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Quantum transport and integrability of the Anderson model for a quantum dot with multiple leads

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We show that an Anderson Hamiltonian describing a quantum dot connected to multiple leads is integrable. A general expression for the nonlinear conductance is obtained by combining the Bethe ansatz exact solution with Landauer-Büttiker theory. In the Kondo regime, a closed form expression is given for the matrix conductance at zero temperature and when all the leads are close to the symmetric point. A bias-induced splitting of the Kondo resonance is possible for three or more leads. Specifically, for N leads, with each at a different chemical potential, there can be $N-1$ Kondo peaks in the conductance.

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I. 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[3,4] provide further evidence for the Kondo effect in QD's. The nonequilibrium density of states (DOS) of the dot has been predicted[5] 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[9] (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 nanoscale electronic devices: Why have not the split Kondo peaks 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.[10–13] 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.

This paper is organized as follows. In Sec. II, the model Hamiltonian is described and a unitary transformation is discussed for the integrability of the Hamiltonian. For the N-lead system, the scattering matrix from integrable excitations is presented in Sec. III. By combining scattering amplitudes from the Bethe ansatz exact solution with Landauer-Büttiker theory, a differential matrix conductance is derived and the Kondo splitting peaks by finite biases are discussed in Sec. IV. As an example, three- and four-lead systems are considered in Sec. V. In Sec. VI, some final remarks will be given.

II. MODEL AND UNITARY TRANSFORMATION

We consider an Anderson model in which N leads are coupled to the QD, as in Fig. 1. The leads are described

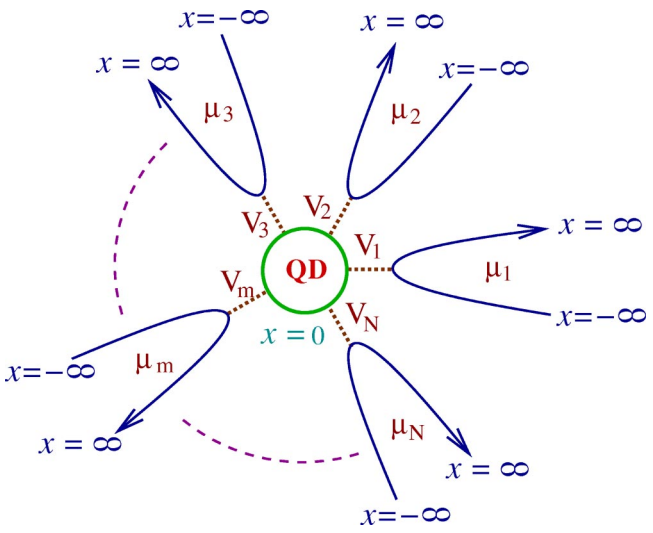

FIG. 1. A quantum dot (QD) coupled to N multiple leads. V_m is the tunneling amplitude between the mth lead and the QD. μ_m is the chemical potential of the mth lead. The leads are presented under the unfolded formalism.

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

$$H=-i\sum_{m=1;\sigma}^{N}\int_{-\infty}^{\infty}dx c_{m\sigma}^{\dagger}(x)\partial_x c_{m\sigma}(x)+\sum_{\sigma}\varepsilon_d d_{\sigma}^{\dagger}d_{\sigma}+Un_{\uparrow}n_{\downarrow}+\sum_{m=1;\sigma}^{N}V_m[c_{m\sigma}^{\dagger}(0)d_{\sigma}+\text{H.c.}], \quad (1)$$

where $n_{\sigma}=d_{\sigma}^{\dagger}d_{\sigma}$ is the number of electrons of spin σ on the dot and U is the on-site Coulomb repulsion. $c_{m\sigma}$ and d_{σ} are the annihilation operators with spin σ for electrons in the lead m and the dot. Σ_m is a sum over the multiple leads ($m=1,\ldots,N$). ε_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.[16] We now generalize this to the case of general N. To do this, one performs a unitary transformation, $\tilde{\mathbf{c}}=\mathbf{U}_N\mathbf{c}$, for the lead electrons, where $\mathbf{c}=(c_1,\ldots,c_N)$ and $\tilde{\mathbf{c}}=(\tilde{c}_1,\ldots,\tilde{c}_N)$. The components of the $N\times N$ matrix $\mathbf{U}_N$ are a function of the hopping amplitudes, V_m. $\mathbf{U}_N$ should satisfy $\mathbf{U}_N^{\dagger}\mathbf{U}_N=I$. If (i) $\Sigma_m V_m[\mathbf{U}_N]_{mm'}=\Sigma_m[\mathbf{U}_N^{\dagger}]_{m'm}V_m$, and (ii) $\Sigma_m V_m[\mathbf{U}_N]_{mm'}=\sqrt{\Gamma}$ 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 $[\mathbf{U}_N]_{1m}=V_m/\sqrt{\Gamma}$ and $\Gamma=\Sigma_m V_m^2$. 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 $(\tilde{c}_2,\ldots,\tilde{c}_N)$, but leaving $\tilde{c}_1$ invariant, which does not affect the physics. A similar unitary transformation was used to study negative resistance fluctuations in quantum Hall conductors.[14]

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

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

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

This is a generalization of the $N=2$ case treated in Ref. 16. 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.[10–13]

III. 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 σ, $\delta_1^{\sigma}(\varepsilon)$, 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 $S_{mm'}^{\sigma}(\varepsilon)$ of electronic excitations, $\{\psi_m\}$, of energy ε between leads in the multiple-lead system. Assuming the relation $\psi_m=\Sigma_{m'}[\mathbf{U}_N]_{mm'}\tilde{\psi}_{m'}$, the scattering matrix is straightforwardly given by

$$S_{mm'}^{\sigma}(\varepsilon)=\delta_{mm'}+2i\Gamma_{mm'}e^{i\delta_1^{\sigma}/2}\sin\frac{\delta_1^{\sigma}}{2}, \quad (6)$$

where $\Gamma_{mm'}=[\mathbf{U}\mathbf{P}_1\mathbf{U}^{-1}]_{mm'}$ and $\mathbf{P}$ is a polarization matrix: $[\mathbf{P}_m]_{mm}=1$ and other entries are zero. For $m\neq m'$, $S_{mm'}^{\sigma}$ is a transmission amplitude $T_{mm'}^{\sigma}$ from m' to m. For $m=m'$, S_{mm}^{σ} corresponds to a reflection amplitude R_{mm}^{σ} from m to m. From $\Gamma_{mm'}=\Gamma_{m'm}$, $T_{mm'}^{\sigma}(\varepsilon)=T_{m'm}^{\sigma}(\varepsilon)$ is automatically preserved.

IV. DIFFERENTIAL MATRIX CONDUCTANCE

In the out-of-equilibrium case, the added chemical potential term destroys the integrability of the model, which may render the applicability of the Bethe ansatz approach questionable.[15] However, as argued by Konik and co-workers[16] (see especially, Sec. V, Ref. 17) for the two-lead case, as far as the computation of the nonequilibrium conductance is concerned, all we need to know is the distribution of particles in each of the leads, and the impact of the different chemical potentials on the scattering amplitudes. Because the particles in different leads do not interact with each other, one may compute the distribution of particles in different leads separately. That is, we may treat the problem as if the particles are still in equilibrium for a certain lead at the corresponding different chemical potential. As for the scattering, the only effect arising from the different chemical potentials is an overall phase factors, which does not contribute to the Landauer-Büttiker conductance. Such a consideration makes it possible to apply the results extracted from the Bethe ansatz approach in the equilibrium case to the out-of-equilibrium conductance. Then the current and the conductance through the QD can be obtained by the Landauer-Büttiker theory[18] for quantum transport through nanodevices.

To describe scattering away from the Fermi energy and calculate the differential conductance, we employ the ansatz[16] verified in Refs. 19 and 20. The ansatz allows us to use the in-equilibrium scattering matrices to calculate the contribution to the current of any given excitation. Konik and coworkers discussed the details of the implementation of the nonequilibrium computation in Ref. 17. With $T^{\sigma}_{mm'}(\varepsilon) = T^{\sigma}_{m'm}(\varepsilon)$, at zero temperature, the current in lead m is given by

$$I_m = \frac{e}{h} \sum_{m' \neq m;\sigma} \int_{\mu_{m'}}^{\mu_m} d\varepsilon |T^{\sigma}_{mm'}(\varepsilon, \{\mu_m\})|^2, \tag{7}$$

where μ_m is the chemical potential at the lead m and

$$|T^{\sigma}_{mm'}(\varepsilon, \{\mu_m\})|^2 = 4\Gamma^2_{mm'} \sin^2\left[\frac{1}{2}\delta^{\sigma}_1(\varepsilon, \{\mu_m\})\right]. \tag{8}$$

To determine δ_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_e multi-particle eigenstates carrying total spin $S_z = N_e/2 - M$ should satisfy the quantization conditions[10–12] as

$$\begin{aligned} e^{ik_jL + i\delta(k_j)} &= \prod_{\alpha=1}^{M} \frac{g(k_j) - \lambda_\alpha + i/2}{g(k_j) - \lambda_\alpha - i/2}, \\ \prod_{\beta=1}^{M} \frac{\lambda_\alpha - \lambda_\beta + i}{\lambda_\alpha - \lambda_\beta - i} &= -\prod_{j=1}^{N_e} \frac{g(k_j) - \lambda_\alpha - i/2}{g(k_j) - \lambda_\alpha + i/2}, \end{aligned} \tag{9}$$

where $g(k) = (k - \varepsilon_d - U/2)^2/2U\Gamma$ and M characterizes the spin projection of the system with the auxiliary parameters, $\{\lambda_\alpha\}$. For $\varepsilon_d > -U/2$, then, N_e total momenta k's form an N_e particle ground state configuration. $N_e - 2M$ of N_e momenta k's is real and $2M$ is complex via M real λ_α's. The $2M$ complex momenta are given by $k^{\pm}_\alpha = x(\lambda_\alpha) \pm iy(\lambda_\alpha)$ with $x(\lambda) = U/2 + \varepsilon_d - \sqrt{U\Gamma}[\lambda + (\lambda^2 + 1/4)^{1/2}]^{1/2}$ and $y(\lambda) = \sqrt{U\Gamma}[-\lambda + (\lambda^2 + 1/4)^{1/2}]^{1/2}$.

According to Andrei's procedure for determining the momentum, p, of an added electron in a periodic system of size L,[21,22] 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 $\delta_1 = p_d$. In adding an electron with spin σ to the system, then, the electron scattering phase shift has two contributions from the charge, p^Q, and the spin sectors, p^S,[16] as given by

$$\delta^{\sigma}_1 = p^{\sigma}_d = p^Q_d(k) + p^S_d(\lambda). \tag{10}$$

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

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

$$\begin{aligned} p^S_d(k) = \tilde{\delta}(k) &+ \int_q^{\tilde{q}} d\lambda' [\theta_2(g(k) - \lambda') - 2\pi]\sigma_d(\lambda') \\ &+ \int_{-D}^{B} dk [\theta_1(\lambda - g(k)) - 2\pi]\rho_d(k), \end{aligned} \tag{12}$$

where $\tilde{\delta} = 2\,\text{Re}[\delta(x(\lambda) + iy(\lambda)]$. q/B are the Fermi surfaces of the seas of k and λ excitations while $\tilde{q}$ is related to the band cutoff, D. Here $\theta_{1,2}$ for describing the dot momentum should be chosen to ensure that $p^Q_d(k \to -\infty) = p^S_d(\lambda \to \infty) = 0$. Moreover, the dot momenta are simply related to the dot density of states:

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

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

$$\delta^{\sigma}_1 = 2\pi \int_{-D}^{B} dk \rho_d(k) + 2\pi \int_q^{\tilde{q}} d\lambda' \sigma_d(\lambda'). \tag{14}$$

This phase shift satisfies the Langreth-Friedel sum rule, $\delta^{\sigma}_1 = 2\pi n_\sigma$, relating the phase shift to the total number of electrons n_d in the dot.[23]

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 $\rho_d(k < 0)$ (Ref. 13) and a direct relation between the phase shifts for the electron with spin $-\sigma$ and the hole with spin σ from a property of electron-hole transformation based on the SU(2) spin symmetry. The phase shift is given by[17]

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

where the Kondo temperature for a lead at chemical potential μ_m is

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

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 ($G_{mm'}=-e\partial_{\mu_{m'}}I_m$) from Eq. (7), (8), and (15). The matrix conductance in the multiple-lead Kondo-dot system is given by

$$G_{mm}=-\sum_{m'\neq m}G_{mm'}, \tag{16}$$

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

where $G_0=2e^2/h$ is the quantum of conductance, and $\Gamma_{mm'}=V_mV_{m'}/\Gamma$. 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.[17] 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 multilead quantum point-contact for free fermions.[24] This unitary scattering limit shows the Fermi liquid nature of the multiple-lead Kondo-dot system.

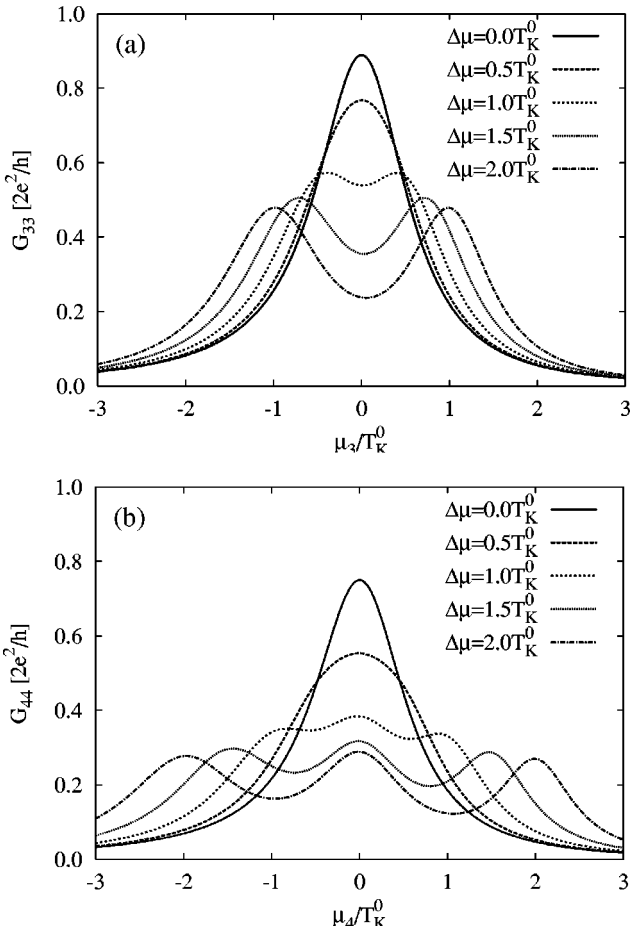

FIG. 2. Splitting of the Kondo resonance by multiple leads. (a) Conductance G_{33} as a function of the chemical potential μ_3 for a quantum dot symmetrically coupled (i.e., $V_1=V_2=V_3$) to the three leads ($N=3$), $\Delta\mu=\mu_2-\mu_1$. (b) Conductance G_{44} as a function of the chemical potential μ_4 for a quantum dot symmetrically coupled to the four leads ($N=4$), $\Delta\mu=\mu_2-\mu_1=\mu_3-\mu_2$. The temperature is zero, $U=100.0\Gamma$, and $\varepsilon_d=-3.0\Gamma$. T_K^0 is the Kondo temperature at equilibrium. Here, at equilibrium, all chemical potentials are set to be zero.

Note that the multiple-lead matrix conductance in Eqs. (16) 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 μ_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 μ_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.

V. 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

$$\mathbf{U}_3=\frac{1}{\sqrt{\Gamma}}\begin{pmatrix}V_1 & V_2 & V_3\\ V_2 & a & b\\ V_3 & b & c\end{pmatrix}, \tag{18}$$

where $a=(-V_1V_2^2+V_3^2\sqrt{\Gamma})/\gamma$, $b=(-V_1V_2V_3-V_2V_3\sqrt{\Gamma})/\gamma$, 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 $\mathbf{U}_4$ for four leads can be determined.

We plot the conductance G_{33} as a function of μ_3 for $N=3$ and the conductance G_{44} as a function of μ_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.

VI. CONCLUSIONS

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.

Note added. Recently, we became aware of work by Simon and Affleck,[25] in which a similar conclusion of a unitary transformation was reached independently for two leads containing multichannels.

ACKNOWLEDGMENT

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