Quantum Transport and Integrability of the Anderson Model for a Quantum Dot with Multiple Leads

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Introduction. Since the first prediction [1] and realization of Kondo physics in a quantum dot (QD) [2], nonequilibrium effects on the Kondo resonance due to a finite bias voltage across the dot have attracted increasing attention. In the experiments, the zero bias peak of the differential conductances has been observed as a signature of the Kondo effect on electron transport through a QD. In the unitary scattering limit, observations of perfect transmission [3] provide further evidence for the Kondo effect in QDs. The nonequilibrium density of states (DOS) of the dot has been predicted [3] to exhibit a splitting of the Kondo peak due to a bias voltage applied between the source and the drain. This splitting has not been observed in transport measurements. To observe the splitting of the Kondo resonance by a finite voltage bias, an experiment with extra leads [6, 7] has been proposed. Very recently, such a splitting was observed in an experiment [8] where a three-lead setup was employed.

In a conventional bulk Kondo system [3] (e.g., a magnetic impurity in a metal), there is a single chemical potential and the Kondo resonance in the DOS appears at the Fermi energy due to the formation of a singlet between the local moments of the impurity and the conduction electrons. If the impurity has available a second conduction band to form singlet states, a second Kondo resonance in the DOS might be expected to occur at the chemical potential of the second conduction band. The splitting of the Kondo resonance of a QD by the differential chemical potentials of the two leads then seems to be reasonable. However, it is not still clear why the differential conductance has only a single peak at zero bias in experiments with two leads. Thus there arises a fundamental question associated with a Kondo resonance in a system with several chemical potentials that can be fabricated in nano-scale electronic devices: why the split Kondo peaks have not been seen in two-lead systems? To help answer this question we consider a QD coupled to multiple leads. The QD is described by an Anderson model generalized to a multiple-lead one. It will be shown that the multiple-lead Anderson model is integrable and exactly solvable by a unitary transformation and the Bethe ansatz [10]. By using the exact solution, a general expression for the conductance of the N-lead system shows that the Kondo resonance at equilibrium is split into N − 1 peaks by increasing the difference between the chemical potentials of the different leads. This then clearly shows why only a single peak of the conductance occurs in the two-lead system.

Model. We consider an Anderson model in which N leads are coupled to the QD, as in Fig. 1. The leads are described under the unfolded formalism with fermions. Within this formalism, fermions incident on the dot (x = 0) from a lead (x < 0) are scattered away from the dot to leads (x > 0). In the continuum limit, the multiple-lead Anderson model Hamiltonian is given by

\[
H = -\frac{i}{\hbar} \sum_{m=1}^{N} \int_{-\infty}^{\infty} dx \left( \sum_{\sigma} \epsilon_{m\sigma}(x) \frac{\partial}{\partial x} c_{m\sigma}^\dagger(x) c_{m\sigma}(x) + \sum_{\sigma} \sum_{\sigma'} \epsilon_{d} \delta_{\sigma\sigma'} d_{\sigma}^\dagger d_{\sigma'} \right) + U n_{+} n_{-} + \sum_{m=1}^{N} V_{m}(c_{m\sigma}^\dagger(0) d_{\sigma} + h.c.),
\]

where \( n_{\sigma} = d_{\sigma}^\dagger d_{\sigma} \) is the number of electrons of spin \( \sigma \) on the dot and \( U \) is the onsite Coulomb repulsion. \( c_{m\sigma} \) and \( d_{\sigma} \) are the annihilation operators with spin \( \sigma \) for electrons in the lead \( m \) and the dot. \( \epsilon_{d} \) is the energy level on the dot. Here the hopping amplitudes between the dot and the lead \( m \), \( V_{m} \), are allowed to be arbitrary.

Previously, it has been shown that, for the \( N = 2 \) case, a unitary (Bogoliubov) transformation can be used to transform the Hamiltonian to a single-lead Anderson Hamiltonian [14]. We now generalize this to the case of general \( N \). To do this, one performs a unitary transformation, \( \mathbf{U} = U_{N} \mathbf{c} \), for the lead electrons, where \( \mathbf{c} = (c_{1\uparrow}, \ldots, c_{N\uparrow}) \) and \( \mathbf{c} = (c_{1\uparrow}, \ldots, c_{N\uparrow}) \). The components of the \( N \times N \) matrix \( U_{N} \) are a function of the hopping amplitudes, \( V_{m} \). \( U_{N} \) should satisfy \( U_{N}^\dagger U_{N} = I \). If (i) \( \sum_{m} V_{m} [U_{N}]_{m m'} = \sum_{m'} U_{N}^{\dagger}_{m} V_{m} \) and (ii) \( \sum_{m} V_{m} [U_{N}]_{m m'} = \sqrt{\Gamma} \) for \( m' = 1 \) and 0 for \( m' \neq 1 \), one
obtains the one-lead Anderson Hamiltonian and \( N - 1 \) free fermion Hamiltonians. Then a \( N \times N \) unitary matrix for the multiple leads has a form satisfying with \([U_N]_{1m} = V_m / \Gamma\) and \( \Gamma = \sum_m V_m^2 \). For \( N > 2 \), actually, there are more freedoms to choose a unitary matrix. The freedoms give us different matrices for a unitary transformation acting only on \((\hat{c}_2, \ldots, \hat{c}_N)\), but leaving \( \hat{c}_1 \) invariant, which does not affect the physics.

As a consequence, the unitary transformation satisfying such conditions decomposes the multiple-lead Hamiltonian into \( N \) independent sub-Hamiltonians, \( \tilde{H}_m \), as

\[
H = \sum_m \tilde{H}_m, \quad (2)
\]

where

\[
\tilde{H}_1 = \sum_{\sigma} \left[ -i \int_{-\infty}^{\infty} dx \, \hat{c}_{1\sigma}^\dagger(x) \partial_x \hat{c}_{1\sigma}(x) + \varepsilon_d d_\sigma^\dagger d_\sigma + U n_{\uparrow} n_{\downarrow} + \sqrt{\Gamma} (\hat{c}_{1\sigma}^\dagger(0) d_\sigma + \text{h.c.}) \right], \quad (3)
\]

\[
\tilde{H}_m = -i \sum_{\sigma} \int_{-\infty}^{\infty} dx \, \hat{c}_{m\sigma}^\dagger(x) \partial_x \hat{c}_{m\sigma}(x) \quad \text{for} \ m \in [2, N]. \quad (4)
\]

This is a generalization of the \( N = 2 \) case treated in Ref. \[14\]. The transformed Hamiltonian can be solved exactly because the sub-Hamiltonian, \( \tilde{H}_1 \), is the one-lead Anderson model that is exactly solvable via the Bethe ansatz \[10, 11, 12, 13\].

**Integrable excitations and scattering amplitudes.** The scattering amplitudes of electronic excitations off the QD coupled to the \( N \) leads can be calculated based on the exact solution of \( \tilde{H}_1 \). In the transformed \( N \) leads, the integrable excitations, \( \{\tilde{\psi}_m\} \), will scatter off the dot with some pure phase shift with spin \( \sigma \), \( \delta_m^\sigma(\varepsilon) \), where in particular \( \delta_m^\sigma(\varepsilon) = 0 \) for \( m \in [2, N] \). With the unfolded formalism, the scattering can be described by the relation

\[
\tilde{\psi}_m(x > 0) = e^{i \delta_m^\sigma} \tilde{\psi}_m(x < 0). \quad (5)
\]

Equation \(5\) leads to the scattering amplitudes \( S_m(\varepsilon) \) of electronic excitations, \( \{\tilde{\psi}_m\} \), of energy \( \varepsilon \) between leads in the multiple-lead system. Assuming the relation \( \tilde{\psi}_m = \sum_{mm'} [U_N]_{mm'} \psi_{mm'} \), the scattering matrix is straightforwardly given by

\[
S_m(\varepsilon) = \delta_{mm'} + 2i \Gamma_{mm'} e^{i \frac{\varepsilon}{\hbar} \sin \frac{\delta_m^\sigma}{2}}, \quad (6)
\]

where \( \Gamma_{mm'} = [UP_1U^{-1}]_{mm'} \) and \( P \) is a polarization matrix: \([P_m]_{mm'} = 1\) and other entries are zero. For \( m \neq m' \), \( S_m(\varepsilon) \) is a transmission amplitude \( T_{mm'}(\varepsilon) \) from \( m' \) to \( m \). For \( m = m' \), \( S_m(\varepsilon) \) corresponds to a reflection amplitude \( R_{mm'}(\varepsilon) \) from \( m \) to \( m' \). From \( \Gamma_{mm'} = \Gamma_{m'm}, T_{mm'}(\varepsilon) = T_{mm'}^\sigma(\varepsilon) \), at zero temperature, the current in lead \( m \) is given by

\[
I_m = \frac{e}{\hbar} \sum_{m' \neq m, \sigma} \int_{-\infty}^{\infty} d\varepsilon \, |T_{mm'}^\sigma(\varepsilon, \{\mu_m}\}|^2, \quad (7)
\]

where \( \mu_m \) is the chemical potential at the lead \( m \) and

\[
|T_{mm'}^\sigma(\varepsilon, \{\mu_m}\}|^2 = 4 \Gamma_{mm'}^2 \sin^2 \left[ \frac{1}{2} \theta_m^\sigma(\varepsilon, \{\mu_m}\) \right], \quad (8)
\]

To determine \( \delta_1 \), we solve \( \tilde{H}_1 \) via the Bethe ansatz for the one-lead Anderson model. The integrability of \( \tilde{H}_1 \) leads to a set of quantization conditions identical to that of the one-lead Anderson model. Single particle excitations with momenta \( \{k_j\} \) are identified by an appropriate basis. Scattered particle eigenstates from the dot picks up the bare phase \( \delta(k) = -2\tan^{-1}[(\Gamma / (k - \varepsilon_d))] \). Calculating two particle eigenstates makes it possible to get the scattering matrices of excitations. The scattering matrices satisfying a Yang-Baxter relationship are identical to that of the one-lead Anderson model. Then a set of \( N_c \) multi-particle eigenstates carrying total spin \( S_z = N_c / 2 - M \) should satisfy the quantization conditions \[10, 11, 12\] as

\[
e^{i(k_jL + i\delta(k_j))} = \prod_{\alpha=1}^{M} \frac{g(k_j) - \lambda_\alpha + i/2}{g(k_j) - \lambda_\alpha - i/2}, \quad \prod_{\beta=1}^{M} \lambda_\alpha - \lambda_\beta + i = -\prod_{j=1}^{N_c} \frac{g(k_j) - \lambda_\alpha + i/2}{g(k_j) - \lambda_\alpha - i/2}. \quad (9)
\]
where \(g(k) = (k - \varepsilon_d - U/2)^2/2UT\) and \(M\) characterizes the spin projection of the system with the auxiliary parameters, \({\lambda}_\alpha\}.\) For \(\varepsilon_d > -U/2,\) then, \(N\) total momenta \(k\)s form an \(N\) particle ground state configuration. \(N = 2M\) of \(N\) total momenta \(k\)‘s is real and \(2M\) is complex via \(M\) real \(\lambda\)’s. The \(2M\) complex momenta are given by \(k_\alpha^\pm = x(\lambda_\alpha) \pm iy(\lambda_\alpha)\) with \(x(\lambda) = U/2 + \varepsilon_d - \sqrt{UT}[\lambda + (\lambda^2 + 1/4)^{1/2}]^{1/2}\) and \(y(\lambda) = \sqrt{UT}[\lambda - (\lambda^2 + 1/4)^{1/2}]^{1/2}\).

According to Andrei’s procedure for determining the momentum \(p\), of an added electron in a periodic system of size \(L\) \[10\], the quantization condition of the system leads to \(p = 2\pi n/L\). Contributions to the momentum come from the bulk of the system and the dot:

\[
p = 2\pi n/L = p_{\text{bulk}} + p_d/L.\]

The dot contribution scaled by the size of the system is identified with the scattering phase of the excitation off the dot, which gives the relation between the phase and the momentum from the dot as \(\delta = \varepsilon_d\). In adding an electron with spin \(\sigma\) to the system, then, the electron scattering phase shift has two contributions from the charge, \(p^Q\), and the spin sectors, \(p^S, [14]\) as given by

\[
\delta_1^\sigma = p^S_\sigma = p^Q_\sigma(k) + p^S_\sigma(\lambda) .
\]

The electronic scattering phase shifts are related to the density of states \(\rho_d(k)\) and \(\sigma_d(\lambda)\) by the equations:

\[
p^Q_d(k) = \delta(k) + \int_q d\lambda [\theta_1(g(k) - \lambda) - 2\pi] \sigma_d(\lambda), \tag{11}
\]

\[
p^S_d(k) = \hat{\delta}(k) + \int_q d\lambda' [\theta_2(g(k) - \lambda') - 2\pi] \sigma_d(\lambda') + \int_D d\lambda [\theta_1(\lambda - g(k)) - 2\pi] \rho_d(k), \tag{12}
\]

where \(\hat{\delta} = 2\text{Re}[\delta(x(\lambda) + iy(\lambda))].\) \(q/B\) are the Fermi surfaces of the seas of \(k\) and \(\lambda\) excitations while \(\hat{\delta}\) is related to the band cutoff, \(D\). Here \(\theta_1,2\) for describing the dot momentum should be chosen to ensure that \(p^Q_d(k \to -\infty) = p^S_\sigma(\lambda \to \infty) = 0\). Moreover, the dot momenta are simply related to the dot density of states:

\[
\partial_k p^Q_d(k) = 2\pi \rho_d(k), \text{ and } \partial_\lambda p^S_\sigma(\lambda) = -2\pi \sigma_d(\lambda). \tag{13}
\]

Integrating the density of states gives us the dot momenta. Consequently, the scattering phase shift is given by

\[
\delta_1^\sigma = 2\pi \int_D d\lambda [\theta_1(\lambda - g(k)) - 2\pi] \sigma_d(\lambda).
\]

This phase shift satisfies the Langreth-Friedel sum rule, \(\delta_1^\sigma = 2\pi n_\sigma,\) relating the phase shift to the total number of electrons \(n_\sigma\) in the dot \[21\].

To obtain the matrix conductance of the multiple-lead system away from the symmetric point \((\varepsilon_d - \mu_m = -U/2),\) we need to do a numerical calculation for the associated integral equations. But at the symmetric point the scattering phase shift is obtained by using an exact expression for \(\rho_d(k < 0) [12]\) and a direct relation between the phase shifts for the electron with spin \(-\sigma\) and the hole with spin \(\sigma\) from a property of electron-hole transformation based on the SU(2) spin symmetry. The phase shift is given by \[18\]

\[
\delta_1(\varepsilon) = \frac{3}{2} \pi - \sin^{-1} \left[ \frac{4T_{K,m}^2 - \pi^2 (\varepsilon - \mu_m)^2}{4T_{K,m}^2 + \pi^2 (\varepsilon - \mu_m)^2} \right] + C(\varepsilon), \tag{15}
\]

where the Kondo temperature for a lead at chemical potential \(\mu_m\) is

\[
T_{K,m} = \sqrt{\frac{UT}{2}} \exp \left[ \frac{\pi}{2TU} \left[ (\varepsilon_d - \mu_m)(\varepsilon_d - \mu_m + U) - \Gamma^2 \right] \right].
\]

Here, \(C(\varepsilon)\) does not give any significant phase shift when the Kondo energy scale is much smaller than the Coulomb interaction \(U\). For \(\mu_m - \mu_m' \ll U,\) we can assume all of the leads are at the symmetric point. This makes it possible to take into account the essence of the physics associated with the splitting of the Kondo resonance in a multiple-lead system. Then one can obtain a simple expression for the matrix conductance \((G_{mm'} = -e\delta_{mm'}\Gamma_m)\) from Eq. \[7, 8\] and \[15\]. The matrix conductance in the multiple-lead Kondo-dot system is given by

\[
G_{mm'} = -\sum_{m'' \neq m} \Gamma'_{mm''} \tag{16}
\]

\[
G_{mm'_{(m \neq m')}} = -4G_0\Gamma'_{mm'} \left[ 1 + \frac{2}{4} \left( \frac{\mu_m - \mu_m'}{T_{K,\max}\mu_m,\mu_m'} \right) \right]^{-1}, \tag{17}
\]

where \(G_0 = 2e^2/h\) is the quantum of conductance, and \(\Gamma'_{mm'} = V_mV_{m'}/T.\) This multiple-lead matrix conductance is the generalized expression of the conductance for the two-lead Kondo-dot system. It reduces to the conductance in the two-lead system \[18\]. For a symmetric coupling \((V_1 = \cdots = V_N)\) and \(\mu_1 = \cdots = \mu_N,\) the matrix conductance is \(G_{mm}/G_0 = 4(N - 1)/N^2\) and \(G_{mm'}/G_0 = -(2/N)^2.\) The resultant matrix conductance agrees with that of a multi-lead quantum point-contact for free fermions \[21\]. This unitary scattering limit shows the Fermi liquid nature of the multiple-lead Kondo-dot system.

Note that the multiple-lead matrix conductance in Eq. \[10\] and \[17\] shows clearly that a conductance peak for the transmission from \(m\) to \(m'\) is developed when the two chemical potentials are tuned to be equal, \(\mu_m = \mu_m'.\) As the chemical potential difference increases, the amplitude of the conductance decreases. In a \(N\)-lead system, if every chemical potential has a different value, the conductance \(G_{mm}\) versus \(\mu_m\) has a total of the \(N - 1\) conductance peaks, one at each of the other chemical potentials. The amplitude of the conductance \(G_{mm'}\) versus
$\mu_m$ has its maximum value for $\mu_m = \mu_{m'}$. The maximum values of $G_{mm'}$s have a one-to-one correspondence to the conductance peaks of $G_{mm'}$. This behavior of the conductances implies that electrons from each lead participate in screening the local moment of the dot and take part in forming a single Kondo resonance at equilibrium. Increasing the difference between the chemical potentials, the electrons from each of the $N$ leads have their own Kondo resonances with the dot. Each resonance is characterized by a Kondo temperature, $T_{K,m}$, depending on the value of the chemical potential of the lead. Since each lead creates a single lead-dot Kondo resonance, the $N$-lead system has $N$ lead-dot Kondo resonances. If the chemical potentials of two of the leads are adjusted to be equal then the two Kondo resonances corresponding to these leads merge together in $G_{mm'}$. Then this results in only a single transmission peak in the conductance $G_{mm}$. Therefore, an electron transport measurement in the two-lead system is able to capture only the single transmission peak even though there are two lead-dot Kondo resonances created by the two leads. Hence, the two-lead system is not a good probe to observe the splitting of the Kondo resonance by finite biases.

Three-lead and four-lead system. Before proceeding to the conclusion, we discuss the conductance for the three leads ($N = 3$) and the four leads ($N = 4$). The unitary transformation for the three-lead system is given by the unitary matrix:

$$U_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} V_1 & V_2 & V_3 \\ V_2 & a & b \\ V_3 & b & c \end{pmatrix},$$

where $a = (-V_1V_2^2 + V_2^2\sqrt{\Gamma})/\gamma$, $b = (-V_1V_2V_3 - V_2V_3\sqrt{\Gamma})/\gamma$, and $c = (-V_1V_3^2 + V_2^2\sqrt{\Gamma})/\gamma$ with $\gamma = V_2^2 + V_3^2$. It can be obtained explicitly under the necessary condition we discussed above. Similarly, the unitary matrix $U_4$ for four leads can be determined.

We plot the conductance $G_{33}$ as a function of $\mu_3$ for $N = 3$ and the conductance $G_{44}$ as a function of $\mu_4$ for $N = 4$ in Fig. 2 (a) and (b), respectively. When all the leads are at the same chemical potential ($\Delta\mu = 0$), the amplitude of the conductance is shown to be reduced as the number of leads increases. The maximum amplitudes are $G_{33}/G_0 = 8/9$ and $G_{44}/G_0 = 3/4$. As the difference between the other chemical potentials, $\Delta\mu$, become larger than the Kondo temperature $T_K^0$ at equilibrium, the single peak at $\Delta\mu = 0$ splits progressively into two and three peaks for three and four leads, respectively. Figure 2 (a) shows that for $\Delta\mu \simeq 2T_K^0$, the amplitudes of the split peaks reduce to around half the value of that of the equilibrium Kondo peak ($\Delta\mu = 0$). The suppression of the Kondo resonance is on a voltage scale $T_K^0$. This behavior agree qualitatively, but not quantitatively, with the experimental results in Ref. [8].

Summary. By using a unitary transformation and the Bethe ansatz, the multiple-lead Anderson model is shown to be integrable. A general expression for the matrix conductance from the integrability has been obtained. The conductance for the $N$-lead system shows $N - 1$ split Kondo peaks located at $N - 1$ different chemical potentials. This shows that a Kondo-dot system with multiple leads provides a good probe to observe the nonequilibrium effects on the Kondo resonance by a voltage bias in transport measurement.

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