigation is made of the behavior of the charge of a small metal particle, tunnel-coupled to a massive electrode, as a function of an external electric field. The step-like field dependence of the charge due to the Coulomb blockade is shown to be smeared out by quantum fluctuations. A relationship established between this and Kondo problems is used to calculate the shape of the smeared-out steps in the case of a low-transparency tunnel barrier.

1. INTRODUCTION

Studies of tunnel junctions formed by two massive metal electrodes joined by tunnel layers containing a small metal particle (granule) have shown that the tunnel current is suppressed at low longitudinal voltages.[1-4] This effect is explained in Ref. 1 as follows: a change in the charge of a metal particle by an amount to equal to an electron charge e in the course of an elementary tunneling event results in a finite change in the electrostatic energy $\Delta E \propto e^2/C$ (here, C is the characteristic capacitance of the granule). Therefore, only electrons with sufficiently high energies $\varepsilon > \Delta E$ can participate in the tunneling processes and their number at low temperatures $T < \Delta E$ is small, which is the reason for suppression of the current (known as the Coulomb tunneling blockade).

In contrast to a large number of investigations of the manifestation of the Coulomb blockade in the current-voltage characteristics of tunnel junctions (see, for example, the review in Ref. 5), our aim will be to consider fluctuations of the granule charge. The investigated system is shown in Fig. 1. The charge carried by a granule 1 may change because of the tunnel coupling to the bank 0. The role of the electrode 2 (gate) is to create an electric field around the granule so that after allowing for this field the electrostatic energy of the system considered as a function of the granule charge Q is

$$E = \frac{Q^2}{2C} + \zeta VQ. \tag{1}$$

Here, V is the voltage applied to the gate 2 (Fig. 2) and the dimensionless factor ζ is governed by the geometry of the system [for details of the derivation of Eq. (1) see, for example, Ref. 6]. We shall limit our task to a calculation of the average charge $\overline{Q}$ of such a granule as a function of V at zero absolute temperature. In fact the $\overline{Q}(V)$ dependence was used by Averin and Likharev[7] to calculate the profile of what are known as one-electron voltage oscillations across a tunnel junction under a given-current conditions. It was assumed in Ref. 7 however that the tunnel coupling is negligible; in this case the charge $\overline{Q}(V)$ can be found by minimizing the electrostatic energy (1) with allowance for the discrete nature of the charge $Q = ne$:

$$\overline{Q}^{(0)}(V) = -e\left[\frac{\zeta VC}{e} + \frac{1}{2}\right] \tag{2}$$

[the square brackets in Eq. (2) enclose an integer]. In view of the energy degeneracy described by Eq. (2) in respect of the value of Q, which appears at $V = V_n$, where

$$\zeta V_n = -(2n-1)\frac{e}{2C}, \tag{3}$$

the charge described by Eq. (2) exhibits a jump by $\pm e$ at the same values of the voltage. We can easily show that these jumps are smoothed out at a nonzero temperature T. We shall show however that because of quantum fluctuations of the charge the $\overline{Q}(V)$ dependence is continuous even at $T = 0$ if the transparency of the insulating layer between the granule and the bank differs from zero.

In Sec. 2 we shall calculate the correction to the dependence (2) in the first order of perturbation theory in terms of this transparency. The results obtained using perturbation theory describe satisfactorily the dependence of the charge on the gate voltage everywhere with the exception of the vicinity of the points (voltages) of charge degeneracy given by Eq. (3), where the correction diverges logarithmically. As pointed out in Ref. 6, the origin of this divergence is the same as in the familiar Kondo problem. It is shown in Sec. 3 that near the charge degeneracy described by Eq. (3) the procedure of calculating the charge $\overline{Q}(V)$ can be reduced formally to finding the magnetic moment of an impurity described by the anisotropic Kondo model. This analogy with the familiar Kondo model allows us solve completely the problem of calculation of the $\overline{Q}(V)$ dependence. We have to distinguish two types of tunnel junction: point contacts and

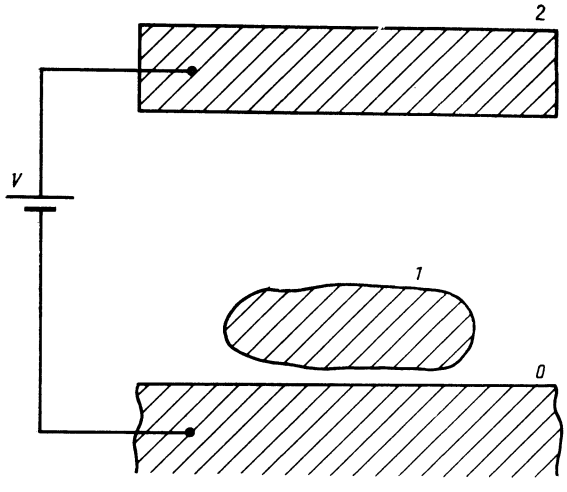

FIG. 1. Metal particle (granule) 1 in the field of two massive electrodes 0 (bank) and 2 (gate). It is assumed that tunneling of electrons is possible only between the granule and the lower electrode.

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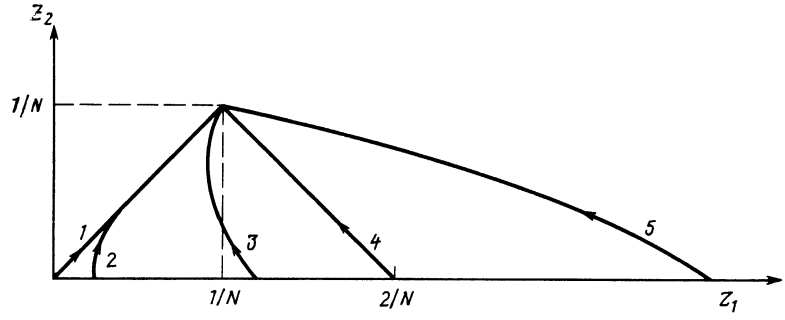

FIG. 2. General form of the solutions of the system of equations (49), (50) obtained for different values of $Z_1(0) = \nu J_0$. All the solutions are in the form of arcs of the hyperbolas (57) and they terminate at the point $Z_1 = Z_2 = 1/N$. The solution 1 corresponds to the limiting case of the isotropic Kondo model $J_\perp = J_z$.

wide junctions. It is shown in Sec. 4 that in the case of a point contact, in which the transparency of the insulating layer differs from zero only in a narrow region with transverse dimensions of the order of the Fermi wavelength λ_F, the problem reduces to the exact solution of the Kondo problem[8-11] obtained by the Bethe method. The opposite limiting case of a wide contact can be investigated by the renormalization group method. The results are summarized in Sec. 5 and the feasibility of verifying them experimentally is considered.

2. PERTURBATION THEORY

We shall calculate the $\bar{Q}(V)$ dependence, allowing for the tunneling of electrons between the granule and the bank and writing down the Hamiltonian of the system in the form

$$H=H_0+H_T, \quad H_0=\sum_k \varepsilon_k a_k^+ a_k+\sum_p \varepsilon_p a_p^+ a_p+\frac{\hat{Q}^2}{2C}+\varphi\hat{Q},$$
$$H_T=\sum_{k,p}(t_{kp}a_k^+ a_p+t_{kp}^* a_p^+ a_k). \tag{4}$$

Here, a_k and a_p are the electron annihilation operators in the bank and in the granule; the corresponding energies ε_k and ε_p are measured from the Fermi level and occupy a band $-W<\varepsilon_k, \varepsilon_p<W$; t_{kp} and t_{kp}^* are the matrix elements that describe the tunneling of electrons from the granule to the bank and vice versa. The Coulomb energy is written in the simplest form of Eq. (1) and the gate voltage V is allowed for by introducing a parameter $\varphi\equiv\zeta V$. The granule charge operator is

$$\hat{Q}=e\sum_p[a_p^+ a_p-\theta(-\varepsilon_p)]. \tag{5}$$

We shall calculate the average charge of the granule

$$\bar{Q}(\varphi)=\langle\Psi|\hat{Q}|\Psi\rangle \tag{6}$$

in the ground state $|\Psi\rangle$ of the Hamiltonian (4). The second term in Eq. (5), which includes the Heaviside function $\theta(x)$, shifts the origin of the charge scale in such a way that $\bar{Q}(\varphi=0)=0$. As a first step, we shall include the tunnel Hamiltonian H_T using perturbation theory and find the second-order correction to the charge (2). We shall confine ourselves to the values of φ in the range

$$-\frac{e}{2C}<\varphi<\frac{e}{2C}, \tag{7}$$

which corresponds to the unperturbed value $\bar{Q}^{(0)}=0$ [see Eq. (2)]. The results can then be generalized to any value of φ employing the obvious relationship

$$\bar{Q}\left(\varphi+\frac{e}{C}\right)=Q(\varphi)-e. \tag{8}$$

Substituting in Eq. (6) the wave function of the ground state $|\Psi\rangle$ in the form of a perturbation-theory series, we obtain

$$\bar{Q}^{(2)}(\varphi)=e\sum_{k,p}|t_{kp}|^2\left\{\frac{\theta(-\varepsilon_k)\theta(\varepsilon_p)}{(\varepsilon_p-\varepsilon_k+e^2/2C+e\varphi)^2}-\frac{\theta(\varepsilon_k)\theta(-\varepsilon_p)}{(\varepsilon_k-\varepsilon_p+e^2/2C-e\varphi)^2}\right\}. \tag{9}$$

It is convenient to replace the matrix elements t_{kp} with a dimensionless parameter

$$g=\sum_{k,p}|t_{kp}|^2\delta(\varepsilon_k)\delta(\varepsilon_p), \tag{10}$$

which represents the conductance $G\equiv G_q g$, of the tunnel layer, reduced to the universal value $G_q\equiv 2\pi e^2/\hbar$. Calculation of the sum in Eq. (9) gives

$$\bar{Q}^{(2)}=eg\ln\frac{e/2C-\varphi}{e/2C+\varphi}. \tag{11}$$

The physical meaning of the correction described by Eqs. (9) and (11) is that the perturbation H_T gives rise to the following two types of virtual transitions: 1) the transfer of an electron from the bank to the granule, increasing the charge of the granule from $Q=0$ to $Q=e$; 2) the transfer of an electron from the granule to the bank, reducing the granule charge from $Q=0$ to $Q=-e$.

Since these two types of transition produce opposite changes of the charge, some of the contributions to Eq. (9) corresponding to high energies $E>e^2/C$ of virtual states cancel out. The correction (11) which then remains is due to the fact that if $\varphi\neq 0$, then one of the possible types of virtual transition is related to a smaller increase in the electrostatic energy of the system.

The small parameter is g and it allows us to use an expansion of $\bar{Q}(\varphi)$ as a perturbation-theory series. We shall assume that everywhere we have $g\ll 1$. Then, Eq. (11) describes correctly the dependence $\bar{Q}(\varphi)$ in a large part of the interval defined in Eq. (7). However, in the vicinity of the points $\varphi=\pm e/2C$ the smallness of the parameter g is compensated by a large logarithmic factor. Therefore, in calculation of $\bar{Q}(\varphi)$ near the ends of the interval (7) we have to allow for the next orders of the perturbation-theory series. We shall consider specifically the vicinity of the point

$\varphi = -e/2C$, i.e., we shall assume that

$$\varphi = -\frac{e}{2C} + U, \tag{12}$$

where $U \ll e/C$. For this selection of φ the electrostatic energies of the states with $Q = 0$ and $Q = e$, given by Eq. (1), are close: $E(0) = 0$ and $E(e) = eU$, whereas the energies of the remaining charge states of the granule are $E(Q) > e^2/C \gg eU$. We have seen already that transitions to states with energies $E > e^2/C$ make no contribution to the average charge. Therefore, in a study of the behavior of $\overline{Q}(\varphi)$ near the point $\varphi = -e/2C$ we can simplify the Hamiltonian (4) by removing from it the states of the granule whose charge differs from $Q = 0$ or $Q = e$, and at the same time limiting the width of the band to e^2/C. The arbitrary nature of this truncation procedure does not affect significantly the value of $\overline{Q}(\varphi)$, which depends logarithmically on e^2/C. The Hamiltonian of the system formed in this way is

$$H = \left(\sum_k \varepsilon_k a_k^+ a_k + \sum_p \varepsilon_p a_p^+ a_p\right)(\hat{P}_0 + \hat{P}_1) + eU\hat{P}_1 + \sum_{k,p}(t_{kp} a_k^+ a_p \hat{P}_1 + t_{kp}^* a_p^+ a_k \hat{P}_0). \tag{13}$$

Here, $\hat{P}_0$ and $\hat{P}_1$ are the operators representing projections, in the eigenstate subspace, of the operator $\hat{Q}$, which correspond to the values $Q = 0$ and $Q = e$, respectively. The energies ε_k and ε_p lie in the interval

$$-\frac{e^2}{C} < \varepsilon_k, \varepsilon_p < \frac{e^2}{C}. \tag{14}$$

Using the Hamiltonians (13) and (14) we can calculate the charge $\overline{Q}(\varphi)$ in the fourth order of perturbation theory using the parameter t_{kp}. It is then found that the dependence of the correction $\overline{Q}^{(4)}$ on the matrix element t_{kp} is not limited to their dimensionless combination (10), as found in the case of the second-order correction $\overline{Q}^{(2)}$. This means that in calculation of the $\overline{Q}(\varphi)$ dependence near the ends of the interval (7) it is generally insufficient to know the conductance of the tunnel layer separating the granule from the bank; we need more information on its structure. However, we can consider two limiting cases when $\overline{Q}(\varphi)$ is expressed solely in terms of the parameter g.

1. Point contact. We shall assume that the transparency of the tunnel layer differs from zero only in a region whose transverse dimensions do not exceed λ_F. Then, a matrix element of the tunnel Hamiltonian, written down in the coordinate representation, is $t(\mathbf{r},\mathbf{r}') = t\delta(\mathbf{r})\delta(\mathbf{r}')$. (Here, $\mathbf{r}$ and $\mathbf{r}'$ are the radius vectors of a point in the bank and in the granule, respectively.) Adopting the momentum representation, we find that $t_{kp} \equiv t$, i.e., the matrix element is independent of the momenta k and p. The parameter g is related to t by

$$g = \nu_0 \nu_1 t^2, \tag{15}$$

where ν_0 and ν_1 are the densities of states in the bank and in the granule. The fourth-order correction to the granule charge, found with logarithmic precision, is described by the following expression in the case of a point contact:

$$\overline{Q}^{(4)}(U) = \frac{4}{3} eg^2 \ln^3 \frac{e}{CU}. \tag{16}$$

2. Wide junction. We shall assume that the surfaces of the insulating layer (spacer) separating the granule from the bank are smooth and parallel and that the area of the spacer A is large: $A \gg \lambda_F^2$. Then, the tunneling process should conserve the components of the electron momentum parallel to the spacer. Bearing in mind this conservation law, we can write down the Hamiltonian of the system as follows:

$$H = \left(\sum_{k,m} \varepsilon_{km} a_{km}^+ a_{km} + \sum_{pm} \varepsilon_{pm} a_{pm}^+ a_{pm}\right)(\hat{P}_0 + \hat{P}_1) + eU\hat{P}_1 + \sum_{k,p,m} t(a_{km}^+ a_{pm}\hat{P}_1 + a_{pm}^+ a_{km}\hat{P}_0). \tag{17}$$

The index m labels the conserved transverse components of the momentum and assumes values from 1 to N, where $N \gg 1$ (we can show that $N \sim A/\lambda_F^2$). In the case of a wide contact the parameter g is

$$g = N\nu_0\nu_1 t^2, \tag{18}$$

where ν_0 and ν_1 are the densities of states with a definite index m. The expression for the fourth-order correction to the granule charge, obtained with the aid of the Hamiltonian (17) in the limit $N \to \infty$, is

$$\overline{Q}^{(4)}(U) = -2eg^2 \ln^2 \frac{e}{CU}. \tag{19}$$

The above expressions (16) and (19) for the correction $\overline{Q}^{(4)}$ do not, naturally, solve the problem of the behavior of $\overline{Q}(\varphi)$ near the ends of the interval (7). They simply indicate that the nature of this function depends strongly on the junction area.

3. RELATIONSHIP TO THE KONDO PROBLEM

We shall now establish a useful analogy between the problem discussed here and the Kondo problem. We shall do this by rewriting the Hamiltonian (13) for the case of a point contact ($t_{kp} \equiv t$) in the form

$$H = H_0 + \hat{V}, \quad H_0 = \sum_{k,\alpha} \varepsilon_k a_{k\alpha}^+ a_{k\alpha}(\hat{P}_0 + \hat{P}_1) + eU\hat{P}_1, \tag{20}$$

$$\hat{V} = t\sum_{k,k'}(a_{k1}^+ a_{k'0}\hat{P}_0 + a_{k'0}^+ a_{k1}\hat{P}_1). \tag{21}$$

Here, the index α indicates the position of an electron: $\alpha = 1$ applies to an electron inside the granule and $\alpha = 0$ represents an electron in the bank. We shall be interested in the ground-state energy $E(U)$ of the Hamiltonian described by Eqs. (20) and (21). This is sufficient for calculation of the average charge of the granule in its ground state, so that the obvious equality $\partial H/\partial U = e\hat{P}_1$ yields

$$\overline{Q}(U) = \partial E/\partial U. \tag{22}$$

We shall represent $E(U)$ as a Brillouin–Wigner series and regard the tunnel Hamiltonian $\hat{V}$ as a perturbation:

$$E = \langle\Phi|\left(\hat{V} + \hat{V}\frac{1}{E-H_0}\hat{V} + \hat{V}\frac{1}{E-H_0}\hat{V}\frac{1}{E-H_0}\hat{V} + \ldots\right)|\Phi\rangle. \tag{23}$$

Here, $|\Phi\rangle$ is the ground state of the Hamiltonian H_0 where $Q = 0$. We can see from Eq. (21) that the operator $\hat{V}$ consists of two parts: the first acts on the states with $Q = 0$ and trans-

forms them to the states with $Q=e$, whereas the second induces transitions from $Q=e$ to $Q=0$. Then, if the first term in Eq. (21) acts on the state with $Q=e$ (or the second term on the state with $Q=0$), the result is nil. The existence of such selection rules can be allowed for in a different way. We can attribute to each state of the system an additional index β (which can have two values: $\beta=0$ and $\beta=1$), so that the eigenstates of the charge operator $\hat{Q}$ correspond to $\beta=Q/e$. Then, the projection operators $\hat{P}_0$ and $\hat{P}_1$ in the Hamiltonian of Eqs. (20) and (21) can be replaced with 2×2 matrices acting in the space of the vectors $\Psi_\beta=\begin{bmatrix}\Psi_0\\ \Psi_1\end{bmatrix}$:

$$H_0=\sum_{k,\alpha}\varepsilon_k a_{k\alpha}^{+}a_{k\alpha}\begin{pmatrix}1&0\\0&1\end{pmatrix}+eU\begin{pmatrix}0&0\\0&1\end{pmatrix}, \tag{24}$$

$$\hat{V}=t\sum_{k,k'}\left\{a_{k1}^{+}a_{k'0}\begin{pmatrix}0&0\\1&0\end{pmatrix}+a_{k'0}^{+}a_{k1}\begin{pmatrix}0&1\\0&0\end{pmatrix}\right\}. \tag{25}$$

We can easily verify that the perturbation-theory series of Eq. (23), written down for the two Hamiltonians described by Eqs. (20), (21) and (24), (25), are identical, i.e., the ground-state energies are the same for the two Hamiltonians.[1)] If we consider β as the abstract spin index (for the spin $S=1/2$), we can describe the matrices in Eqs. (24) and (25) in terms of the components of the corresponding spin operator **S**:

$$H=\sum_{k,\alpha}\varepsilon_k a_{k\alpha}^{+}a_{k\alpha}+eU\left(\frac{1}{2}-S^z\right)$$
$$+t\sum_{k,k'}(a_{k1}^{+}a_{k'0}S^{-}+a_{k'0}^{+}a_{k1}S^{+}), \tag{26}$$

where $S^{\pm}=S^x\pm iS^y$. We shall rewrite Eq. (26) in a more symmetric form using the Pauli matrices $\sigma^i_{\alpha\alpha'}$:

$$H=\frac{1}{2}eU+\sum_{k,\alpha}\varepsilon_k a_{k\alpha}^{+}a_{k\alpha}-\frac{1}{2}eU2S^z$$
$$+t\sum_{\substack{k,k'\\ \alpha,\alpha'}}(\sigma^x_{\alpha\alpha'}S^x+\sigma^y_{\alpha\alpha'}S^y)a_{k'\alpha'}^{+}a_{k\alpha}. \tag{27}$$

Therefore, the ground-state energy of the system $E(U)$ is expressed in terms of the ground-state energy of the Hamiltonian of the anisotropic Kondo model:

$$H=\sum_{k,\alpha}\varepsilon_k a_{k\alpha}^{+}a_{k\alpha}-2hS^z+\sum_{k,\alpha,k',\alpha'}J_0(\sigma^xS^x+\sigma^yS^y)_{\alpha\alpha'}a_{k'\alpha'}^{+}a_{k\alpha}, \tag{28}$$

using the relationship

$$E(U)=\tfrac{1}{2}eU+E_K(h,J_0)|_{h=eU/2,\,J_0=t}. \tag{29}$$

In the Kondo problem the Hamiltonians similar to that given by Eq. (28) describe a localized impurity spin S which is located in a metal matrix and interacts in the exchange manner with conduction electrons. The parameter J_0 is the anisotropic exchange constant and h describes an external magnetic field applied along the z axis. Using Eq. (22) and the corresponding relationship

$$\mu\equiv\langle S^z\rangle=-\frac{1}{2}\frac{\partial}{\partial h}E_K$$

for the Hamiltonian (28), we find from Eq. (29) that

$$\bar{Q}(U)=e[\tfrac{1}{2}-\mu(h,J_0)]|_{h=eU/2,\,J_0=t}. \tag{30}$$

In this way the calculation of the granule charge near the ends of the interval (7) reduces to the determination of the average spin of an impurity in the anisotropic Kondo model of Eq. (28). The following comments should be made.

1. In going over from the Hamiltonian of Eq. (13) to that described by Eqs. (20) and (21), we are assuming that the spectra and, consequently, the densities of states of electrons in the granule and in the bank are identical. This does not affect the results of the present investigation expressed in terms of the parameter g, because the densities of states occur in all the macroscopic quantities in the form of the combination given by Eq. (15).

2. The discussion given in this section can be generalized directly to the case of a wide junction [Eq. (17)]. The granule charge can also be represented in the form of Eq. (30), but the average spin μ of an impurity should now be calculated for the multichannel anisotropic Kondo model:

$$H=\sum_{k,m,\alpha}\varepsilon_{km}a_{km\alpha}^{+}a_{km\alpha}-2hS^z$$
$$+\sum_{k,\alpha,k',\alpha',m}J_0(\sigma^xS^x+\sigma^yS^y)_{\alpha\alpha'}a_{km\alpha}^{+}a_{k'm\alpha'}, \tag{31}$$

where the "color" m assumes the values $m=1,2,\cdots,N$.

3. The "spin" indices α and β introduced by us, as well as the operators σ and **S**, are auxiliary and in no way related to the true electron spins. For example, the "spin" S is reversed when any electron is transferred from the granule to the bank and vice versa; its z component indicates the direction in which we can transfer an electron across the insulating spacer in such a way as to leave the system in the space of the allowed states with the charge $Q=0$ or e. The existence of the true electron spin, which is not affected by the tunneling, can be allowed for in the Hamiltonian (13) as a conservation law additional to the law of conservation of the transverse momentum. Therefore, if we allow for the true electron spins, we find that a point contact should be described by the Hamiltonian (17) or (31) with $N=2$. In the case of wider junctions, which correspond to the value $N\gg 1$, doubling of N to allow for the spin is unimportant.

4. ANALYSIS OF THE MULTICHANNEL ANISOTROPIC KONDO MODEL

It is shown in the preceding section that the problem of calculating the average charge of a granule $\bar{Q}(U)$ reduces to determination of the average spin $\mu(h)$ of an impurity, carried out using the multichannel anisotropic Kondo model of Eq. (31). In this section we shall calculate $\mu(h)$ by the renormalization-group method, which is similar to the scaling procedure proposed by Anderson[12] in a study of the anisotropic Kondo model and used by Nozieres and Blandin[13] in an analysis of the multichannel Kondo model. We shall consider the Hamiltonians

$$H=H_0+\hat{V},\quad H_0=\gamma\sum_{k,m,\alpha}\varepsilon_{km}a^+_{km\alpha}a_{km\alpha}-2h\gamma_s S^z, \tag{32}$$

$$\hat{V}=\sum_{\substack{k,\alpha,m,\\ k',\alpha'}}[J_\perp(\sigma^x S^x+\sigma^y S^y)+J_z\sigma^z S^z]_{\alpha\alpha'}a^+_{km\alpha}a_{k'm\alpha'}, \tag{33}$$

where it is assumed that the electron energies are within the range

$$-D<\varepsilon_k<D. \tag{34}$$

The special case of the Hamiltonian described by Eqs. (32)–(34) is the Hamiltonian H', which is of interest to us and which corresponds to the following set of the parameters:

$$D=D_0\equiv e^2/C,\ \gamma=1\ \ \gamma_s=1,\ J_\perp=J_0,\ J_z=0. \tag{35}$$

In this method the Hamiltonian of Eqs. (32)–(34) is transformed into another Hamiltonian (31) of the same type but with a smaller bandwidth $D'=D/\Lambda\ll D$. We can allow for the scattering effects involving the ignored high-energy states by, firstly, renormalizing the parameters γ, γ_s, $J_\perp$, J_z and, secondly, modifying the rule for calculation of the average impurity spin

$$\mu(h)=\frac{\langle\Psi|S^z|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{36}$$

We can find the explicit form of such renormalizations by writing down the wave function of the ground state $|\Psi\rangle$ in the form of a Brillouin–Wigner series:

$$|\Psi\rangle=(1+G_0P\hat{V}+G_0P\hat{V}G_0P\hat{V}+\ldots)|\Phi\rangle\equiv\frac{1}{1-G_0P\hat{V}}|\Phi\rangle, \tag{37}$$

where $|\Phi\rangle$ is the ground state of the Hamiltonian H_0 whose energy is E_0; the operators P and G_0 are given by[2)]

$$P=1-|\Phi\rangle\langle\Phi|,\ G_0=1/(E_0-H_0).$$

We shall introduce an operator M which projects any state to the subspace that does not include quasiparticle excitations of energies $|\varepsilon_k|\rangle D/\Lambda$. A formal transformation of the series (37) gives

$$|\Psi\rangle=\frac{1}{1-G_0(1-M)\hat{V}}\frac{1}{1-G_0PM\hat{V}[1-G_0(1-M)\hat{V}]^{-1}}|\Phi\rangle.$$

Using the commutative nature of the operators M, P, and G_0, and the obvious property of the unperturbed ground state $M|\Phi\rangle=|\Phi\rangle$, we find that

$$|\Psi\rangle=\frac{1}{1-G_0(1-M)\hat{V}}M|\Psi'\rangle, \tag{38}$$

where

$$|\Psi'\rangle=\frac{1}{1-G_0PM\hat{V}[1-G_0(1-M)\hat{V}]^{-1}M}|\Phi\rangle. \tag{39}$$

It should be noted that Eq. (39) can be regarded as a Brillouin–Wigner series of Eq. (37) for the ground state $|\Psi'\rangle$ of the Hamiltonian

$$H'=H_0+\hat{V}',\quad \hat{V}'=M\hat{V}\frac{1}{1-G_0(1-M)\hat{V}}M. \tag{40}$$

The renormalized perturbation $\hat{V}'$ induces transitions only between the states in a narrow energy band $|\varepsilon_k|<D/\Lambda$. The relationships (38) between the wave functions of the initial and transformed Hamiltonians modify the rule for calculation of the average spin. Substituting Eq. (38) into the definition (36), we find that

$$\mu(h)=\frac{\langle\Psi'|\hat{\Gamma}_s|\Psi'\rangle}{\langle\Psi'|\hat{\Gamma}|\Psi'\rangle}, \tag{41}$$

where

$$\Gamma_s=M\frac{1}{1-\hat{V}(1-M)G_0}S^z\frac{1}{1-G_0(1-M)\hat{V}}M, \tag{42}$$

$$\Gamma=M\frac{1}{1-\hat{V}(1-M)G_0}\frac{1}{1-G_0(1-M)\hat{V}}M. \tag{43}$$

This formal transformation deduces from the initial Hamiltonian (32)–(34) a new Hamiltonian (40) for which the bandwidth is $D'=D/\Lambda$. Calculation of the average spin $\mu(h)$ should be carried out using the rules (41)–(43).

In practical calculations it is not possible to allow rigorously for the renormalization described by Eqs. (40), (42), and (43). We shall therefore limit ourselves to the first few terms of the appropriate series expansions in terms of the perturbation $\hat{V}$:

$$\hat{V}'=M\hat{V}M+M\hat{V}G_0(1-M)\hat{V}M+M\hat{V}G_0(1-M)\hat{V}G_0(1-M)\hat{V}M, \tag{44}$$

$$\hat{\Gamma}_s=MS^zM+M\hat{V}(1-M)G_0S^zG_0(1-M)\hat{V}M, \tag{45}$$

$$\hat{\Gamma}=M+M\hat{V}(1-M)G_0G_0(1-M)\hat{V}M. \tag{46}$$

We shall now substitute in Eq. (44) the operator $\hat{V}$ in the form of Eq. (33) and calculate the correction to the trivial contribution $M\hat{V}M$ to the renormalized perturbation $\hat{V}'$. Retaining only the terms proportional to $\ln\Lambda$, we obtain four different contributions to $\delta\hat{V}'=\hat{V}'-M\hat{V}M$ corresponding to the renormalizations of the four parameters $J_\perp$, J_z, γ, γ_s of the Hamiltonian of Eqs. (32)–(34):

$$\begin{aligned}\delta J_\perp&=(2\nu J_\perp J_z\gamma^{-1}-{}^1/_2N\nu^2J_\perp J_z^2\gamma^{-2})\ln\Lambda,\\ \delta J_z&=(2\nu J_\perp^2\gamma^{-1}-N\nu^2J_\perp^2J_z\gamma^{-2}+{}^1/_2N\nu^2J_z^3\gamma^{-2})\ln\Lambda,\\ \delta\gamma&=N\nu^2(J_\perp^2+{}^1/_2J_z^2)\gamma^{-1}\ln\Lambda,\\ \delta\gamma_s&=-N\nu^2(J_\perp^2-{}^1/_2J_z^2)\gamma^{-2}\gamma_s\ln\Lambda.\end{aligned} \tag{47}$$

It is convenient to represent the renormalizations of the system (47) by differential equations for three dimensionless quantities:

$$Z_1=\nu J_\perp\gamma^{-1},\ Z_2=\nu J_z\gamma^{-1},\ Z_s=\gamma_s\gamma^{-1}. \tag{48}$$

We can do this by replacing $\ln\Lambda$ with $\delta\xi$, where $\xi\equiv\ln(D_0/D)$, which yields

$$dZ_1/d\xi=2Z_1Z_2-N(Z_1^3+Z_1Z_2^2), \tag{49}$$

$$dZ_2/d\xi=2Z_1^2-2NZ_1^2Z_2, \tag{50}$$

$$dZ_s/d\xi=-2NZ_1^2Z_s. \tag{51}$$

This system of equations allows us to calculate the renormalizations of the coefficients of the Hamiltonian of Eqs. (32)–(34) and carry out then several transformations of the type described by Eq. (47). It should be stressed that the values of the average impurity spin μ calculated from Eq.

(36) for the two Hamiltonians, the initial H and renormalized H', are different. In fact, if we calculate $\hat{\Gamma}_S$ and $\hat{\Gamma}$ from Eqs. (45) and (46), we obtain

$$\hat{\Gamma}_S=(1+\gamma_S^{-1}\delta\gamma_S)M,\ \hat{\Gamma}=(1+\gamma^{-1}\delta\gamma)M, \tag{52}$$

where $\delta\gamma_S$ and $\delta\gamma$ are found by renormalization of the Hamiltonian (47). The required relationship between the values of the average spin μ and μ' is now obtained by substituting Eq. (52) into Eq. (41):

$$\mu=(1+\gamma_S^{-1}\delta\gamma_S-\gamma^{-1}\delta\gamma)\mu'=[1+\delta(\ln Z_S)]\mu'. \tag{53}$$

It follows from Eq. (53) that the renormalization of (47) modifies $\ln\mu$ by an increment $\delta(\ln\mu)=-\delta(\ln Z_s)$, i.e., the product μZ_S is not affected. We can find the average spin μ for the initial Hamiltonian (31) by applying consecutively a number of transformations of Eq. (47), which reduce the width of the band D by a factor $\Lambda\gg 1$ until the scale of D becomes of the order of h. This procedure reduces to the solution of the system of equations (49)–(51) subject to the initial conditions of Eq. (35), written in the form

$$Z_1(0)=\nu J_0,\ Z_2(0)=0,\ Z_S(0)=1. \tag{54}$$

Calculation of $\mu\equiv\langle S^z\rangle$ for this Hamiltonian naturally gives $\mu=1/2$. (On a scale of $D\sim h$ a perturbation-theory series contains no large logarithmic factors and we can ignore the perturbation $\hat{V}$.) Therefore, comparing the values of the parameter μZ_S before and after the renormalization, we obtain

$$\mu(h)={}^1/_2 Z_S(\xi_h),\ \xi_h\equiv\ln(D_0/h). \tag{55}$$

We can find the function $Z_S(h)$ by solving the system of differential equations (49)–(51) subject to the initial conditions of Eq. (54). A comparison of Eqs. (50) and (51) shows that

$$Z_S=1-NZ_2. \tag{56}$$

The remaining system of equations (49)–(50) has the first integral

$$f(Z_1,Z_2)=\frac{Z_1^2-Z_2^2}{1-NZ_2}.$$

Its value is found by substituting the initial values from Eq. (54) and it amounts to $f\equiv(\nu J_0)^2$. We therefore have

$$Z_1^2=Z_2^2+(\nu J_0)^2(1-NZ_2). \tag{57}$$

Using Eq. (57) we can represent the solutions of the system (49)–(50) in the plane of the variables Z_1 and Z_2 (Fig. 2). The explicit form of the dependences $Z_1(\xi)$ and $Z_2(\xi)$ will not be needed. Instead, bearing in the task of calculation of the average spin-in accordance with Eq. (55), we shall find $Z_S(\xi)$. Substituting the relationships (56) and (57) into Eq. (51), we obtain

$$\frac{dZ_S}{d\xi}=-\frac{2}{N}[(1-Z_S)^2+(\nu J_0 N)^2 Z_S]Z_S. \tag{58}$$

It is clear from Eq. (58) that its solution $Z_S(\xi)$ falls monotonically from $Z_S(0)=1$ to $Z_S(\xi\to\infty)=0$. Linearization of the right-hand side of Eq. (58) near the point $Z_S=0$ gives $Z_S\propto\exp(-2\xi/N)$ for $\xi\to\infty$. This behavior of $Z_S(\xi)$ is in agrement with the power-law dependence of the average spin of Eq. (55) on the magnetic field:

$$\mu(h)\propto h^{2/N},\ h\to 0. \tag{59}$$

It should be pointed out that the result given by Eq. (59) was obtained by us strictly speaking only for the case when $N\gg 1$. This is due to the fact that Eqs. (49) and (50) are derived by retaining in Eqs. (44)–(46) only the first few terms of the expansion of the exact formulas (40), (42), and (43) as a series in $\hat{V}$. Inclusion of higher terms of the expansion would have given rise to corrections of type NZ^4, N^2Z^5, and similar on the right-hand sides of Eqs. (49)–(51). We can easily see that if $N\gg 1$, then these corrections are small.[3)] If $N\sim 1$, we can use Eqs. (49)–(51) only for moderate values of ξ, as long as $Z_1(\xi)$, $Z_2(\xi)\ll 1$.

Assuming that the number of channels N is large, we can find $Z_s(\xi)$ for any value of the parameter $\nu J_0 N$ by integrating Eq. (58). The problem reduces to the solution of a cumbersome transcendental equation which can be carried out only numerically. An analytic study can be made in the limiting cases $\nu J_0 N\gg 1$ and $\nu J_0 N\ll 1$. In particular, if $\nu J_0 N\gg 1$, the average spin of Eq. (55) is given by

$$\mu(h)=\frac{1}{2}\frac{\exp(-2\xi_h/N)}{(\nu J_0 N)^2[1-\exp(-2\xi_h/N)]+1}. \tag{60}$$

The case $\nu J_0 N\ll 1$ for a wide junction ($N\gg 1$) can be considered simultaneously with the case of a point contact ($N=1$ or 2). The renormalization-group method is a convenient means for investigating the range of high magnetic fields h when the correction $\Delta\mu\equiv 1/2-\mu(h)$ to the average spin of an impurity is small, $\Delta\mu\ll 1$, because the spin is screened by conduction electrons. If h is sufficiently high, it follows from Eqs. (58) and (55) that

$$\mu(h)\approx{}^1/_2[1-\nu J_0 N\,\mathrm{tg}(2\nu J_0\xi_h)]. \tag{61}$$

A reduction in h increases the quantity $\xi_h\equiv\ln(D_0/h)$ and the argument of the tangent in Eq. (61) approaches $\pi/2$. In this range of values of h, Eq. (61) is no longer meaningful, but the first two terms of the asymptotic expansion $\mu(h)$ can still be found from Eq. (58) and are of the form

$$\mu(h)\approx\frac{1}{2}\left\{1-\frac{N}{2}\frac{1}{\ln(h/T_H)}-\frac{N^2}{4}\frac{\ln[\ln(h/T_H)]}{\ln^2(h/T_H)}\right\}. \tag{62}$$

The scale T_H occurring in Eq. (62) is governed by the parameters of the initial Hamiltonian of Eq. (31):

$$T_H=D_0(\nu J_0)^{N/2}\exp\left\{-\frac{\pi}{4\nu J_0}\right\}. \tag{63}$$

The validity of the expansion of (62) is limited to the range of relatively weak magnetic fields $h\gg e^N T_H$, in which the average spin $\mu(h)$ differs little from the unperturbed value $\mu=1/2$.

It should be noted that the dependence (62) is of universal validity. The average spin is governed by the ratio h/T_H and the parameters D_0, J_0, and ν occur in the answer only in the form of the combination described by Eq. (63). This is due to the fact that the renormalization of the parameters $J_\perp$ and J_z of the Hamiltonian (32)–(34) increases them in such a manner that in the case of sufficiently small widths of the band D they are practically equal (curve 2 in Fig. 2). Therefore, the Hamiltonian of Eq. (31) is transformed to the

Hamiltonian of the isotropic Kondo model[4] ($J_\perp = J_z$), for which the universal behavior of $\mu(h)$ is well known.[8,9] Therefore, the average impurity spin when $h \propto e^N T_H$ is identical with $\mu(h)$ for an N-channel isotropic Kondo model with the same value of the parameter T_H.

The multichannel isotropic Kondo model is solved in Refs. 10 and 11 exactly by the Bethe method and the $\mu(h)$ dependence is calculated for any value of the ratio h/T_H. The resultant expressions are very cumbersome and we shall not give them here. We shall simply point out that the behavior of $\mu(h)$ in the limit $h \to \infty$ is identical with that of Eq. (62), whereas in the limit $h \to 0$, it depends on the number of channels N:

$$\mu(h) \sim \begin{cases} h/T_H, & N=1 \\ (h/T_H)\ln(T_H/h), & N=2 \\ (h/T_H)^{2/N}, & N>2 \end{cases}. \tag{64}$$

Therefore, in the absence of a magnetic field ($h = 0$) the impurity spin is screened completely ($\mu = 0$): the power-law dependence of Eq. (59) obtained for the average spin impurity in the limit $N \gg 1$, applies for all values $N > 2$ if $h \to 0$.

5. DISCUSSION OF RESULTS

The above results for the average impurity spin μ in the multichannel anisotropic Kondo model can be reduced with the aid of Eq. (30) to the problem of the charge of a granule in a gate field (Fig. 1). We shall consider only the values of φ in the interval defined by Eq. (7) and in addition to φ we shall employ a new variable

$$\xi_\varphi \equiv \ln \frac{e/2C - \varphi}{e/2C + \varphi},$$

with the aid of which we can write down some of the results for the charge $\bar{Q}(\varphi)$. In particular, in the case of a wide junction in the limit $N \to \infty$ we find from Eq. (60) that

$$\bar{Q}(\varphi) = e \frac{g\xi_\varphi}{1 + 2g|\xi_\varphi|}. \tag{65}$$

It follows from Eq. (65) that if $\varphi \to \varphi_1 \equiv -e/2C$, the granule charge is $e/2$ and $\bar{Q}(\varphi)$ approaches this limiting value logarithmically:

$$\bar{Q}(\varphi) \approx \frac{e}{2}\left\{1 - \frac{1}{2g\ln[\varphi_1/(\varphi_1 - \varphi)]}\right\}, \quad \varphi \to \varphi_1.$$

For finite values $N \gg g^{-1}$ the dependence (65) is valid throughout the interval described by Eq. (7), with the exception of narrow regions near the ends of the interval, where $|\xi_\varphi| > N$. Within these narrow regions the charge differs little from the limiting values $\pm e/2$, but it obeys a power law:

$$\bar{Q}(\varphi) \approx \frac{e}{2}\left[1 - \frac{1}{gN}\left(\frac{\varphi_1 - \varphi}{\varphi_1}\right)^{2/N}\right], \quad \varphi \to \varphi_1.$$

In the limit $N \ll g^{-1}$, which includes also the case of a point contact ($N = 1$ or 2), the dependence $\bar{Q}(\varphi)$ has the characteristic scale

$$U^* = \frac{e}{C}\left(\frac{g}{N}\right)^{N/4} \exp\left\{-\frac{\pi}{4}\left(\frac{N}{g}\right)^{1/2}\right\},$$

which is an analog of the Kondo temperature (63). For values of φ within the interval (7), but separated from the ends of the interval by more than U^*, we find that the average granule charge is small, $\bar{Q} \ll e$, and it amounts to

$$\bar{Q} = {}^1/_2 e (gN)^{1/2} \operatorname{tg}\left(2(g/N)^{1/2}\xi_\varphi\right). \tag{66}$$

(This expression is obtained in Ref. 6 for the case when $N = 1$.) On approach of φ to the ends of the interval (7), for example, when $\varphi + e/2C \propto U^*$, we find that the average granule charge rises reaching values of the order of e. The dependence of $\bar{Q}$ on the parameter φ or, which is equivalent, on $U \equiv \varphi + e/2C$ can be found from the expression for the average spin N using the N channel Kondo model[10,11] and it is given by

$$\bar{Q} = \frac{e}{2} - \frac{e}{4\pi^{1/2} i}\int_{-\infty}^{+\infty} \frac{d\omega}{\omega - i0} \exp\left(2i\omega \ln \frac{U}{U^*}\right)$$

$$\times \left(\frac{i\omega N + 0}{e}\right)^{i\omega N} \frac{\Gamma(1 - i\omega N)\Gamma({}^1/_2 - i\omega)}{\Gamma(1 - i\omega)}.$$

It is clear from Eq. (64) that in the limit $U \to 0$ the granule charge approaches $e/2$ in accordance with the following power law:

$$e/2 - \bar{Q} \propto \begin{cases} eU/U^*, & N=1 \\ (eU/U^*)\ln(U^*/U), & N=2 \\ e(U/U^*)^{2/N}, & N>2 \end{cases}. \tag{67}$$

Experimental verification of the $\bar{Q}(\varphi)$ dependences can be made by, for example, measuring the capacitance between the gate and the substrate (Fig. 1) as a function of a constant bias V applied to the gate. Such a dependence should exhibit periodic maxima at the points defined by Eq. (3) where, as is clear from Eq. (67), the capacitance reaches the value e/U^* for $N = 1$ and diverges for $N > 1$.

The author is grateful to L. I. Glazman and A. I. Larkin for valuable discussions.

[1)] A more general conclusion is also valid: the Hamiltonians of Eqs. (20), (21), and (24), (25) are equivalent if we consider the Hamiltonian of Eqs. (24), (25) in the subspace of such states for which we have $\beta = Q/e$. This is possible since the operator $\beta\delta_{\beta\beta'} - \hat{Q}/e$ commutes with the Hamiltonian of Eqs. (24) and (25).

[2)] In fact, the unperturbed energy E_0 which occurs in the series (37) should be replaced with the true ground-state energy E. We shall assume that the shift of E_0 is compensated by adding to the perturbation (33) a counterterm $E_0 - E$, the presence of which, however, is not manifested in any way in the subsequent expressions.

[3)] We have to satisfy also the condition $N(\nu J_0)^2 \ll 1$, which—as is clear from Eqs. (30) and (18)—implies (when the language of fluctuations of the granule charge is used) smallness of the conductance of the tunnel layer, $g \ll 1$, and thoughout this treatment this condition is assumed to be true.

[4)] It is clear from Eq. (57) that the approximate equality $Z_1 \approx Z_2$ begins to be satisfied when $Z_1 \sim Z_2 \sim \nu J_0 \ll 1$ and the system of equations (49)–(51) can then be applied even in the case of a point contact, (i.e., when $N \sim 1$).

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Translated by A. Tybulewicz