Kondo shuttling in a nanoelectromechanical single-electron transistor

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We investigate theoretically a mechanically assisted Kondo effect and electric charge shuttling in a nanoelectromechanical single-electron transistor. It is shown that the mechanical motion of the central island (a small metallic particle) with the spin results in a time-dependent tunneling width $\Gamma(t)$ which leads to an effective increase of the Kondo temperature. The time-dependent oscillating Kondo temperature $T_K(t)$ changes the scaling behavior of the differential conductance, resulting in the suppression of transport in a strong-coupling and its enhancement in a weak-coupling regime. The conditions for fine-tuning of the Abrikosov-Suhl resonance and possible experimental realization of the Kondo shuttling are discussed.

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Kondo resonance tunneling predicted in Ref. 1 and observed experimentally[2] has attracted a great deal of current attention as a possible base for manipulating spin transport. Nanomechanical shuttling[3] (NMS) offers a unique platform for design of a single-electron transistor (SET) in which spin switch and transfer can be controlled electromechanically; the first successful experimental implementation of NMS was reported in Refs. 4 and 5. In this paper we develop a theory of a nanomechanical shuttling device that utilizes the Kondo resonance (KR) effect and thus breaks ground for a class of effects integrating both phenomena.

The Kondo effect in electron tunneling results from the spin exchange between electrons in the leads and the island (quantum dot) that couples the leads and manifests itself as a sharp zero-bias anomaly (ZBA) in low-temperature tunneling conductance. Many-particle interactions and tunneling renormalize the electron spectrum, enabling KR both for odd-[2] and even-[6,7] electron occupations. In the latter case the KR is caused by the singlet-triplet crossover in the ground state (see Ref. 8 for a review).

A general shuttle mechanism for a charge transfer described in Ref. 3 implies periodic charging and decharging of the oscillating nanoparticle. As the bias exceeds some threshold value, the shuttling particle oscillates with constant amplitude along a classical trajectory. A model for a nanoelectromechanical single-electron transistor (NEM-SET), where either a small (nanoscale) metallic particle or a single molecule oscillate under the external time-dependent electric field was studied theoretically in Refs. 9–14. In experimental realizations, the moving dot was mounted as a electromechanical pendulum formed by a gold clapper[5] or a silicon nanopillar.[4] Single-electron tunneling in a molecular conductor with center of mass motion was realized in Ref. 15 and discussed theoretically in Ref. 16. The vibration-induced Kondo effect in metal-organic complexes was further explored in Ref. 17. Experimental realization of the Kondo effect in electron shuttling is becoming one of the most challenging tasks of current nanophysics.

In this paper we investigate the effect of the spin degrees of freedom on single-electron transport through the NEM-SET. We show that mechanical shuttling of a nanoparticle between the leads causes a sequential-in-time reconstruction of its tunnel electronic states and gives rise to the Kondo effect. By analogy with the effect of sequential-in-time recharging of the particle in an ordinary charge shuttling effect[3] we call this phenomenon *Kondo shuttling*.

Building on the analogy with shuttling experiments of Refs. 4 and 5, we consider a device where an isolated nanomachined island oscillates between two electrodes. We are, however, interested in a regime where the applied voltage is low enough so that the field emission of many electrons, which was the main mechanism of tunneling in those experiments, should be neglected. Note further that the characteristic de Broglie wavelength associated with the dot should be much shorter than typical displacements, allowing thus for a classical treatment of the mechanical motion of the nanoparticle. The condition $\hbar\Omega \ll T_K$, necessary to eliminate decoherence effects, requires for, e.g., planar quantum dots with the Kondo temperature $T_K \gtrsim 100$ mK, the condition $\Omega \lesssim 1$ GHz for oscillation frequencies to hold; this frequency range is experimentally feasible.[4,5] The shuttling island then is to be considered as a "mobile quantum impurity," and transport experiments will detect the influence of mechanical motion on a differential conductance. If the dot is small enough, then the Coulomb blockade guarantees the single-electron tunneling or cotunneling regime, which is necessary for realization of the Kondo effect.[1,8] The cotunneling process is accompanied by a change of spin projection in the process of charging and discharging of the shuttle and therefore is closely related to the spin and charge pumping problem.[18]

We apply our theory to planar quantum dots in semiconductor heterostructures.[19] In these systems KR tunneling may be realized both for odd- and even-electron occupation N.[7,8] If N is odd, the last occupied level in the island is occupied by a single electron [Fig. 1(a)]. In this case the Kondo effect occurs and the corresponding Kondo temperature T_K^0 is that of a static regime. The question we wish to address is how T_K is *influenced* by the adiabatic mechanical motion of the

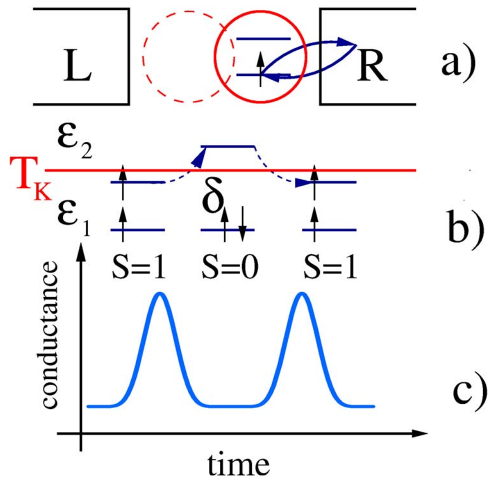

FIG. 1. (Color online) (a) Nanomechanical resonator with an odd number of electrons as a "mobile quantum impurity." (b) Time evolution of the level spacing for the shuttle with an even number of electrons measured with respect to evolving Kondo temperature. (c) Pulse ZBA in tunneling conduction for Kondo shuttling with the singlet-triplet transition.

island. If, on the contrary, N is even, the ground state of the nanoparticle is singlet $S=0$ whereas the excited state is triplet $S=1$ [Fig. 1(b)]. Under the assumption that the energy difference between the singlet and triplet states, $\Delta_{ST}=\delta-J_{ex}$, exceeds the actual Kondo temperature, $\Delta_{ST}>T_K$, the Kondo effect is absent in the static limit (here $\delta=\epsilon_2-\epsilon_1$, J_{ex} is ferromagnetic exchange, and $\epsilon_{i=1,2}$ are the energies of single-electron states for the last occupied and first empty levels). However, the *mechanically induced* Kondo effect may arise provided the inequality $\Delta_{ST}<T_K(t)$ is satisfied due to mechanical motion of the dot.

Now we turn to a quantitative description of Kondo shuttling. The Hamiltonian $H=H_0+H_{tun}$ is given by

$$H_0=\sum_{k,\alpha}\varepsilon_{k\sigma,\alpha}c^{\dagger}_{k\sigma,\alpha}c_{k\sigma,\alpha}+\sum_{i\sigma}[\epsilon_i-e\mathcal{E}x]d^{\dagger}_{i\sigma}d_{i\sigma}+Un^2,$$

$$H_{tun}=\sum_{ik\sigma,\alpha}T^{(i)}_{\alpha}(x)[c^{\dagger}_{k\sigma,\alpha}d_{i\sigma}+\text{H.c.}],\qquad(1)$$

where $c^{\dagger}_{k\sigma}$ and $d^{\dagger}_{i\sigma}$ create an electron in the lead $\alpha=L,R$ or the dot level $\varepsilon_{i=1,2}$, respectively, $n=\Sigma_{i\sigma}d^{\dagger}_{i\sigma}d_{i\sigma}$, and $\mathcal{E}$ is the electric field between the leads. The tunneling matrix element $T^{(i)}_{L,R}(x)=T^{(i,0)}_{L,R}\exp[\mp x(t)/\lambda_0]$ depends exponentially on the ratio of the time-dependent displacement $x(t)$ (which is considered to be a given harmonic function of the time) and the electronic tunneling length λ_0.

We begin with a discussion of an odd-N, $S=1/2$, case [Fig. 1(a)]. Then only the state with $i=1$ is retained in (1), and hereafter we omit this index. In order to find an analytic solution, we assume that if $x(t)$ varies adiabatically slow (on the scale of the tunneling recharging time), there is no charge shuttling due to multiple recharging processes,[3] but the KR cotunneling occurs. The time-dependent tunneling width is $\Gamma_{\alpha}(t)=2\pi\rho_0|T_{\alpha}(x(t))|^2$ (Ref. 20), where ρ_0 is the density of states at the lead Fermi level. The adiabaticity condition reads $\hbar\Omega\ll T_K\ll\Gamma$, with $\Gamma=\min[\sqrt{\Gamma^2_L(t)+\Gamma^2_R(t)}]$. We apply the time-dependent Schrieffer-Wolff transformation and obtain the time-dependent Kondo Hamiltonian[20] as

$$H=H_0+\sum_{k\alpha\sigma,k'\alpha'\sigma'}\mathcal{J}_{\alpha\alpha'}(t)\left[\vec{\sigma}_{\sigma\sigma'}\vec{S}+\frac{1}{4}\delta_{\sigma\sigma'}\right]c^{\dagger}_{k\sigma,\alpha}c_{k'\sigma',\alpha'},\qquad(2)$$

where $\mathcal{J}_{\alpha,\alpha'}(t)=\sqrt{\Gamma_{\alpha}(t)\Gamma_{\alpha'}(t)}/[\pi\rho_0E_d(t)]$ and $\vec{S}=\frac{1}{2}d^{\dagger}_{\sigma}\vec{\sigma}_{\sigma\sigma'}d_{\sigma'}$. Without a loss of generality, we can restrict ourselves to the symmetric Anderson model ($\epsilon_0=-U/2$ in the static limit) and neglect the renormalization of a single-electron level position by tunneling ($\Gamma/U\ll1$) and also by its shift from the equilibrium position $[(e\mathcal{E}A)/U\ll1]$ such as $E_d(t)\approx E^0_d=U/4$.

As long as the nanoparticle is not subjected to the external time-dependent electric field, the Kondo temperature is given by $T^0_K=D_0\exp[-(\pi U)/(8\Gamma_0)]$ [for simplicity we assumed that $\Gamma_L(0)=\Gamma_R(0)=\Gamma_0$; $D_0=\sqrt{2\Gamma_0U/\pi}$ plays the role of effective bandwidth]. As the nanoparticle moves adiabatically, $\hbar\Omega\ll\Gamma$, the decoherence effects are small provided $\hbar\Omega\ll T^0_K$ (see the discussion below). In this case the time can be treated as an external parameter and the renormalization group equations for the Hamiltonian (2) can be solved in the same manner as those for the equilibrium.[20] As a result, the Kondo temperature becomes time oscillating:

$$T_K(t)=D(t)\exp\left[-\frac{\pi U}{8\Gamma_0\cosh[2x(t)/\lambda_0]}\right].\qquad(3)$$

Neglecting the weak time dependence of the effective bandwidth $D(t)\approx D_0$, we arrive at the following expression for the time-averaged Kondo temperature:

$$\langle T_K\rangle=T^0_K\left\langle\exp\left[\frac{\pi U}{4\Gamma_0}\frac{\sinh^2[x(t)/\lambda_0]}{1+2\sinh^2[x(t)/\lambda_0]}\right]\right\rangle.\qquad(4)$$

Here $\langle\cdots\rangle$ denotes averaging over the period of the mechanical oscillation. The expression (4) acquires especially transparent form when the amplitude of mechanical vibrations A is small: $A\lesssim\lambda_0$. In this case the Kondo temperature can be written as $\langle T_K\rangle=T^0_K\exp(-2W)$, with the Debye-Waller-like exponent $W=-\pi U\langle x^2(t)\rangle/(8\Gamma_0\lambda^2_0)$, giving rise to the enhancement of the static Kondo temperature. This counterintuitive exponentially *large* Debye-Waller factor results from the strong asymmetry in the tunneling rate at the turning points of the nanoparticle trajectory. Note that taking the formal limit of the large-amplitude oscillations $A\gg\lambda_0$ one obtains $\langle T_K\rangle\to T^{max}_K(A)\gg T^0_K$ for the time-averaged Kondo temperature if $\Gamma^{max}_{L,R}\ll U$ (see the inset in Fig. 2). In the opposite limit $\Gamma_{L,R}(t_1<t<t_2)\gtrsim U$ the system falls into a mixed-valence regime where the Kondo temperature is the poorly defined quantity. The result (4) survives as long as the large-amplitude limit holds provided that the condition $\langle T_K\rangle/D_0\ll1$ is still fulfilled. We conclude that the Kondo temperature considerably increases as compared to T^0_K when the shuttling particle approaches one of the leads. The relative variation of the Kondo temperature oscillations at small shuttling amplitudes is given by

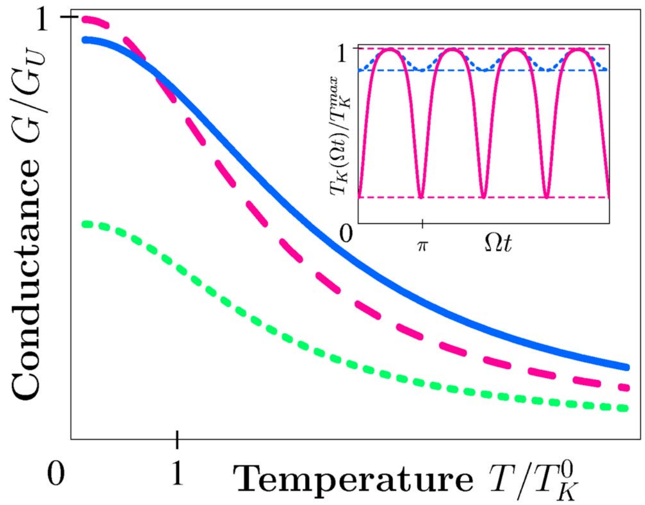

FIG. 2. (Color online) Differential conductance of a Kondo shuttle $\Gamma_0/U=0.4$. Solid line denotes G for the shuttle $\Gamma_L=\Gamma_R$, $A=\lambda_0$. Dashed line: the static nanoisland $\Gamma_L=\Gamma_R$, $A=0$. Dotted line: $\Gamma_L/\Gamma_R=0.5$, $A=0$. The inset shows the time oscillations of T_K for small $A=0.05\lambda_0$ (dotted line) and large $A=2.5\lambda_0$ (solid line) shuttling amplitudes.

$$\frac{\delta T_K}{T_K^0}=\frac{\langle T_K\rangle - T_K^0}{T_K^0}=2\frac{\langle x^2(t)\rangle}{\lambda_D^2}, \tag{5}$$

where $\lambda_D=\lambda_0/\sqrt{\ln(D_0/T_K^0)}\ll\lambda_0$ is the effective tunneling length which accounts for the Kondo renormalizations.

Let us discuss the temperature behavior of the differential conductance $G(T,V_{dc}\to 0)=dI/dV_{dc}$. In the strong coupling Kondo limit $T\ll T_K^0$,

$$G=\frac{2e^2}{h}\left\langle\frac{4\Gamma_L(t)\Gamma_R(t)}{[\Gamma_L(t)+\Gamma_R(t)]^2}\right\rangle=\frac{2e^2}{h}\left(1-2\frac{\delta T_K}{T_K^0}\frac{\lambda_D^2}{\lambda_0^2}\right). \tag{6}$$

The conductance does not reach the unitary limit $G_U=2e^2/h$ due to the asymmetry in the respective couplings to the leads. If, however, the shuttling island was not centrally positioned when starting its motion, the effective magnitude of the conductance can grow as compared to its value at the starting position (see Fig. 2).

In the weak-coupling regime $T_K^{max}\ll T\ll D_0$ the ZBA in the tunneling conductance is given by

$$G(T)=\frac{3\pi^2}{16}G_U\left\langle\frac{4\Gamma_L(t)\Gamma_R(t)}{[\Gamma_L(t)+\Gamma_R(t)]^2}\frac{1}{\{\ln[T/T_K(t)]\}^2}\right\rangle. \tag{7}$$

Although the central position of the island is most favorable for the Breit-Wigner (BW) resonance ($\Gamma_L=\Gamma_R$), it corresponds to the minimal width of the Abrikosov-Suhl resonance. The turning points correspond to the maximum of the Kondo temperature given by Eq. (3) while the system is away from the BW resonance. These two competing effects lead to the effective enhancement of G at high temperatures:

$$G(T)=G_K^0\left\langle\left(\frac{1}{1-2\alpha^2(T)\sinh^2[x(t)/\lambda_0]}\right)^2\right\rangle, \tag{8}$$

where $G_K^0=G_U(3\pi^2)/[16\ln^2(T/T_K^0)]$ is the conductance of the static island in the central position (Fig. 2), $\alpha^2(T)=\ln(D_0/T)/\ln(T/T_K^0)$, and $\lambda_T=\lambda_0/\alpha(T)$ is the temperature-dependent tunneling length. Evaluating Eq. (8) for the small-amplitude limit under the condition $\lambda_T\ll\lambda_0$, we obtain

$$\frac{\delta G_K}{G_K^0}=\frac{G(T)-G_K^0}{G_K^0}=2\frac{\delta T_K}{T_K^0}\frac{1}{\ln(T/T_K^0)}. \tag{9}$$

Formally, the correction to the conductance δG_K, Eq. (9), must be compared with the regular term $O(C/[\ln^3(T/T_K^0)])$. The latter, however, has a much smaller amplitude provided that $C\sim\ln[\ln(T/T_K^0)]\ll(A/\lambda_0)^2\ln(D_0/T)$. Thus, Eq. (9) describes the leading correction to the conductance.

In the limit $T_K^0\ll\hbar\Omega\ll\Gamma$ the differential conductance in the weak-coupling regime is given by

$$G_{peak}=\frac{3\pi^2}{16}G_U\frac{1}{\{\ln[\hbar/(\tau T_K^0)]\}^2}, \tag{10}$$

where $\hbar/\tau\sim\hbar\Omega$ is determined by the decoherence effects associated with the nonadiabaticity of the motion of the shuttling particle and by the Q factor of the NEM device. In general, the behavior of the differential conductance at low temperatures has a form $G_{peak}/G_U=F[(\delta T_K/T_K^0)f(\hbar\Omega/T_K^0)]$, where $F(x)$ and $f(y)$ are two universal functions, each of them depending on one variable similar to Ref. 20. In the large-voltage limit $eV\gg T_K^0$ the finite current transferred by the shuttle and therefore the noise created by this current lead to $\hbar/\tau\sim eV$ destroying the Kondo effect. We will present more detailed discussion on the decoherence effects in the "antiadiabatic" Kondo regime elsewhere.

Next we turn to the case of even N in the island [Fig. 1(b)]. In this case one may refer to the *excited-state Kondo features*,[8,21] where the KR tunneling is possible only during the time intervals where

$$\Delta_{ST}(t)=\delta(t)-J_{ex}(t)<T_K(t). \tag{11}$$

The level spacing $\delta(t)=\epsilon_2(t)-\epsilon_1(t)$ may reduce due to the tunneling-induced Friedel shift

$$\epsilon_i(t)=\epsilon_i^0-\sum_{\alpha=L,R}|T_\alpha^{(i)}(t)|^2\,\mathrm{Re}\left(\int\frac{\rho_0 d\varepsilon}{\epsilon_i-\epsilon_\alpha}\right), \tag{12}$$

provided $T_\alpha^{(2)}>T_\alpha^{(1)}$, which is usually the case.[8] This effect is maximal near the turning points of shuttle motion. Similar second-order tunnel processes result in the so-called Haldane renormalization[22] of J_{ex}. In close analogy with Ref. 7, it is easy to see that the reduction of exchange gap in a dot with even occupation obeys the renormalization group flow equation

$$d\Delta_{ST}/d\eta=\rho_0\sum_\alpha[|T_\alpha^{(2)}|^2-|T_\alpha^{(1)}|^2], \tag{13}$$

where $\eta=\ln(D_0/D)$ is the scaling variable describing the reduction of the energy scale D of the band electrons in the leads. An additional contribution to this reduction originates from the mixture of the excited state with two electrons on the level ε_2 with the ground-state singlet.[7] These effects are also maximal around the turning points of the shuttle trajectory.

Thus, if the condition (11) is valid for the certain time intervals during the oscillation cycle [Fig. 1(b)], Kondo tunneling is possible for a part of this cycle, where the shuttle is close to one of the leads. It should be emphasized that in this regime only the weak-coupling Kondo effect may be observed at $T \gg T_K$, whereas at $T \to 0$ the triplet state is quenched and the dot behaves as a zero-spin nanoparticle.[21] The full-scale Kondo effect may arise only if the variation of $|T_\alpha^{(i)}(t)|^2$ induces a crossover from a singlet to a triplet ground state of a shuttle. The singlet-triplet crossover induced by the variation of gate voltages was observed on a static planar dot.[23] Unlike conventional level crossings, this crossover does not violate adiabaticity because it conserves the SO(4) symmetry of the singlet-triplet manifold.[7,8]

In the excited-state Kondo regime $T_K(t)$ is described by a one-parametric scaling function $T_K(\Delta_{ST}(t)/T_K^*)$, with a maximum at $T_K^* = T_K(\Delta_{ST}=0)$.[7,8] Thus, we conclude that the Kondo shuttling in the case of even N may be observed as a *pulse ZBA in tunnel conduction* [Fig. 1(c)], which emerges in time intervals δt, where the condition (11) is fulfilled. Assuming the linear dependence $\Delta_{ST}(x(t))$,[23] we estimate these intervals as $\delta t \sim \delta x/(\Omega\sqrt{\langle x^2\rangle})$, where δx is the distance from the turning point at which the Kondo shuttling is possible.[24]

The Kondo shuttling differs from the Kondo effect in molecular conductors with center-of-mass motion.[16] In that case the shift of the center-of-mass is caused by single-electron transport and the *nonadiabatic* phonon-assisted processes interfere with the Kondo tunneling.

In conclusion, we have found that the Kondo shuttling in a NEM-SET increases the Kondo temperature due to the asymmetry of coupling in the turning points compared to the central position of the island. As a result, in the case of odd N the differential conductance is enhanced in the weak-coupling regime and is suppressed in the strong-coupling limit. In the case of even N, Kondo tunneling exists only as a shuttling effect.

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