Kondo Physics and Exact Solvability of Double Dots Systems

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We study two double dot systems, one with dots in parallel and one with dots in series, and argue they admit an exact solution via the Bethe ansatz. In the case of parallel dots we exploit the exact solution to extract the behavior of the linear response conductance. The linear response conductance of the parallel dot system possesses multiple Kondo effects, including a Kondo effect enhanced by a nonperturbative antiferromagnetic RKKY interaction, has conductance zeros in the mixed valence regime, and obeys a non-trivial form of the Friedel sum rule.

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The continual advance in the ability to engineer devices on the nanoscale level has led to the recent fabrication of double quantum dot (DQD) devices [1, 2, 3, 4, 5, 6, 7, 8, 9], both from semiconducting heterostructures [1, 2, 3, 4, 5, 6, 7, 8, 9] and from carbon nanotubes [6, 8]. Like their single dot cousins [10], these devices are highly tunable. This tunability makes DQDs both a leading candidate for a solid state realization of a quantum qubit and an ideal laboratory to observe strongly correlated Kondo phenomena.

Single dot devices have long been known to exhibit Kondo physics [3, 10]. By the use of a gate voltage, the number of electrons on the dot can be adjusted so that it is odd. By virtue of Kramers degeneracy, the dot, through hybridization with electrons in connecting leads, becomes a realization of a single impurity Kondo system. Transport measurements are the most striking signatures of Kondo physics in such devices, where, for example, the observed finite temperature linear response conductance [3] matches that predicted theoretically [11, 12].

With different possible dot geometries, Kondo physics in DQD devices is necessarily more rich. Dots arranged in series have been shown to exhibit Kondo physics in DQD devices [1, 2, 3, 4, 5, 6, 7, 8]. Like their single dot cousins [9, 10], these devices are highly tunable and an ideal laboratory to observe strongly correlated Kondo phenomena.

In this letter, we present a powerful theoretical approach to DQD systems. We study two models of such systems, one with dots in parallel, one with dots in series. We argue both models admit exact solutions via the Bethe ansatz. The model of dots in series possesses an SU(4) symmetry [18] and is relevant to the study of the Kondo effect in carbon nanotubes [10]. For the model of dots in parallel, we explicitly demonstrate that transport properties may be extracted from the exact solution. Transport in the system of parallel dots exhibits two interesting features: i) at the particle-hole symmetric point, we find a cooperative combination of Kondo and RKKY physics where a non-perturbative antiferromagnetic RKKY effect serves to mediate the formation of a Kondo like singlet; and ii) in the dots’ mixed valence regime, we discover a form of the Friedel sum rule where contributions to the scattering phase come both from electrons in the dots and the leads.

Models Defined: We examine two generalized Anderson models coupling two leads (l = 1, 2) to two DQDs (α = 1, 2) in two distinct configurations. In the first configuration (denoted by PD), the dots are arranged in parallel. The corresponding Hamiltonian is taken to be

\[ H_1 = H_0 + H_{\text{int}} \text{ with } H_0 = -i \sum_{\sigma} \int_{-\infty}^{\infty} dx c_{\sigma}^\dagger \partial_x c_{\sigma} + \sum_{\sigma} \epsilon_{\sigma} n_{\sigma} \]

\[ H_{\text{int}} = \sum_{\alpha, \alpha'} V_{\alpha \alpha'} (c_{\alpha}^\dagger d_{\alpha} + \text{h.c.}) + \sum_{\alpha, \alpha'} U_{\alpha \alpha'} n_{\alpha} n_{\alpha'} \]. (1)

Here the \( c_{\alpha} / d_{\alpha} \) specify electrons living in the leads and the dots. \( V_{\alpha \alpha'} \) measures the tunneling strength between the dot \( \alpha \) and lead \( l \). \( U_{\alpha \alpha'} \) characterizes the Coulombic repulsion between electrons of opposite spin living on dots \( \alpha \) and \( \alpha' \).

\[ Dots \text{ in Parallel (PD)} \]

\[ Dots \text{ in Series (SD)} \]

In the second model (denoted SD) the dots are arranged in series. The corresponding Hamiltonian has a similar form to the first \( H_2 = P(H_0 + H_{\text{int}})P \). Here \( H_{\text{int}} \) is of the form

\[ H_{\text{int}} = \sum_{\sigma, l} V_l (c_{\sigma}^\dagger d_{\sigma l} + \text{h.c.}) + \sum_{(\alpha \sigma) \neq (\alpha' \sigma')} n_{\alpha \sigma} n_{\alpha' \sigma'} \]

\[ \times \left( U + i \lim_{\alpha \to \infty} \sum_{l, \sigma} \int_{-\infty}^{\infty} dx c_{\sigma}^\dagger(x) \partial_x c_{\sigma}(x) \right) \]. (2)

\( P \) is a projection operator which forbids total occupancy of both dots from exceeding two electrons. In a regime...
where fewer than two electrons sit on the dots, the role played by both the projection operator and the correlated hopping terms will be minimal. We note that the addition of an interdot hopping term, i.e. $\delta H_2 = t_+$, does not spoil integrability [21].

**Integrability of PD:** To analyze PD (two dots in parallel) we first map the problem to an Anderson model involving a single effective lead. To do so need to assume the ratio of left/right lead couplings are equal, i.e. $V_{L_0}/V_{R_0} = V_{L_0}/V_{R_0}$. Writing $c_{e/}(\alpha) = (V_{L_0}/V_{R_0})V_{R_0}/V_{L_0}$, with $\Gamma_0 = (V_{L_0}^2 + V_{R_0}^2)/2$, the Hamiltonian factorizes into an even and an odd sector, $H_1 = H_e + H_o$. Only $H_e$ couples to the dot and is given by $H_e = H_{e0} + H_{eint}$, with $H_{e0} = -i \sum_\sigma \int^\infty_{-\infty} dx c^\dag_{\sigma\alpha} \partial_x c_{\sigma\alpha} + \sum_{\sigma} c_{\sigma\alpha} n_{\sigma\alpha}$ and

$$H_{eint} = \sum_{\sigma} \sqrt{2 \Gamma_0 (e_{c\sigma} n_{\sigma\alpha} + h.c.)} + \sum_{\alpha\alpha'} U_{\alpha\alpha'} n_{\sigma\alpha} n_{\sigma\alpha'}.$$  \hfill (3)

In contrast, $H_o$ is trivial: $H_o = H_{e0}(e \rightarrow \alpha, \epsilon_{do} = 0)$. The integrability of PD is then equivalent to the exact solvability of $H_e$.

To determine under what conditions $H_e$ admits eigenfunctions of the Bethe ansatz form, we begin by computing both the one and two electron eigenstates. The one particle wave function appears as

$$|\psi_\alpha\rangle = \left[ \int^\infty_{-\infty} dx \{ g_\alpha(x) c^\dag_{\alpha\alpha}(x) \} + e_{\sigma\alpha} d_{\alpha\sigma}^\dag \right]|0\rangle.$$  \hfill (4)

Solving the Schrödinger equation, $H_e|\psi\rangle = q|\psi\rangle$, we find $g_\alpha(x) = \theta(x)e^{i\pi x + \pi/2} + \theta(-x)e^{-i\pi x - \pi/2}$ with $\delta(q)$, the impurity scattering phase, to be $\delta(q) = -2\tan^{-1}(\sum_{\sigma}(\Gamma_\sigma/\epsilon_{\sigma\alpha})).$ To compute the effective scattering between electrons, we study the two particle eigenfunction with spin projection, $S_z = 0$:

$$|\psi\rangle = \left[ \int^\infty_{-\infty} dx_1 dx_2 g(x_1, x_2) c^\dag_{\alpha\alpha}(x_1) c_{\alpha\alpha}(x_2) + \sum_{\alpha} \int^\infty_{-\infty} dx \left[ c_\alpha(x) \{ c^\dag_{\alpha\alpha}(x) d_{\alpha\alpha}^\dag - c_{\alpha\alpha}(x) d_{\alpha\alpha}^\dag \} \right] \right]|0\rangle.$$  \hfill (5)

Again solving the Schrödinger equation $H_e|\psi\rangle = (q + p)|\psi\rangle$ gives $g(x_1, x_2) = g_1(x_1)g_2(x_2)\phi(x_{12}) + (x_1 \leftrightarrow x_2)$, with $x_{12} = x_1 - x_2$. Here $g_1/2(p)(x)$ are one particle wavefunctions with energies $p,q$. $\phi(x)$ governs the scattering when two electrons are interchanged. It takes the form $\phi(x) = 1 + i\gamma(q,p)sgn(x)$. We find that $\gamma(q,p)$ is consistently determined to be

$$\gamma(q,p) = \frac{1}{q - p} \sum_{\alpha\alpha'} \epsilon_\alpha e_{\alpha\alpha'} U_{\alpha\alpha'}.$$  \hfill (6)

if either

$$U_{\alpha\alpha'} = \delta_{\alpha\alpha'} U_{\alpha}; \quad U_{\alpha \Gamma_\alpha} = c; \quad U_{\alpha} + 2\epsilon_{do} = c';$$  \hfill (7)

where $c$ and $c'$ are $\alpha$-independent constants or

$$U_{\alpha\alpha'} = U; \quad \Gamma_\alpha = \Gamma_{\alpha'}; \quad \epsilon_\alpha = \epsilon_{\alpha'}.$$  \hfill (8)

The first set of conditions describes single level dots absent an interdot coupling while the second dots with degenerate levels with a highly finely tuned interdot interaction. We will thus focus on the first.

Exact solvability is predicated on how $\gamma(q,p)$ determines the scattering matrix of the two electrons. The scattering matrix has the general spin (SU(2)) invariant form, $S_{ab}^{\lambda\mu} = \bar{b}(p,q)F_{ab}^{\lambda\mu}$, where $\lambda, \mu = \uparrow, \downarrow$ and $I/P$ are the identity/permutation matrices. The coefficients, $b(p,q)$ and $c(p,q)$, are determined by $\gamma(q,p)$ from the relation, $b(p,q) - c(p,q) = \phi(x > 0)/\phi(x < 0) = (1 + i\gamma(p,q))/(1 - i\gamma(p,q))$, together with $b(p,q) + c(p,q) = 1$ which arises from considering the eigenfunction in $S_z = \pm 1$ sector where interactions are absent.

In order for the Hamiltonian, $H_e$, to be integrable, a minimal condition is that the above S-matrix satisfy the Yang-Baxter relation. The Yang-Baxter relation governs the scattering of three electrons and it enforces the equivalence of different scattering orders. It is well known in the case of an $SU(2)$ symmetry that the validity of the Yang-Baxter relations is equivalent to the condition, $b(p,q) - c(p,q) = i(g(p) - g(q))$, where $g(p)$ is an arbitrary function [22]. In the case at hand, $g(p)$ is given by $g(p) = (p - \epsilon_{do} - U_\alpha - 2\epsilon_{do})/2(2\epsilon_{\alpha\alpha})$.

Having determined under what conditions the dot-lead Hamiltonian is exactly solvable, we are now in a position to construct N-particle eigenstates in a controlled fashion. An eigenfunction with spin, $S_N = N - 2M$, is characterized by a sea of N electrons each carrying momenta $(q|N|_{j=1})$ and so total energy $E = \sum_\alpha q_\alpha$. In a periodic system of length L, integrability allows us to write down in a compact form the $q_\alpha$-quantization conditions (the Bethe ansatz equations):

$$e^{i\alpha L + i\delta(q_\alpha)} = \frac{M}{\alpha = 1} g(q_\alpha) - \lambda_\alpha + i/2.$$  \hfill (9)

These equations are identical to those for the ordinary Anderson model [22] but for the form of $\delta(q)$. The M dependent $\lambda_\alpha$‘s appearing in the above equations are indicative of the spin degrees of freedom.

There are two integrable generalizations of the PD model: i) N-dots in parallel and ii) a pair of dots in a T-junction. These systems, to be integrable, must satisfy a set of constraints similar to Eqs. 7 and 8.

**Integrability of SD:** We demonstrate the generic integrability of SD along similar lines – it was already known to be exactly solvable for infinite $U$ [22]. Here, however, we do not transform to an even/odd sector. We thus have four different types of fermions/dot degrees of freedom.
This will ultimately lead to the model having an exact $SU(4)$ symmetry at all energy scales.

Constructing the two particle eigenfunctions as before leads to an $SU(4)$ S-matrix provided $V_l = V$ for all $l$ and $\epsilon_{da} = \epsilon_d$ for all $\alpha$. (This latter constraint can be relaxed enabling one to study non-degenerate dots where the $SU(4)$ symmetry is broken, say by a magnetic field or a gate voltage.) The S-matrix takes the same form as Eq. [21] but with $a$, $b$ one of four values, $(1, \uparrow), (1, \downarrow), (2, \uparrow)$, $(2, \downarrow)$. Again we have $b(p,q)/e(p,q) = i(g(p) - g(q))$, sufficient for the Yang-Baxter relation to be satisfied, but with $g(p) = (p - \epsilon_d - U/2)^2/(V^2U)$.

To construct the N-particle eigenfunctions, we again employ a nested Bethe ansatz [22]. Crucial to these eigenfunctions being of the Bethe form are both the projectors, $P$, and the correlated hopping term (Eq. 2) of $H_2$. This demonstrates that in the case of dot systems with orbital degeneracies and a finite $U$ Coulomb repulsion, and unlike Hubbard models with orbital degeneracies, it is possible to find a simple Hamiltonian which is exactly solvable. As was demonstrated in Ref. [24], the $(N > 2)$-particle wavefunctions of any simple finite $U$ orbitally degenerate Hubbard model are not of the Bethe type.

The quantization conditions of an N-electron state carrying momenta $\{q_\alpha\}_{\alpha=1}^N$ are of the form

$$e^{iq_\alpha L + i\delta_2(q_\alpha)} = \prod_{\alpha=1}^N \lambda_\alpha^0 - \lambda_\alpha^1 + \frac{i}{2} \prod_{\alpha=1}^{M_\alpha-1} \lambda_\alpha^0 - \lambda_\alpha^{-1} - \frac{i}{2} = \prod_{\lambda_\alpha^0 = \lambda_\alpha^{-1}} \lambda_\alpha^0 - \lambda_\alpha^{-1} - \frac{i}{2} \prod_{\lambda_\alpha^0 = \lambda_\alpha^{-1}} \lambda_\alpha^1 - \lambda_\alpha^{-1} - \frac{i}{2}$$

Here $\delta_2(q) = -2\tan^{-1}(V/2(q-\epsilon_d))$. The quantum numbers, $\{\lambda_\alpha^k\}, k = 0, 1, 2, 3$ (with $\lambda^0 = g(q)$) correspond to both spin and orbital degrees of freedom. In a preliminary analysis of Eqs. [21], we have verified the $SU(4)$ Kondo physics expected in a regime where one electron sits on the dots [18]. Thus the marginal correlated hopping term in Eqn. (2) does not influence the universality class into which the physics falls. We also note that the integrability of SD can be generalized to N-dots arranged in triangles (N=3), squares (N=4), etc.

**T=0 Conductance of PD**: In the remainder of the paper, we focus on extracting the features of the $T = 0$ linear response conductance of the parallel dots (PD). The structure of the linear response conductance, $G$, for the parallel dots is much richer than that of a single dot containing distinct Kondo effects, novel applications of the Friedel sum rule, and quantum critical behavior.

To compute the linear response conductance of the dots we closely follow Ref. [12]. The approach is based on the observation that the impurity scattering phase, $\delta_{\text{imp}}$, of an electron is determined by the shift in the electron’s momentum due to the presence of the impurity, i.e. $p \rightarrow p + \delta_{\text{imp}}/L$. From the Bethe ansatz the full momentum $p$ of the excitations are readily extracted. Then isolating the term in the momentum scaling as the inverse system size, $L^{-1}$, allows the $\delta_{\text{imp}}$ to be computed. In the geometry we have chosen, $G$ is given by $2e^2/h \sin^2(\delta_{\text{imp}}/2)$.

**FIG. 2**: The total conductance and number of displaced electrons per spin species vs. $\epsilon_{d1}$, $\Delta \epsilon$ fixed, for two dots in parallel.

We plot an example of the linear response conductance for two dots in parallel in Fig. 2. We consider the asymmetric case where $\Delta \epsilon = \epsilon_{d1} - \epsilon_{d2} \gg \Gamma_1, \Gamma_2$. The conductance is plotted as a function of $\epsilon_d$, keeping $\Delta \epsilon$ fixed from the particle-hole symmetric (p.h.s.) point of the system (i.e. $U_\alpha = -2\epsilon_d$) where two electrons sit on the dots to a point where both dot levels are well above the Fermi level and the dots are nearly empty. In this plot, the structure of the linear response conductance, in comparison with that for a single level dot, is more complex. This reflects both the presence of interference [14] as well as distinct types of Kondo physics.

At the p.h.s. point, (i.e. $\epsilon_{d1}/\Gamma_1 = -10$ in Fig. 2) the two electrons residing on the dots together with electrons in the leads form a singlet. With no bare direct exchange, singlet formation is mediated solely by virtual hopping processes which here promote antiferromagnetic correlations. We thus term this formation the RKKY-Kondo effect to mark the role of electron itinerancy. This phenomena is distinct from the ferromagnetic RKKY effect arising in fourth order perturbation theory for two closely spaced dots and is thought to compete with Kondo physics. In particular, the RKKY-Kondo effect is non-perturbative in virtual hopping processes. We find that the RKKY-Kondo effect is generically present provided $\epsilon_{d1} \neq \epsilon_{d2}$ and so there are unequal numbers of electrons on each dot (as indicated in the cartoon in Figure 2).

This antiferro-RKKY Kondo effect is, in a sense, unsurprising. The Friedel sum rule (FSR) dictates that at the p.h.s. point, the scattering phase equal $\pi$ and $G$ vanish. If we were instead to have a ferro-RKKY effect, and so an underscreened spin 1 impurity, $G$ would be maximal and so violate the FSR. Our finding of a
Fermi liquid fixed point is supported indirectly by earlier work on the two impurity Anderson model \[26\]. Although there the focus is upon two electron channels coupled to two impurities, the finding is both that the physics is Fermi liquid and that the one to two channel crossover is smooth. We have verified singlet formation both by demonstrating from the Bethe ansatz equations that the entropy vanishes in the zero temperature limit and, separately, from a slave boson mean field analysis.

The Abrikosov-Suhl resonance associated with this RKKY-Kondo effect can be computed along the lines of Ref. \[12\] (up to a multiplicative constant):

\[
\rho(\epsilon) = \cos(\beta\pi)(T_{RRK}^{-1}(\epsilon^2 + 1)))(2\epsilon^2 \cos(2\beta\pi) + \epsilon^4 + 1),
\]

where \(\epsilon = \epsilon/T_{RRK}\) and \(T_{RRK}\) is the RKKY Kondo temperature, \(T_{RRK} \sim \sqrt{U_1 \Gamma_1} \exp(-\pi U/8\Gamma_1)\). The parameter \(\beta\) is 0 if \(\Delta \epsilon \gg \Gamma_{1,2}\) and is 1/2 if \(0 < \Delta \epsilon \ll \Gamma_{1,2}\). As \(\Delta \epsilon \to 0\), the resonance evolves from a Lorentzian centered at zero energy to a structure with split peaks. The scale \(T_{RRK}\) governs the leading corrections to the conductance as a function of Zeeman field (H) and temperature (T). For \(\Delta \epsilon \gg \Gamma_{1,2}\), we compute these at the p.h.s. point to have the Fermi-liquid form (in units of \(2e^2/h\)): \(G(T/T_{RRK}) = \pi^4(T/T_{RRK})^2/4\) and \(G(H/T_{RRK}) = \pi^2(H/T_{RRK})^2/4\).

As we move away from the p.h.s. point through increasing the gate voltage, we begin to empty the dots. With the assumed asymmetry in \(\epsilon_{d1}\) and \(\epsilon_{d2}\), we arrive at a point where the dot system has roughly one electron predominantly on dot 1. At this value of the gate voltage, we expect ordinary Kondo physics to be operating. Defining \(T_K\) via its relation to the static impurity susceptibility, i.e. \(\chi_{\text{imp}} = (4T_K)^{-1}\), the corresponding leading contributions to the conductances (in units of \(2e^2/h\)) are \(G(T/T_K) = 1 - (\pi^2/16)(T/T_K)^2\) \[11\] \[12\] and \(G(H/T_K) = 1 - (\pi^2/16)(H/T_K)^2\) \[12\]. From a numerical analysis, we know that \(T_K\) has a single dot form, i.e. \(T_K \sim \sqrt{UT_1/2}\exp(\pi\epsilon_{d1}(\epsilon_{d1} + U)/2U_1\Gamma_1)\) \[22\] \[23\].

As \(\epsilon_{d1}\) is further increased, we see both a vanishing of the conductance and an unusual form of the FSR, a mark of the effects of interference. The vanishing of the conductance may reflect interference alone: it is present as well in the non-interacting case. However the form the FSR takes reflects both interference and interactions. The FSR relates the scattering phase to the number of displaced electrons, i.e. \(\delta_x = \pi n_{\text{dis}}\). \(n_{\text{dis}}\) is defined to be

\[
n_{\text{dis}} \equiv n_{\text{dis}} + \int dx \left[ (c_{\sigma}^{\dagger} x c_{\sigma}(x)) - \rho_{\text{bulk}\sigma} \right], \tag{10}
\]

and contains contributions from both the occupancy of the dots, \(n_{\text{dis}}\), and deviations in the lead electron density from coupling the dots to the leads \[27\]. As is evident in Figure 2, we have an unusual situation where both contributions to \(n_{\text{dis}}\), and not merely \(n_{\text{dis}}\), are finite: \(n_{\text{dis}}\) is always manifestly positive while \(n_{\text{dis}}\) is negative over a range of \(\epsilon_{d1}\).

One last feature to the linear response conductance we wish to point out is the disappearance of the Abrikosov-Suhl resonance at precisely \(\epsilon_{d1} = \epsilon_{d2}\). The transition is first order as \(T_{RRK}\) itself does not vanish as \(\epsilon_{d1} \to \epsilon_{d2}\). The origin of this critical point lies in the decoupling of one dot degree of freedom (d.o.f) if \(\epsilon_{d1} = \epsilon_{d2}\) (and only if), as can be seen via a change of basis \(d_{e/0} = (\Gamma_1/2d_1 + \Gamma_2/d_2)/(|\Gamma_1^2 + \Gamma_2^2|)^{1/2}\). This discontinuous behavior at \(\epsilon_{d1} = \epsilon_{d2}\) however can be transformed into a smooth crossover by weakly coupling a second channel of electrons to the dot \[28\] and so recoupling the odd dot d.o.f.

Apart from the behavior at \(\epsilon_{d1} = \epsilon_{d2}\), we generally expect the above physics to be robust against small violations of the integrability constraints (Eqn. 9) for a number of reasons \[21\]: i) the ground state of the dot-lead system is already robustly established (unlike when perturbation theory in \(V\) is done for a single dot-lead); and ii) a Schrieffer-Wolfe transformation in the Kondo regime is unaffected by (weak) violations of Eqn. (7).

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