Zero-bias anomaly of point-contact resistance due to adiabatic electron renormalization of dynamical defects

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We study the effect of the adiabatic electron renormalization on the parameters of the dynamical defects in the ballistic metallic point contact. The upper energy states of the ''dressed'' defect are shown to make a smaller contribution to a resistance of the contact than the lower-energy ones. This holds both for the ''classical'' renormalization related to defect coupling with average local-electron density and for the ''mesoscopic'' renormalization caused by the mesoscopic fluctuations of electronic density the dynamical defects are coupled with. In the case of mesoscopic renormalization, one may treat the dynamical defect as coupled with Friedel oscillations originated by the other defects, both static and mobile. Such coupling lifts the energy degeneracy of the states of the dynamical defects making a different mesoscopic contribution to resistance, and provides a model for the fluctuator that pictures it as the object originated by the electronic mesoscopic disorder rather than by the structural one. The correlation between the defect energy and the defect contribution to the resistance leads to zero-temperature and zero-bias anomalies of the point-contact resistance. A comparison of these anomalies with those predicted by the two-channel Kondo model (TCKM) is made. It is shown, that although the proposed model is based on a completely different from TCKM physical background, it leads to a zero-bias anomalies of the point-contact resistance, which are qualitatively similar to TCKM predictions. [S0163-1829(97)06501-6]

I. INTRODUCTION

Recent advances in nanofabrication technology have made it possible to visualize single defects with internal degrees of freedom - ''fluctuators,''[1,2] which lead to a ''telegraph'' resistance noise of nanometer-scale systems. In metals these defects are believed[3–7] to be structural defects, which at low temperatures are seen as the well-known two-level tunneling states (TLS).[8] TLS's are typical objects for strongly disordered amorphous solids [8] that switch by tunneling between their two possible configurations. Although the microscopic nature of the fluctuators remains unclear (especially for ballistic devices made of pure metals), the experiments allow us to study various phenomenological parameters of these objects, in particular the interlevel spacing.

Kondo[9] pointed out that in metals the parameters of the dynamical defects are strongly renormalized by electrons. One can discriminate between adiabatic electron ''dressing,'' which is related to a static electron response on the defect potential, and a nonadiabatic one, which affects the tunneling process and leads to a renormalization of the TLS tunneling matrix element (''dissipative tunneling''). It is this nonadiabatic effect that has attracted most attention (see e.g., Ref. 10) due to its evident importance for defect dynamics. As for the adiabatic renormalization of the defect parameters, it is customary to include it in the bare values. This procedure is usually justified by the fact that the adiabatic effects are related to a response of the whole electron systems, while only a small strip of electron energies, close to the Fermi surface, is responsible for transport properties and sensitive to external factors like temperature or applied fields. However, as was demonstrated in Refs. 4 and 6, the adiabatic ''dressing'' of the fluctuator, in particular, the adiabatic renormalization of the fluctuator energy splitting E, can be important, and depends on the state of the electron system (e.g., on superconducting properties). Furthermore, very recently the surprising ''magnetic tuning'' of the TLS interlevel spacing observed[11] for TLS's in Bi nanoconstrictions was explained[12] as a direct result of the adiabatic renormalization of TLS parameters by electrons, whose states are affected strongly by the magnetic field.

The purpose of the present paper is to show that *the adiabatically renormalized energy of the fluctuator state correlates with the fluctuator contribution to the resistance*. That is, the conductance is *larger* for the fluctuator on its *upper* level. This fact causes, in particular, Kondo-like zero-temperature and zero-bias anomalies in differential conductance of the metallic point contacts. Indeed, an increase of temperature leads, on average, to an increase of occupation numbers of the fluctuator upper levels. The above-mentioned correlation causes a corresponding conductance *increase with temperature*, which imitates the Kondo-like behavior. The same holds for an applied bias increase.

II. ADIABATIC RENORMALIZATION OF THE PARAMETERS OF THE DYNAMICAL DEFECTS IN METALS

Two mechanisms of the adiabatic renormalization can be considered. The first is due to the possible difference of electron-fluctuator coupling potentials V for the two of the

fluctuator states ($|V^{(1)}| \neq |V^{(2)}|$), and was studied in Refs. 4,6 and 12. We will show that for this mechanism (which will be referred to as the ''classical'' one) the above-mentioned correlation is due to the fact that expressions for the conductance and for the electron contribution to defect energy include the same strength of the electron-defect coupling.

The second mechanism of adiabatic renormalization of dynamical defects parameters was suggested by Altshuler and Spivak.[13] It implies mesoscopic electron-density fluctuations, which lead to a difference, even for $|V^{(1)}| = |V^{(2)}|$, of electron-fluctuator coupling strengths for different fluctuator states due to their spatial resolution. The same correlation occurs for this ''mesoscopic'' contribution as for the classical one. We will show it for the experimentally important situation of ballistic point contact, where a description in terms of ''local'' interference, which involves a finite number of scatterers, is possible.

A. Renormalization due to difference in defect-electron coupling potentials

Let us start from the classical effect. TLS energy splitting E depends[7] on the TLS tunneling parameter Δ_0 and on the TLS asymmetry Δ:

$$E = \sqrt{\Delta_0^2 + \Delta^2}. \tag{1}$$

Interaction of TLS's with conduction electrons leads to the renormalization of both TLS asymmetry[4,6,12] and of the tunneling parameter.[9] For asymmetrical TLS's with large enough barriers, $\Delta \gg \Delta_0$, the renormalization of TLS asymmetry makes the major contribution to E. As a result, [4,6,12] the electron-TLS coupling leads to the renormalization of TLS ''bare'' energy splitting E which has a form $E \to E + E_{\rm el}$, where $E_{\rm el} = E_{\rm el,2} - E_{\rm el,1}$,

$$E_{{\rm el},i} = \sum_{\mathbf{k},\mathbf{k}'} |V_0^{(i)}|^2 \frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k}'})}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}} \approx - \frac{|V_0^{(i)}|^2}{\varepsilon_F}. \tag{2}$$

Here $V_0^{(i)}$ is the electron-TLS coupling constant for the ith TLS configuration. The electron bandwidth is assumed to be of the order of ε_F, and the electron distribution $f(\varepsilon)$ to have an equilibrium Fermi form $f(\varepsilon) = f_0(\varepsilon) = \{\exp[(\varepsilon - \varepsilon_F)/T] + 1\}^{-1}$. Applicability of the second-order perturbation theory approximation is justified for Eq. (2) when $V_0^{(i)} \ll \varepsilon_F$. In contrast to Kondo-like corrections, Eq. (2) depends weakly on temperature. The renormalization $E_{\rm el}$ is due to the difference in the values of the total electron energy, renormalized by the presence of TLS's, for the TLS's in states 1 and 2, respectively. It is important, that $E_{\rm el}$ is not, due to adiabaticity, sensitive to the details of the interstate transition mechanism. Thus the problem is reduced to estimates of energies $E_{{\rm el},i}$ corresponding to different configurations of the defect which for this case can be considered as its independent realizations. Therefore, Eq. (2) holds both at low temperatures, when the fluctuator transitions are due to tunneling, and at higher temperatures when thermal activation dominates. [7,14]

According to Eq. (2) the energy E is *lowered* from the ''bare'' value. The lowering is larger the stronger is the coupling of the state with the electrons. On the other hand, the presence of the defect in state i inside a ballistic point contact with a characteristic size d causes a reduction of the contact conductance[5]

$$\delta G_i \approx - \frac{|V_0^{(i)}|^2}{\varepsilon_F^2} \left(\frac{\lambda_F{}^2}{d^2} \right) G, \tag{3}$$

where λ_F is the Fermi wavelength, and $G \approx (e^2/h)(d^2/\lambda_F^2)$ is the Sharvin conductance. Making use of Eq. (2) one obtains $\delta G_i \approx (e^2/h)(E_{{\rm el},i}/\varepsilon_F)$. Therefore, if the defect asymmetry is completely controlled by the conduction electrons, the conductance, which corresponds to the defect in its lower state (larger absolute value of the electron contribution to the defect energy) is smaller than that for the defect in the upper state.

B. Interference contribution to the renormalization

Let us now consider the electronic interference. For adiabatic effects different states of ''active'' defects, fluctuators, can be considered as independent realizations. Thus we can choose some configuration of some active defect as a ''reference'' scatterer i, and consider its properties in the presence of ''background'' scatterers. We will analyze both the interference contribution to conductance due to the defect i and the ''mesoscopic'' renormalization of the energy of this defect, which is equal to a change of the electron system energy due to a presence of interference pattern involving defect i.

The ballistic point contact contains a finite number of scatterers. Therefore the interference contribution to the contact conductance is provided by a *local* interference (involving trajectories with small number of scatterers) rather than by a *global* one [which leads to well-known Universal Conductance Fluctuations (Ref. 16)]. This ''local'' interference contribution was to some extent analyzed in Ref. 17. In what follows, for simplicity we will restrict ourselves mainly to the interference patterns involving only pairs of scatterers. However, as is shown in Appendix A 1, our results can be generalized for the case of an arbitrary number of scatterers.

As is shown in Appendix A 1 [Eq. (A9)], the contribution to the conductance due to a pair of scatterers, namely the ''reference'' scatterer i and the ''background'' m, is

$$\delta G_{im} = A_{G,im} \xi_{im}, \quad A_{G,im} \approx \frac{e^2}{h} \frac{|V_0|^2}{\varepsilon_F^2} \left(\frac{\lambda_F}{R_{im}} \right)^2. \tag{4}$$

Here $\xi_{im} = \cos(2k_F R_{im})$, and $\mathbf{R}_{im} \equiv \mathbf{R}_i - \mathbf{R}_m$ is the vector, which connects two scatterers. For simplicity we assume that the scattering potentials for all scatterers, both ''active'' and ''passive'' ones, depend only on the coordinate $\mathbf{R}_i$ of the scatterer: $V_{i\mathbf{k}\cdot\mathbf{k}'} = V_0 \exp[i(\mathbf{k} - \mathbf{k}')\mathbf{R}_i]$.

Let us now find a contribution to the energy of ''reference'' scatterer i, which represents one state of some fluctuator, due to its being involved in electron interference along with another scatterer m. Following the scheme implied by Eq. (2), it is given by a renormalization of electron system energy due to this pair of scatterers. In the second-order perturbation theory approximation, we obtain, collecting all terms proportional to $V_{i\mathbf{k}\cdot\mathbf{k}'} V^*_{m\mathbf{k}\cdot\mathbf{k}'}$

$$E_{\mathrm{el},im}=\mathrm{Re}\sum_{\mathbf{k},\mathbf{k}'}|V_0|^2\exp[i(\mathbf{k}-\mathbf{k}')\mathbf{R}_{im}]\frac{f(\varepsilon_{\mathbf{k}})-f(\varepsilon_{\mathbf{k}'})}{\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}}. \tag{5}$$

A straightforward calculation for a spherical Fermi surface and zero temperatures gives [see Appendix A 1, Eq. (A9)]:

$$E_{\mathrm{el},im}=A_{E,im}\xi_{im}, \quad A_{E,im}\approx\frac{|V_0|^2}{\varepsilon_F}\frac{\lambda_F^3}{R_{im}^3}. \tag{6}$$

The obtained renormalization is due to interaction of defect m with the Friedel oscillation of electron density originated by the defect i.

Both δG_{im}, Eq. (4), and $E_{\mathrm{el},im}$, Eq. (6), are proportional to the *same* phase factor $\xi_{im}=\cos(2k_FR_{im})$. Correspondingly,

$$\frac{[\delta G_{im}/(e^2/h)]}{(\delta E_{\mathrm{el},im}/\varepsilon_F)}\sim\frac{\lambda_F}{R_{im}}>0, \tag{7}$$

and thus, in analogy with the ''classical'' effect, the larger the energy of a configuration, the larger the contact conductance. As it can be shown (see Appendix A 1), the proportionality to the same phase factor and, therefore, Eq. (7), holds not only for pairs of scatterers but for an arbitrary number of scatterers as well.

To estimate a total interference contribution due to the defect i, both to the conductance δG_i and to the defect energy $E_{\mathrm{el},i}$, one must sum over all ''background'' scatterers m. Due to a random distribution of $\mathbf{R}_{im}$, this results in some mesoscopic fluctuations for both quantities with respect to realizations of the system. However, the fact that both quantities are linearly related to the same set of random factors ξ_{im} leads to the correlation between them, namely

$$\langle\delta G_iE_{\mathrm{el},i}\rangle=C\overline{\delta G}\ \overline{E_{\mathrm{el}}}, \tag{8}$$

where $\bar{x}\equiv\sqrt{\langle x^2\rangle}$, $C\approx1$, and $\langle\rangle$ denotes the ensemble average. More detailed argumentation of this is given in Appendix B. For a given value of $E_{\mathrm{el},i}=E$, one has

$$\langle\delta G_i\rangle_E=C\overline{\delta G}\frac{E}{E_{\mathrm{el}}}. \tag{9}$$

Keeping in mind factors $1/R_{im}^2$ (for the conductance) and $1/R_{im}^3$ (for the energy), one may suggest the main contribution to both these quantities to stand from the nearest neighbors. In this case both the energy renormalization and the contribution to the resistance are related to a few neigboring defects, and thus could be estimated by Eqs. (4) and (6) with R_{im} of the order of most probable interdefect distance $N_i^{-1/3}$ (where N_i is the background defect concentration). Note that if we take an average over all possible realizations of the background scatterers we would find a problem with a singular behavior of the averaged quantities when $R_{im}\to0$. This means that the average is mainly controlled by (rare) realizations corresponding to a very close neighboring background defect, and one has $R_{im}>k_F^{-1}$ which would give $|\delta G|\sim e^2/h$, $E_{\mathrm{el},i}\sim E_F/(k_Fl)^{1/2}$. However, in the case of small ballistic contact we deal with some given contact realization, so that we deal with the most probable quantity rather than with an average quantity (compare with Ref. 15).

For the ballistic point contact the number of defects in the contact is small, so that the dominant contribution is expected to be from the trajectories, which involve a boundary of the contact. Assuming the contact to be a short channel with a length $\approx d$, this boundary may be considered as an array of scatterers at a distances $\approx d$ from the defect i with a total number $\approx(d/\lambda_F)^2$. For this case

$$\overline{\delta G}\approx\left(\frac{\lambda_F}{d}\right)\frac{e^2}{h}, \quad \overline{E_{\mathrm{el},i}}\approx\varepsilon_F\left(\frac{\lambda_F}{d}\right)^2. \tag{10}$$

Taking values of d typical of nanofabricated ballistic point contacts, $d\approx5$–10 nm, one obtains $|\delta G|\approx(0.05-0.1)e^2/h$ and $E_{\mathrm{el},i}\approx30$–$100$ K.

The mesoscopic interference renormalization has some special features as compared with the ''classical'' one. First, mesoscopic disorder lifts the energy degeneracy of the defect states, which have different spatial positions. Thus it causes a formation of fluctuators from otherwise symmetric defect configurations (that is, interstitials which have symmetrical lattice positions).

In this case one expects the temperature and bias behaviors of the resistance to depend on an external magnetic field, which affects the electron interference (see, e.g., Ref. 16).

In addition, the interference contribution both to the defect energy and to the conductance depends on the electron distribution. The finite applied bias makes this strongly nonequilibrium, which at high enough biases causes a ''direct'' effect of bias on both quantities. The physical picture of the mesoscopic renormalization is much richer than that provided by the ''classical'' one, and it is this mechanism that we will concentrate on in the rest of the paper.

III. ZERO-BIAS AND ZERO-TEMPERATURE RESISTANCE ANOMALIES

Let us consider defect i, which occupies either of the *two* neighboring positions 1 and 2 with close energies. For simplicity we will assume that the energy asymmetry of these defect states is completely determined by the electron renormalization. This object is a sort of two-level fluctuator caused by the *electronic* disorder rather than by the lattice one. It is important that, due to the correlation discussed above, the upper state of such a fluctuator, which corresponds to a defect position with higher energy, makes a smaller contribution to the contact resistance. A conductance increase, which accompanies a transition from the lower to the upper level of such a fluctuator, $\delta G_{(i)}=\delta G_{(i)1}-\delta G_{(i)2}$, is, according to Eq. (9), scaled with the energy asymmetry $E_{(i)}=E_{\mathrm{el},(i)1}-E_{\mathrm{el},(i)2}$. Here index i now denotes the fluctuator.

A summation over all fluctuators gives their total contribution to the average contact conductance,

$$\Delta G=\sum_i\delta G_{(i)}n_{(i)}=\int\langle\delta G_{(i)}\rangle_EP(E)n(E)dE. \tag{11}$$

Here $n_{(i)}=n(E_{(i)})$ is the ith fluctuator upper level occupation number and $P(E)$ a density of states given by statistical properties of $E_{\mathrm{el},i}$. For the mesoscopic system it is reasonable to take the values of $E_{\mathrm{el},i}$ for the neighboring defect positions to be statistically independent. In this case $P(E)$ is

approximately constant at small $E \ll \overline{E_{\rm el}}$. Making use of Eq. (9) and of the expression $n(E)=[1+\exp(E/T)]^{-1}$, at small temperatures $T \ll \overline{E_{\rm el}}$ one has the conductance enhancement

$$\Delta G \propto T^{\beta}, \tag{12}$$

where $\beta=2$.

For some defects, like light interstitials or some defect complexes, the probabilities of defect hopping between spatially symmetric positions are relatively high.[18] For these ''delocalized'' defects the effect of electronic disorder provides a many-site ''potential relief'' instead of two-site fluctuator picture. Assuming that any site can be occupied by only one defect, one deals with ''Fermi-type'' statistics, so at $T \to 0$ sites with the lowest energies are occupied by the mobile defects while those with energies higher than the ''Fermi level'' are free. At finite temperature Eq. (11) can be applied, where the site occupation number again has the form $n(E)=[1+\exp(E/T)]^{-1}$ if one takes the Fermi level as the origin of the energy E. In this case the total number of available sites is much larger than the number of defects, N, and for finite temperatures the ''Boltzmann-type'' statistics holds rather than the ''Fermi type:''

$$n(E)=\frac{N\exp(-E/T)}{\int P(E)\exp(-E/T)\mathrm{d}E}. \tag{13}$$

In this case a change of T does not affect the number of rearranged defects (because any of them can change its energy) and leads only to a change of the average defect energy. As a result, in this case we have in Eq. (12) $\beta=1$ independently of the form of the density of states $P(E)$.

Let us turn now to the effect of finite bias $eV \gg T$. For TLS's it was first considered in Refs. 5 and 19. It was shown that for low-energy TLS's with small enough energy splitting E, for which the coupling with electrons dominates,[20] the TLS occupation numbers are sensitive to the electron distribution. For the contact region this is strongly nonequilibrium and for a central point of symmetric contact has a form

$$f(\mathbf{k})=\theta(k_x)f_0(\varepsilon_{\mathbf{k}}+eV/2)+\theta(-k_x)f_0(\varepsilon_{\mathbf{k}}-eV/2), \tag{14}$$

where OX is the main axis of the contact and $\theta(x)$ the theta function. The ''energy width'' of this distribution, eV, plays a role of the effective temperature. In particular, the upper levels of the TLS are empty if $eV<E$, while for $eV \gg E$ the occupation numbers of TLS levels are almost equal[5,19] and $n(E)\approx\frac{1}{2}[1-(E/eV)]$.

For larger E the coupling with phonons becomes important, [20,14] due to the rapid increase of the density of states for actual phonons with an increase of E. For the two-state case the fluctuator relaxation rate due to electron-assisted tunneling is[5,20] $W_{\rm el}(E,V)\approx(|V_0^-|/\varepsilon_F)^2[(eV-E)/\hbar]\mathcal{T}$, where $V_0^-=(V_0^{(2)}-V_0^{(1)})/2$. For the phonon-assisted process[7] $W_{\rm ph}(E,T)\approx(\Lambda^2E^2/\mathcal{E}\Theta_D^3)(E/\hbar)\coth(E/2T)\mathcal{T}$. Here Λ is the fluctuator deformational potential, and $\mathcal{E}$ and Θ_D are the atomic and Debye energies, respectively. $\mathcal{T}=\exp(-\lambda)$, where λ is the tunneling constant.

Let us define the characteristic energy E^* for which $W_{\rm el}(E^*,(eV-E^*)\approx E^*)=W_{\rm ph}(E^*,T=0)$; for the reasonable values of the parameters (see e.g., Ref. 20), E^* is expected to be ≈ 1–3 K. For $eV \gg E^*$ a probability of electron-assisted tunneling to the upper level $W_{\rm el}$ exceeds the probability of phonon-assisted decay of the upper level $W_{\rm ph}$ up to some threshold energy $E=E_{\rm th}=E^*(eV/E^*)^{1/3}$, at which an increase of the electron phase volume with bias ($\propto eV$) is compensated for by a corresponding increase of phonon phase volume ($\propto E^3$). For the crude estimates let us take the occupation numbers $n(E)\propto\theta(E_{\rm th}-E)$. Now, making use of Eq. (11) and assuming the density of states $P(E)$ to be constant, one obtains the following interpolation formula for the interference contribution to the conductance:

$$\Delta G \propto \left[E^*\left(\frac{eV}{E^*}\right)^{1/3}+T\right]^{\beta}, \tag{15}$$

with $\beta=2$.

The same considerations can be applied to the case of ''delocalized'' defects. Although the probabilities $W_{\rm el}$ and $W_{\rm ph}$ for this case can differ from ones for the two-level fluctuators, the scaling $W_{\rm el}/W_{\rm ph}\sim eV/E^3$ (relation between relevant electron and phonon phase volumes) holds for ($eV \gg E \geqslant T$), and thus Eq. (15) is valid, but with $\beta=1$.

IV. DIRECT EFFECT OF THE APPLIED BIAS ON THE FLUCTUATOR PARAMETERS

When a large enough bias V is applied to the point contact, one should take into account the nonequilibrium electron distribution in the course of estimates Eqs. (4), (6), and (9). For the distribution given by Eq. (14) one obtains (see Appendix A 2) for $\Delta E_{{\rm el},im}$ the phase factor

$$\Delta E_{{\rm el},im}\propto\cos[2k_FR_{im}+\phi(V,R_{im},k_F)]\cos(2\Delta kR_{im}), \tag{16}$$

and for δG_{im} a factor

$$\delta G_{im}\propto\cos[2k_FR_{im}+\phi(V,R_{im},k_F)]\cos(2\Delta kR_{im}) + \frac{\partial\phi}{\partial V}\frac{1}{2R(\partial\Delta k/\partial V)}\sin[2k_FR_{im} + \phi(V,R_{im},k_F)]\sin(2\Delta kR_{im}), \tag{17}$$

where $\Delta k\equiv k_FeV/\varepsilon_F$. This is the ''direct'' effect of bias on the fluctuators parameters in addition to tuning a of fluctuator level occupation numbers.

As seen, the first term in Eq. (17) is correlated with the phase factor of Eq. (16), while the second is not, and thus will sum out. As for the correlated cosine terms, the effect of bias initially (at $\Delta kR \ll 1$) leads to their decrease due to a decrease of the corresponding cosine factors, while for $\Delta kR \gg 1$ (when the factors are random with respect to parameter R_{im}) they are suppressed due to additional (with respect to the case $V=0$) averaging over R_{im}:

$$(\overline{\Delta E_{\rm el}},\overline{\Delta G})\propto(\Delta kR)^{-1/2}.$$

Actually we deal here with the well-known energy averaging effect, suppressing any mesoscopic phenomena.

It is important to note that these effects can lead to resistance anomalies even if the defect structure is not rearranged in the course of the bias application; the only condition is

that the defects occupy the positions with the lowest energies available and thus with the largest mesoscopic contribution to resistance $\overline{\delta G_i}$. For these defect configurations, on average on obtains $\overline{\delta G}<0$. The total interference contribution to the conductance due to N defects is

$$\Delta G \sim N\mathcal{F}(V)\overline{\delta G}, \tag{18}$$

where $\mathcal{F}\sim\cos(\Delta kR)$ for $\Delta kR<1$, and $\mathcal{F}\sim(\Delta kR)^{-1/2}$ for $\Delta kR\gg 1$. The result we obtained is that the bias increase leads to a systematic conductance increase. It is interesting that in combination with the effects discussed for relatively small V—occupation of states with higher energies—this ''direct'' effect can form configurations with *smaller* resistances than those available for a simple temperature increase. Indeed, it can suppress (negative in average) a mesoscopic contribution to the conductance due to configurations with a large enough energy gap between the available realizations which cannot be rearranged at relatively small temperatures when the phonon contribution to the resistance (obviously masking the effects in question) is still small. Note that, as we saw above, bias values allowing the same occupation states of the defects and at the same time the same efficiency of electron-phonon processes as in the equilibrium state with a temperature T, are scaled with T as $eV\approx T(T/E^*)^3$. Thus the energy averaging effects can become pronounced for large-gap configurations when the filling of the upper level is still negligible. Certainly, the temperature increase can also lead to an energy averaging, but the necessary temperatures are too large and correspond to a significant phonon contribution to resistance.

V. DISCUSSION

In this section we would like to make several remarks about the limitations and possible complications of our model. First, until now, we considered the defect energy density of states to be constant. The limitation of the defect energy band leads to a saturation of $\Delta G(T)$ and $\Delta G(V)$ dependencies at $T>T_{\rm sat}$ and $V>V_{\rm sat}$, respectively. These quantities scale as $eV_{\rm sat}\approx T_{\rm sat}(T_{\rm sat}/E^*)^3$ and $\Delta G_{\rm sat}\approx N_f\overline{\delta G}$, where N_f is a total number of fluctuators. As for the estimate for $T_{\rm sat}$, taking $\varepsilon_F\approx 10^4$–$10^5$ K and $(d/\lambda_F)\approx 50$, and making use of Eq. (10), we obtain $T_{\rm sat}\approx\overline{E_{{\rm el},i}}\approx 4$–$40$ K. Note that the ''saturation'' value $\Delta G_{\rm sat}$ corresponds to a random realization of different interference patterns involving the fluctuators, while the values of ΔG at lower temperatures correspond to a preferable occupation of larger resistance states, and thus are systematically smaller than typical for mesoscopic disorder.

Second, it is important that the picture discussed is sensitive to the external magnetic field. In particular, it is known that in homogeneous diffusive conductors the interference particle-particle channel is suppressed in a strong enough magnetic field $H>\Phi_0/L_c^2$ where Φ_0 is the quantum of the magnetic flux and L_c is the coherence length, while in our case we use a contact size d. This suppression reduces the magnitude of mesoscopic fluctuations nearly twice.[13,16] The point contact is a strongly inhomogeneous system, and the main contribution to the mesoscopic fluctuations is due to local interference. However, despite the fact that the effect of magnetic field implies a contribution of configurations which involve more than two scatterers, this contribution is relatively large due to the rather high probability of the boundary scattering, and leads to a decrease of ΔG with the field increase.

Another important feature is related to a coupling between different ''active'' defects i and j, due to a dependence of the defect i energy on a position of defect j. This dependence is given by Eq. (6). For a large enough concentration of ''active'' defects one may expect the formation of self-organized aggregates in the defect system (of spin-glass type). Indeed, defect positions corresponding to maxima of the Friedel oscillations caused by the other defects become energetically preferrable, which introduces some ''ordering'' into the defect system. Thus a formation of ''coherently scattering'' aggregates can be possible, leading to a significant enhancement of the interference contribution to resistance. The increase of bias is expected first to suppress this contribution to the resistance in a way similar to discussed above. On the other hand, at higher biases the direct bias-induced decrease of ''coupling potentials'' $E_{{\rm el},ij}$ [see Eq. (16)] can destroy such aggregates, which can lead to sharp resistance changes.[21]

Finally, it is instructive to compare results of our model with the two-channel Kondo model (TCKM), [22,23] which also predicts zero-bias resistance anomalies of a nonmagnetic nature. Despite the fact that these two models are based on completely different physical backgrounds, they predict qualitatively similar resistance behaviors at low T and V: the negative temperature and bias resistance coefficients affected by a magnetic field. However, quantitative predictions of the two models differ. Our model does not predict a singular T behavior at $T\to 0$—in contrast to the TCKM. As for bias dependence, our model predicts a singular behavior $V^{2/3}$ for biases $V\gtrsim 1$–3 mV [see Eq. (15)] and saturation at smaller biases. This saturation can imitate the ''restoration of the Fermi-liquid behavior'' predicted by the TCKM. On the other hand, the TCKM, being related to the nonadiabatic effect, is relevant to fluctuators of a rather special type (with a small asymmetry and large tunneling probability), while our predictions hold for any sort of mobile defect. Our model also predicts special features at higher temperatures and biases; in particular, the saturation of the zero bias anomaly at large V and T, and a principal possibility to reach larger values of conductance in the course of a bias increase with respect to the ones available for a temperature increase.

VI. CONCLUSIONS

To conclude, we predict a mechanism of zero-bias resistance anomalies in metallic point contacts based on a correlation found between energies of defects with an internal degree of freedom and their contributions to resistance. The correlation lifts to some extent the ''random'' character of mesoscopic disorder, and breaks the symmetry of the defect states with respect to the signs of the mesoscopic contribution to resistance. We suggest a model of a fluctuator related to a purely electronic disorder, which provides insight into the nature of fluctuators in the perfect point contacts.

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APPENDIX A:

1. Calculation of the mesoscopic contribution to the conductance and to the defect energy at small applied biases

To calculate mesoscopic contributions both to the conductance and energy of the electron system due to the presence of some finite number of scatterers, we will make use of the ''wave-optics'' approach.[24] The approach is based on perturbation theory in real space. Let us consider an electron, the wave function of which initially is a plane wave with the wave vector $\mathbf{k}$. After n successive scattering events involving scatterers $1,\ldots,n$ the electron wave function becomes

$$|1,\ldots,n\rangle \equiv \psi_{1,\ldots,n}(\mathbf{r}) = \frac{f^n}{|\mathbf{r}-\mathbf{R}_n|\cdot\cdots\cdot|\mathbf{R}_2-\mathbf{R}_1|} e^{i\mathbf{k}\cdot\mathbf{R}_1}\exp(ik[|\mathbf{r}-\mathbf{R}_n| + \cdots + |\mathbf{R}_2-\mathbf{R}_1|]) \tag{A1}$$

where $\mathbf{R}_1,\ldots,\mathbf{R}_n$ are the positions of the scatterers. For the short-range scatterers the scattering amplitude f in the Born approximation takes the form

$$f = -\frac{m}{2\pi\hbar^2}\int d^3r V(\mathbf{r}), \tag{A2}$$

and is assumed the same for all scatterers. The contribution of the scatterers to the conductance is determined by their backscattering efficiency. The interference contribution to the backscattering current due to trajectories involving scatterers $1,\ldots,n$ and $1',\ldots,n'$ is

$$\delta\mathbf{j} = \frac{ie\hbar}{2m}(\langle 1',\ldots,n'|\nabla|1,\ldots,n\rangle + \text{c.c.}). \tag{A3}$$

To obtain a contribution to the conductance, one should integrate this equation over $\mathbf{r}$ within some reference plane remote from the scatterers system. It is important that only position of last scatterers n and n' are relevant for this integration, and one deals with a factor

$$\int d^2\rho \exp[ik(|\mathbf{r}-\mathbf{R}_n| - |\mathbf{r}-\mathbf{R}_{n'}|)].$$

Here ρ is a projection of $\mathbf{r}$ on the plane in question. Taking the plane to be normal to $\mathbf{R}_n-\mathbf{R}_{n'}$, and expanding the exponent as $[\ldots]\sim|\mathbf{R}_n-\mathbf{R}_{n'}|+\rho^2|\mathbf{R}_n-\mathbf{R}_{n'}|/r^2$ one obtains the result of the integration in the form:

$$\frac{1}{ik|\mathbf{R}_n-\mathbf{R}_{n'}|}\exp(ik|\mathbf{R}_n-\mathbf{R}_{n'}|).$$

The next step is the integration over $\mathbf{k}$ directions. In its turn, this integration is relevant only to coordinates of the ''first'' scatterers in the chains; that is to $\mathbf{R}_1$ and $\mathbf{R}_{1'}$, which enter the exponential factor $\exp[\mathbf{k}(\mathbf{R}_1-\mathbf{R}_{1'})]$. Correspondingly, the integration over $\cos\theta$, where $\theta=\angle(\mathbf{k},\mathbf{R}_1-\mathbf{R}_{1'})$, gives the factor

$$\frac{1}{ik|\mathbf{R}_1-\mathbf{R}_{1'}|}\exp(ik|\mathbf{R}_1-\mathbf{R}_{1'}|).$$

Finally one arrives at the following estimate for the mesoscopic contribution to the conductance:

$$\frac{\delta G}{G} \sim \frac{f^{n+n'}}{k^2a^2R^{n+n'}} \times\cos[\varphi(n,n',n'-1,\ldots,1',1;n',n,n-1,\ldots,1)] \tag{A4}$$

where the phase φ is

$$\varphi(n,n',n'-1,\ldots,1',1;n,n-1,\ldots,1) = k(|\mathbf{R}_{1'}-\mathbf{R}_1| + |\mathbf{R}_{n'}-\mathbf{R}_n| + |\mathbf{R}_{n'}-\mathbf{R}_{n'-1}| + \cdots + |\mathbf{R}_{2'}-\mathbf{R}_{1'}| - |\mathbf{R}_n-\mathbf{R}_{n-1}| - \cdots - |\mathbf{R}_2-\mathbf{R}_1|). \tag{A5}$$

Here R is a typical interscatterer distance within the chains, while d is the contact size appearing as a result of normalization of the backscattering efficiency on the incident electron flow.

The picture discussed can be interpreted as a contribution to scattering due to the presence of the scatterer n affecting the superposition of states formed by successive scattering by chains $1,\ldots,n-1$ and $1',\ldots,n'$. The phase φ, after the integration over $\mathbf{k}$ directions, is the phase difference for the paths $n,n',n'-1,\ldots,1',1$ and $n,n-1,\ldots,1$, correspondingly. One should also note that in course of derivation of Eq. A4 we have taken into account that only those electrons with energies close to the Fermi energy contribute to the conductance, and used $k=k_F$ in Eq. (A4).

Now let us estimate the mesoscopic contribution to the electron energy due to the presence of the same system of scatterers finally affecting the electron state in the position of scatterer n. In the lowest approximation, one has

$$\delta E_{el}=\langle 1',\ldots,n'|V(\mathbf{r}-\mathbf{R}_n)|1,\ldots,n-1\rangle, \quad \text{(A6)}$$

where V is a scattering potential assumed to be short ranged: $V=V_0\delta(r)$. As a result of averaging over the direction of $\mathbf{k}$, we obtain

$$\delta E_{\mathrm{el}}\approx -V_0\frac{f^{n+n'-1}}{kR^{n+n'+1}} \times\sin[k\varphi(n,n',n'-1,\ldots,1',1;n,n-1,\ldots 1)]. \quad \text{(A7)}$$

This is important, since the structure of the expression for δE_{el} and that for δG, the phase difference for the interference pattern φ, are exactly the same.

In order to obtain the interference correction to the energy of the whole electron system we should sum Eq. (A7) over all occupied electronic states. For $T=0$, one has

$$\delta E_{\mathrm{el}}\sim -\frac{V_0}{\pi^2}\frac{f^{n+n'-1}}{R^{n+n'+1}}\int_0^{k_F}k\,dk\sin[k\varphi(n,n',n'-1,\ldots,1',1;n,n-1,\ldots 1)]$$

$$=-\frac{V_0}{\pi^2}\frac{f^{n+n'-1}k_F}{R^{n+n'+2}(n+n')}\cos[\varphi(n,n',n'-1,\ldots,1',1;n,n-1,\ldots 1)]. \quad \text{(A8)}$$

Thus we conclude that the mesoscopic contributions of the same system of scatterers to the conductance and to the electron energy renormalization depend on the *same* phase factor and, therefore, *are correlated*.

For the simplest case of two scatterers (positioned in $\mathbf{R}_1$ and $\mathbf{R}_{1'}$), site $\mathbf{R}_1$ plays the same a role as site $\mathbf{R}_n$. The phase factor in this case is

$$\cos(k|\mathbf{R}_{1'}-\mathbf{R}_1|+k|\mathbf{R}_{1'}-\mathbf{R}_1|)=\cos(2k|\mathbf{R}_{1'}-\mathbf{R}_1|),$$

and, correspondingly,

$$\frac{\delta G}{G}\sim\frac{f^2}{a^2k_F^2R^2}\cos(2kR), \quad \delta E_{\mathrm{el}}\sim -\frac{fV_0k_F}{R^3}\cos(2kR), \quad \text{(A9)}$$

which gives Eqs. (4) and (6).

2. Direct effect of bias on the interference contributions

In this subsection we will study the ''direct'' effect of bias on the renormalization of the fluctuator energy and on the interference contribution to the conductance for the simplest case of two scatterers. We start by deriving E_{el}. For the steplike electron distribution given by Eq. (14) for the integral over k [instead of Eq. (A8)] one obtains

$$\frac{1}{2}\int_{k_F-\Delta k}^{k_F+\Delta k}dk\sin(2kR+\phi(V,R,k_F))+\int_0^{k_F-\Delta k}dk\sin(2kR+\phi(V,R,k_F))$$

$$=\int_0^{k_F+\Delta k}dk\,k\sin(2kR+\phi(V,R,k_F))-\frac{1}{2}\int_{k_F-\Delta k}^{k_F+\Delta k}dk\,k\sin(2kR+\phi(V,R,k_F)) \quad \text{(A10)}$$

Here $\Delta k = eV/\hbar v_F$. An additional V-dependent phase ϕ is related to a dependence of k on a coordinate due to the presence of an electric field $[(\hbar k)^2/2m + \varphi(\mathbf{r}) = \varepsilon = \text{const}]$. Calculation of the integral gives the phase factor

$$\cos[2(k_F+\Delta k)R + \phi(V,R,k_F)] + \sin(2k_F R + \phi)\sin(2\Delta k R) = \cos[2k_F R + \phi(V,R,k_F)]\cos(2\Delta k R) \tag{A11}$$

instead of the factor $\cos(2k_F R)$ obtained for $V \to 0$.

In the same way we estimate the contribution to the conductance at $T=0$:

$$\begin{aligned}\delta I &\propto \int_{k_F-\Delta k}^{k_F+\Delta k} \cos(2kR + \phi(V,R,k_F)), \delta G \\ &= \frac{dI}{dV} \propto \frac{\partial \Delta k}{\partial V}[\cos(2(k_F+\Delta k)R + \phi(V,R,k_F)) + \cos(2(k_F-\Delta k)R + \phi(V,R,k_F))] \\ &\quad - \frac{\partial \phi}{\partial V}\int_{k_F-\Delta k}^{k_F+\Delta k} \sin(2kR + \phi(V,R,k_F)) \\ &\sim \frac{\partial \Delta k}{\partial V} 2\cos(2k_F R + \phi(V,R,k_F))\cos(2\Delta k R) + \frac{\partial \phi}{\partial V}\frac{1}{2R} 2\sin(2k_F R + \phi(V,R,k_F))\sin(2\Delta k R)\end{aligned} \tag{A12}$$

Taking into account that $\phi \sim \Delta k R R/a$, one sees that the second and the first terms on the right-hand side of Eq. (A12) are of the same order provided that $R/a \approx 1$. However, the first term completely correlates with the corresponding phase factor for the energy renormalization, Eq. (A11), while the second term does not.

APPENDIX B

For each ''active'' defect i the interference contribution to the conductance, G_i, as well as to the energy, $E_{\text{el},i}$ contains a summation over ''background'' scatterers m. The contribution of each scatterer m gives some phase factor $\xi(\mathbf{R}_{im}) \equiv \xi_{im} = \xi_{mi}$ which depends on the distance of the scatterer m from the defect. Hence one can rewrite the expressions for δG_i and $E_{\text{el},i}$ in a form

$$\delta G_i \equiv \sum_m G_{im}\xi_{im} \equiv (\mathbf{G}_i, \vec{\xi}_i), \tag{B1}$$

$$E_{\text{el},i} \equiv \sum_m E_{im}\xi_{im} \equiv (\mathbf{E}_i, \vec{\xi}_i). \tag{B2}$$

Here we have introduced some ''vector space,'' where vector $\vec{\xi}_i$ contains the set of the corresponding phase factors, and vectors $\mathbf{E}_i$ and $\mathbf{G}_i$ contain the sets of the prefactors [given by Eqs. (3) and (5), correspondingly]. For the ensemble of defects i, the vector $\vec{\xi}_i$ should be considered random, while all components of $\mathbf{E_i}$ and $\mathbf{G_i}$ are positive. We may rewrite the vectors $\mathbf{E}_i$ and $\mathbf{G}_i$ as

$$\mathbf{E}_i = \frac{\mathbf{E}_i}{\overline{E_i}}\overline{E_i}, \quad \mathbf{G}_i = \frac{\mathbf{G}_i}{\overline{G_i}}\overline{G_i} \tag{B3}$$

where we have introduced the ''norms'' of the vectors $\mathbf{E}_i$ and $\mathbf{G}_i$. The correlator $\langle \xi_m, \xi_n \rangle = \gamma \delta_{m,n}$ (where for the cosine phase factors $\gamma = \frac{1}{2}$), and we obtain

$$\langle \delta G_i, E_{\text{el},i} \rangle = \langle (\mathbf{G}_i, \boldsymbol{\xi}_i)(\mathbf{E}_i, \boldsymbol{\xi}_i) \rangle = \gamma \overline{E_i G_i} \left(\frac{\mathbf{E}_i}{\overline{E_i}}, \frac{\mathbf{G}_i}{\overline{G_i}} \right). \tag{B4}$$

The scalar product of the normalized positively defined vectors in the brackets is of the order of unity, and one comes to the estimate for the average, Eq. (8), $\langle\ \rangle = C\,\overline{\delta G}\,\overline{E_{\text{el}}}$ [according to definitions given in front of Eq. (7), $E = E_{\text{el}}$ and $G = \delta G$].

Representing vector $\mathbf{G}$ as a sum of components ''parallel'' and ''normal'' to the vector $\mathbf{E}$: $\mathbf{G} = \mathbf{G}_E + \mathbf{G}_\perp$, one has $(\mathbf{G}_E, \mathbf{E}) = (\mathbf{G}, \mathbf{E})$, $(\mathbf{G}_\perp, \mathbf{E}) = 0$, and, finally,

$$\mathbf{G}_E = \frac{(\mathbf{G}, \mathbf{E})}{E^2}\mathbf{E} = C\frac{\overline{\delta G}}{\overline{E}}\mathbf{E}$$

Decomposing in the same way the random vector $\vec{\xi}_i$ on the components ''parallel'' and ''normal'' to $\mathbf{E}$ (ξ_E and $\xi_\perp$) and taking into account that

$$\langle \delta G \rangle_E = \langle (\mathbf{G}_E + \mathbf{G}_\perp, \vec{\xi}_E + \vec{\xi}_\perp) \rangle_E,$$

$$(\mathbf{G}_E, \vec{\xi}_\perp) = (\mathbf{G}_\perp, \vec{\xi}_E) = 0,$$

and $\langle (\mathbf{G}_\perp, \vec{\xi}_\perp) \rangle = 0$, we finally have

$$\langle \delta G \rangle_E = \langle (\mathbf{G}_E, \vec{\xi}_E) \rangle = C\frac{\overline{\delta G}}{\overline{E}}(\mathbf{E}, \vec{\xi}) = C\frac{\overline{\delta G}}{E}E,$$

which corresponds to Eq. (9). This means that δG has a linear regression with respect to E_{el}.

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