Adiabatic pumping in the mixed-valence and Kondo regimes

Tomosuke Aono
Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel
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We investigate adiabatic pumping through a quantum dot with a single level in the mixed-valence and Kondo regimes using the slave-boson mean field approximation. The pumped current is driven by a gauge potential due to time-dependent tunneling barriers as well as by the modulation of the Friedel phase. The sign of the former contribution depends on the strength of the Coulomb interaction. Under finite magnetic fields, the separation of the spin and charge currents peculiar to the Kondo effect occurs.

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Introduction.— Adiabatic pumping in a quantum dot system occurs when the dot is under slowly varying external gate voltages with zero bias voltage. After a certain period when the system returns to its initial state, a finite charge is transferred by electron interference through the system. In recent experiments, both charge \(^2\) and spin \(^1\) are realized in open quantum dot systems. This pumping has been investigated theoretically; charge pumping \(^3\), \(^4\), \(^5\), \(^6\), \(^7\), \(^8\), \(^9\), \(^10\), \(^11\) as well as spin pumping \(^12\), \(^13\), \(^14\), \(^15\), \(^16\), \(^17\), \(^18\). It has been elucidated that the pumping can be understood in terms of the Berry phase argument in Ref. \(^17\) and Refs. \(^19\), \(^20\), \(^21\), \(^22\).

Adiabatic pumping is investigated for the systems under electron-electron interactions \(^12\), \(^13\), \(^14\), \(^15\), \(^16\), \(^17\), \(^18\). In quantum dots, the interactions introduce a prominent feature, the Kondo effect \(^27\), \(^28\), \(^29\), \(^30\), where the spin-exchange between electrons in the leads and the dot results in an enhancement of the conductance at low temperatures. We investigate the adiabatic pumping in the mixed-valence and the Kondo regimes to demonstrate an interplay between the Kondo effect and a gauge potential associated with the Berry phase, though this system itself is partly studied in Ref. \(^27\). To this end, we will show explicitly the appearance of the Berry phase term due to time-dependent tunneling barriers and elucidate the connection with the adiabatic pumping under the electron correlations. We will then show that the spin-charge separation peculiar to the Kondo effect emerges as the separation of pumped spin and charge under a finite magnetic field.

Model.— We consider a system which consists a quantum dot which has a single energy level and couples to two leads, described by the Anderson model \(^27\), \(^28\), \(^29\), \(^30\)

\[
H = \sum_{k,\sigma=L,R} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma=L,R} V_\sigma(t) \left( c_{k\sigma}\sigma \right) d_\sigma + h.c. \right) + H_{\text{dot}}
\]

\[
H = \sum_{k,\sigma,s=\pm} b_{k\sigma s}^\dagger (\varepsilon_k - (\mu(t) + sh(t))) b_{k\sigma s} + \frac{V(t)}{\sqrt{2}} \sum_{k,\sigma,s=\pm} b_{k\sigma s} d_\sigma + h.c. + H_{\text{dot}}.
\]

Equation (2) defines that the gauge potential \(a(t)\), which originates from the time-dependent barriers, acts as a finite bias voltage between \(b_{k\sigma s} \) and \(b_{k\sigma t} \) fields. Hence a finite current flows through the dot even when a real bias voltage is zero. In the following, we assume \(u = 0\) for a while.

Adiabatic Current and pumped charge.— The current \(I_\sigma = (I_{\sigma,L} - I_{\sigma,R})/2\) with \(I_{\sigma,\alpha} = ie/h \sum_k V_\alpha(t) \left( d_\sigma^\dagger c_{k\alpha} - c_{k\alpha}^\dagger d_\sigma \right)\) can be represented by \(b_{k\sigma s}^\dagger d_\sigma \) fields:

\[
I_\sigma = \frac{ieV(t)}{2\sqrt{2h}} \sum_{k,s=\pm} \left[ (\xi + is\eta)^2 \langle b_{k\sigma s}^\dagger b_{k\sigma s} \rangle - (\xi - is\eta)^2 \langle b_{k\sigma s}^\dagger d_\sigma \rangle \right].
\]
We investigate the current in the adiabatic limit that the frequency \( \Omega \) of external time-dependent sources is much smaller than the dot-lead coupling \( \Gamma(t) = \pi \rho |V(t)|^2 \), where \( \rho \) is the density of states at the Fermi energy in the leads: \( \Omega \ll \Gamma(t)/\hbar \). This condition is consistent with both of the two models appears when the electron interaction is treated as weak. However, it determines an adiabatic limit and can be disregarded. Thereby, \( q = \sigma_\delta \eta \). In the following, we choose \( V_g \) and \( \theta \) as the pumping parameters.

Equations (4) and (5) are also derived by the conventional scattering matrix approach of the pumping \( I_{\sigma,B} \), which has been successfully applied for the regimes. We assume \( u \to \infty \) to exclude the double occupancy of electrons in the dot. In this situation, the annihilation operator \( d_\sigma \) of electron is the dot is written as \( d_\sigma = b_\sigma f_\sigma \) with the slave boson operator \( b_\sigma \) and the pseudo fermion operator \( f_\sigma \), with the constraint term of \( H_u = \lambda \sum \sigma f_\sigma^\dagger f_\sigma + b_\sigma^\dagger b_\sigma - 1 \), where \( \lambda \) is a Lagrange multiplier. We assume that \( b_\sigma \) and \( \lambda \) are constant, determined by the self-consistent equations as a function of the gate voltage \( V_g \) and \( \delta \). The current is therefore given by the sum of Eqs. (4) and (5) with these renormalized values. Note that to keep the adiabatic condition, we need a smaller value of \( \Omega \): \( \Omega \ll \Gamma/\hbar \) since \( \Gamma > \Gamma_u \). Let us show that Eq. (6) is satisfied by \( I_{\sigma,B} \).

The first term corresponds to Eq. (4) and the second to Eq. (5). These are due to (i) the relation of \( \exp(2i\delta') = 1 - 2i\Gamma G^R(t) = 0 \), and (ii) the Friedel sum rule on the dot.

Pumped charge \( Q_\sigma \) per cycle is

\[
Q_\sigma = \frac{e}{2\pi} \int dt (1 - T_\sigma) \frac{d\delta_\sigma}{dt} \equiv \int dt I_{\sigma,S}(t)
\]

with the transmission probability \( T_\sigma \) and the phase of the reflection coefficient \( \alpha_\sigma \) through the dot. The scattering matrix of the dot is given by

\[
U(0, \delta) = \begin{pmatrix}
\xi^2 + \eta^2 & \xi \eta (e^{2i\delta} - 1) \\
\xi \eta (e^{2i\delta} - 1) & \xi^2 + \eta^2 e^{2i\delta}
\end{pmatrix}
\]

with the Friedel phase \( \delta' \) at the Fermi energy in the leads. It determines \( T_\sigma = 4\xi^2 \eta^2 \sin^2 \delta_\sigma \), and \( \alpha_\sigma = \arctan (\xi^2 - \eta^2) \tan \delta_\sigma \). Hence

\[
I_{\sigma,S} = \frac{e}{2\pi} 2\xi \eta \sin 2\delta_\sigma = \frac{e}{\pi} (\xi^2 - \eta^2) \frac{d\delta_\sigma}{dt}
\]

The second term is given by

\[
Q_{\sigma} = \frac{e}{2\pi} \int dt \sin 2\delta_\sigma + \frac{e}{2\pi} (\xi^2 - \eta^2) \frac{d\delta_\sigma}{dt}
\]

These are due to (i) the relation of \( \exp(2i\delta) = 1 - 2i\Gamma G^R(t) = 0 \), and (ii) the Friedel sum rule on the dot.

Let us show that \( I_{\sigma,B} \) can flow in the opposite direction depending on the strength of \( u \). To this end, we choose the pumping path as shown in Fig. (a), where \( Q = Q_\sigma = \frac{e}{2\pi} \sin^2 \frac{\delta - \delta'}{2} \sin (\delta_1 + \delta_2) \).
we choose the path as in Fig. 1(b), only the contribution from \( I_{\sigma, F} \) remains and \( \mathcal{Q} = \frac{e}{2} (\delta_2 - \delta_1) \). Then the sign change of \( \mathcal{Q} \) does not happen. The conductance also does not show such a change of sign.

Spin pumping in the Kondo regime. — Let us look at the Kondo effect under a finite magnetic field, where the Zeeman energy \( E_Z \) lifts spin degeneracy of the dot level: \( E_0 \rightarrow E_0 \pm E_Z \). In Fig. 1(a), the Friedel phases \( \delta_\pm \) are plotted as a function of the gate voltage \( V_0 \) under \( E_Z = 5.0 \times 10^{-3} \Gamma \). When \( V_0 < -\Gamma \), the Zeeman effect competes with the Kondo effect, and

\[
\delta_\pm \sim \pi/2 \pm \Delta \delta, \quad (10)
\]

with a certain phase \( \Delta \delta \). This phase shift is peculiar to the Zeeman splitting of the Kondo state; the center of the splitting peaks is fixed at the Fermi level in the leads. Pumped charge \( \mathcal{Q}_\sigma \) depends on the spin \( \sigma \) accordingly.

Now we investigate the pumping in the Kondo regime along the path shown in Fig. 1(c), where \( \mathcal{Q}_\sigma \) is given by

\[
\mathcal{Q}_\sigma = \frac{e}{2 \pi} \left( 2 (\delta_{2,\sigma} - \delta_{1,\sigma}) - (\sin 2 \delta_{2,\sigma} - \sin 2 \delta_{1,\sigma}) \right) \quad (11)
\]

with \( \delta_{j,\sigma} = \delta_\sigma (V_j) \) \((j = 1, 2)\). In Fig. 1(b), the pumped charge \( \mathcal{Q}_c = \mathcal{Q}_+ + \mathcal{Q}_- \) (the broken line) and pumped spin \( \mathcal{Q}_s = \mathcal{Q}_+ - \mathcal{Q}_- \) (the solid line) are plotted as a function of \( V_1 \) for a fixed \( V_2 = -2\Gamma \) \((-2\Gamma < V_1 < -\Gamma)\). We obtain \( \mathcal{Q}_c \sim 0 \) and \( \mathcal{Q}_s \neq 0 \); the spin pumping without the charge pumping is realized by Eq. 11. The effect of \( \Delta \delta \) is cancelled for \( \mathcal{Q}_c \) and doubled for \( \mathcal{Q}_s \).

The absence of charge pumping is a generic feature in the Kondo regime, and in contrast to the conductance, which is the maximum of \( 2e^2/h \). On the other hand, the finite pumped spin proves that the spin degree of freedom is active. These results are consistent with the fact that in the Kondo regime, the spin excitations freeze while the spin excitations are active. Thereby the pumping seizes this separation peculiar to the Kondo effect.

We further demonstrate this separation in the pumping by investigating the pumping along the path shown in Fig. 2: Pumped charge \( \mathcal{Q} \) (in the unit of \( e/2\pi \)) for the path in Fig. 1(a) as a function of \( V_2 \) for \( V_1 = \Gamma \). The solid and broken lines stand for the interacting \((u \rightarrow \infty)\) and non-interacting \(u = 0)\) models, respectively.

FIG. 2: Pumped charge \( \mathcal{Q} \) (in the unit of \( e/2\pi \)) for the path in Fig. 1(a) as a function of \( V_2 \) for \( V_1 = \Gamma \). The solid and broken lines stand for the interacting \((u \rightarrow \infty)\) and non-interacting \(u = 0)\) models, respectively.

FIG. 3: Electron pumping under the Zeeman effect; \( E_Z = 5.0 \times 10^{-3} \Gamma \). (a) \( \delta_{\sigma \sigma} \) as a function of the gate voltage \( V_g \). (b) The pumped charge \( \mathcal{Q}_c = \mathcal{Q}_+ + \mathcal{Q}_- \) (the solid line), and pumped spin \( \mathcal{Q}_s = \mathcal{Q}_+ - \mathcal{Q}_- \) (the broken line) (in the unit of \( e/2\pi \)) for the path in Fig. 1(c) as a function of \( V_1 \) for a fixed \( V_2 = -2.0 \Gamma \).

The absence of charge pumping is a generic feature in the Kondo regime described above. On the other hand, the peak of \( \mathcal{Q}_s \) appears in the Kondo regime described above. In Fig. 2(b), the amplitudes of the charge and spin pumping, \( A_c = A_+ + A_- \) (the broken line) and \( A_s = A_+ - A_- \) (the solid line), are plotted as a function of \( V_1 \). Around \( V_1 \sim 0 \), \( A_c \) has a peak and decreases to zero as \( V_1 \) decreases. On the other hand, \( A_s \) is zero for high gate voltage and increases as \( V_1 \) decreases, and it has a peak around \( V_1 \sim -2 \Gamma \).

The separation of the peak structures between \( A_c \) and \( A_s \) is a direct evidence of the separation of the spin and charge excitations peculiar to the Kondo effect. The peak of \( A_s \) appears in the Kondo regime described above. On the other hand, the peak of \( A_c \) appears in the mixed-valence regime, where the number of electrons in the dot can fluctuate; the charge excitations are active. In this way, the pumping reveals the intrinsic nature of electronic states in the Kondo effect. Note that when \( V_1 \ll \Gamma \), where the spin polarized state appears, both \( A_c / A_s \) are zero.

Keldysh Green functions. — We now discuss the derivation of the Keldysh Green functions. Equation 3 is expressed in terms of the Keldysh Green functions 3: \( I_{\sigma} = I_{\sigma, B} + I_{\sigma, F} \) with

\[
I_{\sigma, B} = \frac{2ieV\xi\eta}{4\hbar} V(G_{\sigma}^R g_{\sigma A}^< + g_{\sigma A}^< G_{\sigma}^A), \quad (12)
\]

\[
I_{\sigma, F} = \frac{eV(\xi^2 - \eta^2)}{4\hbar} \times V(G_{\sigma}^R g_{\sigma S}^< - g_{\sigma S}^< G_{\sigma}^R + G_{\sigma}^R g_{\sigma S}^< - g_{\sigma S}^< G_{\sigma}^R), \quad (13)
\]

where we have introduced the Keldysh Green functions in the dot and leads, \( G_{\sigma}^R \) and \( g_{\sigma k}^R \) \((j = R, A, <)\), and \( g_{\sigma S}^R / A = \sum_k (g_{\sigma k}^R + g_{\sigma k}^-) \). The notation of \( V G_{\sigma}^R g_{\sigma A}^< \) stands for \( \int dt_1 V(t_1) G_{\sigma}^R(t_1, t_1) g_{\sigma A}^< (t_1, t) \) for example.
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[36] When the system is in the Kondo regime, \( \tilde{E}_0 \) gives the position of the Kondo resonance, \( \tilde{E}_0 \simeq 0 \), and \( \tilde{\Gamma} \) gives the Kondo temperature \( T_K = \frac{\Delta}{\pi} \exp\left(\frac{\pi V_g}{\Delta}\right) \).
[37] When \( V_g \ll -\Gamma \), the system in the spin-polarized state rather than the Kondo state, and as a result, \( \delta_+ = \pi \) and \( \delta_- = 0 \). [This regime is not included in the Fig. 3a.]
[38] The discrete sum of \( k \) in \( \sum_k \) can be expressed as \( \rho \int d\epsilon \). We have also used the relations of \( g_{R/A}(\omega) = \mp i \theta (\pm t \mp t') \exp[-i\epsilon_k(t - t')] \).