Thermoelectric resonant transport through the Anderson impurities

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The low-temperature thermoelectric resonant transport through the Anderson impurities under the Kondo resonance conditions is studied. It is shown that for the smooth Anderson impurity (AI) density of states the thermoelectric current is parametrically larger than that in the absence of on-site Coulomb correlation, which is the signature of the Kondo effect. In the case of singular AI density of states some new characteristic temperature appears. For temperatures smaller than this, the Kondo-type contributions to the thermoelectric current are important, while in the opposite case the conventional picture of thermoelectric transport returns.

Recently, transport in mesoscopic systems with a strong electron-electron interaction has received considerable interest.[1–3,7–11] In particular, in small tunneling systems, this interaction suppresses tunneling in certain temperature and voltage regimes. This so-called Coulomb blockade[1,2] leads to various anomalies in transport coefficients including the conductance[1,2] and the thermopower.[3]

As one further reduces a sample size, a problem of the resonant tunneling through an Anderson localized state[4] with an on-site Coulomb repulsion arises. At sufficiently high temperatures, this on-site electron-electron interaction leads to a shift of the resonance energy. At small temperatures and small applied voltages, the Kondo resonance anomaly becomes important and dominates the tunneling transport.[5–11] The first time the importance of the Kondo anomaly for tunneling transport was pointed out and studied above the Kondo temperature by Appelbaum[5] and Anderson.[6] For a wide temperature range, both higher and lower than the Kondo temperature of Anderson impurity (AI), this problem has been reexamined by Glazman and Raikh[7] and Ng and Lee[8] within the linear response approximation. Very recently, the nonlinear current response on an applied voltage[9,10] and effects of the external magnetic field on this[11] were studied.

At the same time, all research on the low-temperature transport through the Anderson impurities has been focused on the current-voltage characteristics, while the thermal and the thermoelectric transport have not been under discussion. This is mainly due to the fact that the latter are more difficult to measure. However, recent experiments on different nanometer-size structures showed that it is, in fact, possible to study in these structures the "off-diagonal" transport coefficients like the thermopower and the Peltier coefficient. In particular, the thermoelectric transport through the quantum point contact,[12–14] and through the quantum dot in the Coulomb blockade regime[3,15] were analyzed both experimentally[14,15] and theoretically.[12,13,3]

The purpose of the present paper is to study the low-temperature thermoelectric transport through the Anderson impurities under the Kondo resonance conditions. It is well known that in such typical Kondo systems as the dilute magnetic alloys, the thermoelectric transport is anomalously effective and is characterized by a giant thermopower.[16] This makes it attractive to study thermoelectric resonant-tunneling transport via an ensemble of Anderson impurities. The important difference between these two systems is that while the dilute magnetic alloy can be characterized by one Kondo temperature T_K, AI with levels being scattered in energy space have a *distribution* of Kondo temperatures $\{T_K^{\rm AI}\}$. We will show that the thermoelectric current is sensitive to this distribution. For a smooth AI density of states the thermoelectric current has a large additional factor $\approx \tilde{\Gamma}/T$, with respect to that in the absence of the on-site Coulomb interaction, which is the signature of the Kondo effect; $\tilde{\Gamma}$ is the characteristic level broadening (see below), T is the temperature. In the case of singular AI density of states, we show that a new characteristic temperature $\tilde{T}^{\rm AI} \gg T_K^{\rm AI}$ appears. If $T \ll \tilde{T}^{\rm AI}$ the Kondo contributions to the thermoelectric current are important, while if $T \gg \tilde{T}^{\rm AI}$ the many-body effects are unimportant and the conventional picture of thermoelectric transport returns.

We consider the system in the standard setup. Electrons tunnel resonantly via AI levels positioned in a barrier of the device (see Fig. 1). The Hamiltonian of such a system, taking account for on-site Coulomb repulsion (W is the Coulomb energy), has a form:[4]

$$\begin{aligned} H = &\sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} a^\dagger_{L\mathbf{k}\sigma} a_{L\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} a^\dagger_{R\mathbf{k}\sigma} a_{R\mathbf{k}\sigma} \\ &+ \sum_i \left[\varepsilon_i \sum_\sigma d^\dagger_{i\sigma} d_{i\sigma} + W d^\dagger_{i\sigma} d_{i\sigma} d^\dagger_{i-\sigma} d_{i-\sigma} \right] \\ &+ \sum_{\mathbf{k}\sigma} \left(V_L^i a^\dagger_{L\mathbf{k}\sigma} d_{i\sigma} + V_L^{i*} d^\dagger_{i\sigma} a_{L\mathbf{k}\sigma} \right) \\ &+ \sum_{\mathbf{k}\sigma} \left(V_R^i a^\dagger_{R\mathbf{k}\sigma} d_{i\sigma} + V_R^{i*} d^\dagger_{i\sigma} a_{R\mathbf{k}\sigma} \right) . \end{aligned} \quad (1)$$

Here, $a_{L\mathbf{k}\sigma}$, $a_{R\mathbf{k}\sigma}$, and $d_{i\sigma}$ are the second-quantization operators for the electrons with the wave vector $\mathbf{k}$ and spin σ in the left, right leads, and on the ith AI correspondingly; ε_i—energy of the ith AI level; V_L^i and V_R^i hybridization constants.

Thermoelectric current through the junction is a result of the applied temperature shift[17] between left and right

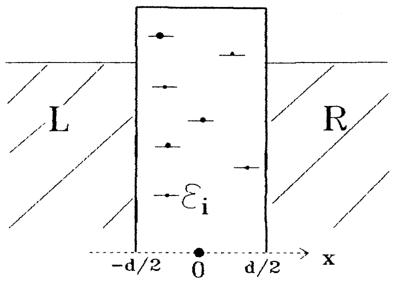

FIG. 1. Resonant tunneling through the Anderson impurities.

leads of the device $\Delta T \equiv T_L - T_R$, which is considered as small $\Delta T \ll T_L, T_R \approx T$. In the spirit of Landauer approach,[18] we express this current in terms of the transmission probability $D(\varepsilon, T)$ of the electron with energy ε through the barrier:

$$I_T = 2\frac{e}{h}\,\Delta T \int D(\varepsilon,T)\frac{\varepsilon-\varepsilon_F}{T}\left(-\frac{\partial f}{\partial \varepsilon}\right)d\varepsilon, \tag{2}$$

where $f(\varepsilon, T)$ is the Fermi distribution function.

If the tunnel barrier is thin enough, one can neglect the processes involving two or more AI simultaneously and consider them all as independent transmission channels. That gives $D(\varepsilon,T) = \sum_i D^i(\varepsilon,T)$, where i indices the AI with the energy ε_i and the coordinate x_i.

In the absence of the on-site Coulomb interaction ($W = 0$), Eq. (1) describes standard resonant tunneling. As it is well-known, the transmission coefficient $D^i(\varepsilon,T)$ in this case is given by the Breit-Wigner formula and does not depend on temperature if one neglects many-body effects in the leads:

$$D^i(\varepsilon,T) = D^i(\varepsilon) = \frac{4\Gamma_L^i\Gamma_R^i}{(\varepsilon-\varepsilon_i)^2 + (\Gamma_L^i + \Gamma_R^i)^2}, \tag{3}$$

where $\Gamma^i_{L(R)} = \pi|V^i_{L(R)}|^2\nu_F$ is a width of quasilocal level ε_i, with respect to electron decay from ε_i to the left (right) lead, ν_F is the density of electron states at the Fermi level in the leads. Widths Γ_L^i and Γ_R^i depend exponentially on x_i:

$$\Gamma_L^i + \Gamma_R^i = 2\Gamma_0 \cosh\left(\frac{2x_i}{\lambda}\right),$$

where $\Gamma_0 \equiv (\Gamma_L^i\Gamma_R^i)^{1/2} \propto \exp(-d/\lambda)$ does not depend on i, λ is the tunneling constant, d-barrier thickness. From Eq. (3), it is clear that resonant transport via those impurities close to the Fermi level $|\varepsilon_i - \varepsilon_F| < \Gamma_L^i + \Gamma_R^i$ is mostly effective.

In the case $W = 0$, the transmission coefficient as a function of ε changes weakly in the T vicinity of chemical potential, and we expand D in powers of $\varepsilon - \varepsilon_F$. Leading nonvanishing term of this expansion gives from Eq. (2),

$$I_T^{W=0} = \Delta T \frac{2\pi^2 e}{3h} T \left.\frac{\partial D(\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon=\varepsilon_F}. \tag{4}$$

The thermoelectric current, Eq. (4) is proportional to $T/\max\{|\varepsilon_i - \varepsilon_F|, (\Gamma_L^i + \Gamma_R^i)\}$, which is due to the particle-hole symmetry, characteristic for degenerate Fermi systems.

Finite on-site Coulomb interaction ($W \neq 0$) makes the many-body effects important. In particular, for the AI level positioned far below ε_F and with large enough on-site Coulomb constant $W \gg \varepsilon_F - \varepsilon_i \gg \Gamma_0$, an increase of junction conductance[6–11] with the temperature decrease, in analogy with the well-known Kondo effect in dilute magnetic alloys, takes place. Let us study this quantitatively. For the sake of simplicity consider first only one AI, with parameters ε_0, x_0, V_L^0, and V_R^0. Following Glazman and Raikh,[7] we introduce new second-quantization operators $\alpha_{\mathbf{k}\sigma}$ and $\beta_{\mathbf{k}\sigma}$:

$$\alpha_{\mathbf{k}\sigma} = u a_{L\mathbf{k}\sigma} + v a_{R\mathbf{k}\sigma}, \tag{5}$$

$$\beta_{\mathbf{k}\sigma} = u a_{R\mathbf{k}\sigma} - v a_{L\mathbf{k}\sigma}, \tag{6}$$

where $u = V_L^0/V^0$, $v = V_R^0/V^0$, $V^0 = (|V_L^0|^2 + |V_R^0|^2)^{1/2}$. This transforms the Hamiltonian, Eq. (1), to a form

$$\begin{aligned} H = &\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}\sigma}\alpha^\dagger_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}\sigma}\beta^\dagger_{\mathbf{k}\sigma}\beta_{\mathbf{k}\sigma} + \varepsilon_0\sum_\sigma d^\dagger_{0\sigma}d_{0\sigma} \\ &+ W d^\dagger_{0\sigma}d_{0\sigma}d^\dagger_{0\,-\sigma}d_{0\,-\sigma} + V^0\sum_{\mathbf{k}\sigma}\left(\alpha^\dagger_{\mathbf{k}\sigma}d_{0\sigma} + d^\dagger_{0\sigma}\alpha_{\mathbf{k}\sigma}\right), \end{aligned} \tag{7}$$

in which only one sort of quasiparticles (α) is coupled with the AI. This Hamiltonian (without $\beta^\dagger\beta$ terms) is equivalent to the standard Kondo sd Hamiltonian,[19] with both the potential scattering constant $\mathcal{V}_\varepsilon^i$ and the exchange scattering constant $\mathcal{J}_\varepsilon^i$ depending on the electron energy ε and being of the same order. For the electrons with energies close to the Fermi level, they are estimated as[19]

$$\mathcal{J}_\varepsilon^i \approx \mathcal{V}_\varepsilon^i \approx \frac{2}{\pi\nu_F}\frac{\Gamma_L^i + \Gamma_R^i}{\varepsilon_i - \varepsilon_F}. \tag{8}$$

The quasiparticle scattering amplitude $S_{\alpha\mathbf{k}\to\alpha\mathbf{k}'}$ in the new representation is related to the tunneling amplitude as $S_{L\mathbf{k}\to R\mathbf{k}'} = [V_L^0 V_R^{0*}/(V^0)^2]S_{\alpha\mathbf{k}\to\alpha\mathbf{k}'}$. As a result, with taking into account only elastic electron scattering on AI, the transmission coefficient $D^i(\varepsilon,T)$ has a form[7]

$$D^i(\varepsilon,T) = D_0(\varepsilon_F)\,\frac{4\Gamma_L^i\Gamma_R^i}{(\Gamma_L^i+\Gamma_R^i)^2}\,[\sin(\delta^i_{\varepsilon,T})]^2, \tag{9}$$

where $D_0(\varepsilon)$ is the transmission coefficient under the full resonance conditions ($x^i = 0$, $\varepsilon_i = \varepsilon_F$), and $\delta^i_{\varepsilon,T}$ is a scattering phase in terms of which the scattering amplitude $S_{\alpha\mathbf{k}\to\alpha\mathbf{k}'}$ in a "homogeneous metal" is expressed. This phase is determined by the relationship between T and the so-called Kondo temperature[20,7] of AI T_K^i:

$$\begin{aligned} T_K^i &= \frac{2}{\pi}\left[2\varepsilon_i^{**}(\Gamma_L^i+\Gamma_R^i)\right]^{1/2}\exp\left(-\frac{\pi\varepsilon_i^{**}}{2(\Gamma_L^i+\Gamma_R^i)}\right), \\ \varepsilon_i^{**} &+ \frac{\Gamma_L^i+\Gamma_R^i}{\pi}\ln\left(\frac{W}{4\varepsilon_i^{**}}\right) = \varepsilon_F - \varepsilon_i, \\ W &\gg \varepsilon_i^{**} > \Gamma_L^i + \Gamma_R^i. \end{aligned} \tag{10}$$

In the case $T \gg T_K^i$, the Born approximation [$\delta^i_{\varepsilon,T} = \delta^{i(1)}_{\varepsilon,T} + \delta^{i(2)}_{\varepsilon,T} + \cdots$, and, correspondingly, $D^i(\varepsilon,T) = D^{i(1)}(\varepsilon,T) + D^{i(2)}(\varepsilon,T) + \cdots$] is valid. The first-order value of the transmission coefficient $D^{i(1)}(\varepsilon,T)$ coincides with Eq. (3) in the lowest approximation and does not depend on temperature:

$$D^{i(1)}(\varepsilon) \approx D_0 \frac{4\Gamma_L^i \Gamma_R^i}{(\varepsilon - \varepsilon_i)^2}. \tag{11}$$

In the next-order approximation, the temperature-dependent terms appear. For the electrons with $\varepsilon \approx \varepsilon_F$, they are

$$D^{i(2)}(\varepsilon,T) \approx D_0 \Gamma_L^i \Gamma_R^i \left\{ \frac{(\Gamma_L^i + \Gamma_R^i)}{(\varepsilon_F - \varepsilon_i)^3} \ln\left(\frac{\varepsilon_F}{T}\right) + \frac{(\Gamma_L^i + \Gamma_R^i)^2}{(\varepsilon_F - \varepsilon_i)^4} [2f(\varepsilon,T) - 1] \right\}. \tag{12}$$

The first, logarithmic, term in Eq. (12) is proportional to the exchange scattering constant $\mathcal{J}^i_\varepsilon$ squared and is responsible for the low-temperature Kondo-type conductance enhancement. The second, $[2f(\varepsilon,T) - 1]$ term is proportional to $(\mathcal{J}^i_\varepsilon)^3 \mathcal{V}^i_\varepsilon$ and gives smaller contribution to the conductance. However, only the latter term is odd, with respect to $\varepsilon - \varepsilon_F$, lifts the particle-hole symmetry and, thus, gives rise to the thermoelectric current.[16]

When T becomes smaller than T_K^i, Anderson impurity becomes strongly screened by the electron cloud. The scattering phase for electron scattering on such a "complex" tends to $\pi/2$ (unitary limit) and may be written as[20]

$$\delta^i_{\varepsilon,T} = (\pi/2)[1 - \gamma(T/T_K^i)^2], \tag{13}$$

where γ is constant of order unity. In this case, particle-hole symmetry recovers and thermoelectric current due to tunneling via ith AI vanishes.

Strictly speaking, Eq. (9) is valid only at zero temperature, when only elastic electron scattering is present. In the case $T \neq 0$, electrons can be scattered inelastically[20] on a complex "Anderson impurity + screening cloud" via a polarization of the screening cloud. This scattering channel also gives rise to the transmission coefficient. In the limit of small temperatures, $T \ll T_K^i$ AI is nearly completely screened by the electron cloud and the inelastic scattering contribution to the temperature-dependent part of D^i is of the order of[20] the elastic scattering contribution, Eq. (13). However, this temperature limit does not contribute to the thermopower under discussion. In the case $T \gg T_K^i$, screening of the impurity by electrons is very weak. The inelastic scattering contribution to the transmission probability is correspondingly weak, and it can be neglected. Therefore, studying thermopower we will not take the inelastic electron scattering channel into account.

Let us now turn to the calculation of the thermoelectric current via an ensemble of AIs. This has a form[21]

$$I_T = S_0 \int_{-d/2}^{d/2} dx_i \int d\varepsilon_i \, g(\varepsilon_i, x_i) \frac{2e}{h} \, \Delta T \times \int D^i(\varepsilon,T) \frac{\varepsilon - \varepsilon_F}{T} \left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon, \tag{14}$$

with $D^i(\varepsilon,T)$ given by Eq. (9); $g(\varepsilon_i, x_i)$ is the AI density of states, S_0 the cross section of the contact. We will consider two limiting cases for $g(\varepsilon_i, x_i)$: constant density of states and singular distribution of ε_i. These cases are most likely to happen in real structures.

(1) Constant density of states $g(\varepsilon_i, x_i) = g_0$. According to Eq. (12) the dominant contribution to the thermoelectric current is due to those AI with $(\varepsilon_F - \varepsilon_i) \approx (\Gamma_L^i + \Gamma_R^i)$, for which the odd, with respect to $\varepsilon - \varepsilon_F$, contribution to the transmission coefficient becomes large. On the other hand, in the region $T \ll T_K^i$, particle-hole symmetry recovers and the contribution of the ith AI to the thermoelectric current vanishes. With account of the equality $\int (2f-1)[(\varepsilon - \varepsilon_F)/T](-\partial f/\partial \varepsilon) d\varepsilon = 1/2$ thermoelectric current, Eq. (14) in this case can be estimated as

$$I_T^{W\neq 0} \approx -\frac{e}{h} \tilde{D} \, \Delta T, \tag{15}$$

where $\tilde{D} \approx \pi^2 S_0 \lambda g_0 \Gamma_0 D_0$ is the resonant transmittance without accounting for collective effects.

It is important to mention that neglecting the on-site Coulomb interaction we would obtain estimate for the thermoelectric current, which has an additional small factor T/Γ_0. Thus, we obtain a strong enhancement of the thermoelectric transport efficiency under the Kondo resonance conditions similar to that in the dilute magnetic alloys.

(2) Singular density of states. For small contacts, the number of AIs is small and their distribution is strongly inhomogeneous. In this case, it is convenient to model AI density of states as a sum of singular terms. For simplicity, we take $g(\varepsilon_i, x_i) = (\mathcal{N}/S_0 d)\delta(\varepsilon_i - \tilde{\varepsilon})$, where $\mathcal{N}$ is a total number of AIs, which all have the same energy $\tilde{\varepsilon}$.

In order to find the thermoelectric current, we have to compare the contribution due to usual potential scattering, Eq. (11), with the Kondo contribution, Eq. (12). For the potential scattering one obtains, combining Eq. (11) and Eq. (4),

$$I_T^{\rm pot} \approx -\frac{e}{h} \Delta T \, \tilde{D} \, \frac{T}{\varepsilon_F - \tilde{\varepsilon}}, \tag{16}$$

where $\tilde{D} = \mathcal{N} D_0 \Gamma_0^2 / (\varepsilon_F - \tilde{\varepsilon})^2$ is the resonant transmittance without account for collective effects. The Kondo contribution gives from Eq. (14), (12) for $T > T_K(x^i = 0, \varepsilon^i = \tilde{\varepsilon})$,

$$I_T^{\rm Kondo} \approx \frac{e}{h} \Delta T \, \tilde{D} \, \frac{\lambda}{d} \exp(2d/\lambda) \frac{\Gamma_0^2}{(\varepsilon_F - \tilde{\varepsilon})^2}. \tag{17}$$

For $T \ll T_K(x^i = 0, \varepsilon^i = \tilde{\varepsilon})$, the Kondo contribution to the thermoelectric current tends to zero.

One sees that there are two regions separated by a characteristic temperature $\tilde{T}(\tilde{\varepsilon}) = [\Gamma_0^2/(\varepsilon_F - \tilde{\varepsilon})](\lambda/d)\exp(2d/\lambda) \approx \mathcal{V}_{\tilde{\varepsilon}}^{x_i=d/2} \mathcal{J}_{\tilde{\varepsilon}}^{x_i=d/2} (\lambda/d)\nu_F$. For $T \gg \tilde{T}(\tilde{\varepsilon})$ the potential scattering dominates, and the thermoelectric current has the usual factor $T/(\varepsilon_F - \tilde{\varepsilon})$ characteristic for the degenerate Fermi systems. For the temperatures $T \ll \tilde{T}(\tilde{\varepsilon})$, the Kondo contribution dominates.

To conclude, the low-temperature thermoelectric transport through the Anderson impurities under the Kondo resonance conditions is studied. It is shown that for the smooth AI density of states, the thermoelectric current is parametrically larger than that in the absence of on-site Coulomb correlation, which is the signature of the Kondo effect. In the case of singular AI density of states, some new characteristic temperature $\tilde{T}(\tilde{\varepsilon}) \gg T_K^{\mathrm{AI}}$ appears. If $T \ll \tilde{T}(\tilde{\varepsilon})$, the Kondo-type contributions to the thermoelectric current are important, while if $T \gg \tilde{T}(\tilde{\varepsilon})$ the conventional picture of thermoelectric transport is restored.

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[17] The question arises, what the estimate for ΔT in real tunneling structures is. For the structures with massive metallic banks, ΔT can be estimated as $\Delta T \approx l^{\text{el-ph}} \nabla T$, where ∇T is the applied temperature gradient in the banks far away from the contact region, $l^{\text{el-ph}}$ is the electron-phonon diffusion length for actual electron energies. For the microjunctions, where the temperature shift ΔT is reached by a local heating (for instance, by current), ΔT is determined by the actual experimental setup.

[18] For a review see, e.g., C.W.J. Beenakker and H. van Houten, in *Solid State Physics: Advances in Research and Applications*, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1991), Vol. 44, p. 1.

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[21] Note that in contrast to the case $W = 0$, where one can expand D in powers of $\varepsilon - \varepsilon_F$ [see Eq. (4)], here D contains terms varying rapidly in the T vicinity of chemical potential, which makes a simple expansion wrong.