Discrete charging of a quantum dot strongly coupled to external leads

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The discrete features of a quantum dot with strongly attached leads are examined both analytically and numerically for varying dimensionless conductance g of the leads, i.e., varying number of channels. It is shown that for strong couplings between the dot and the leads the number of remaining bound states on the dot (akin to subradiant states in optics) is reduced by no more than g. The remaining states in the dot show discrete charging and strong Coulomb blockade behavior as function of the chemical potential.

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It is well known that the number of electrons in a weakly coupled quantum dot changes discretely as function of the chemical potential. This phenomenon is the basis for the application of such dots as single electron transistors [1]. As long as the coupling to the external leads is weak, it may be treated as a perturbation and results in a broadening $\Gamma = \pi N \nu |V|^2$ of the original states of the uncoupled dot, given by Fermi's golden rule. (ν is the density of states in a lead, N the number of leads, and V is the overlap matrix element between a state in the dot and a typical state of the leads.) Usually, one expects the discrete features of the dot to be lost once Γ is larger than the typical level spacing Δ in the dot. This corresponds to the requirement that the dimensionless conductance through the dot, $g_{\rm dot} = \Gamma/\Delta$, should be larger than one.

Electron-electron interaction in the dot results in the Coulomb blockade phenomenon [1]. Within the "orthodox model" [2], the chemical potential change needed to add an additional electron to a weakly coupled dot is no longer Δ but rather $\Delta + e^2/C$, where C is the capacitance of the dot. For stronger coupling to the leads, suppression of the Coulomb blockade is predicted [3], and once $\Gamma \sim \Delta$ only a weak remnant of the discreteness of the dot is expected [4].

In this picture the only relevant parameter which predicts the appearance of discrete features in the dot is $g_{\rm dot} < 1$. Nevertheless, one may extrapolate from the Dicke effect [5, 6] (atoms strongly coupled via the radiation field exhibit new sharp resonances known as subradiant states) that a quantum dot strongly coupled to a lead will also show strong resonances. Indeed, a resonance in a two orbital dot strongly coupled to two leads was seen in Ref. [7]. The tunneling density of states of a non-interacting two-orbital dot strongly coupled to a single lead tends towards a delta-like peak when $g_{\rm dot} \to \infty$ [8]. It was later shown [9] that when a dot of $N_{\rm dot}$ states is strongly connected to a single lead, $N_{\rm dot} - 1$ delta-like peaks in the tunneling density of states remain for $g_{\rm dot} \to \infty$. The case of two leads connected to a dot with $N_{\rm dot} = 2$ shows interesting dependence on the overlap matrix element $V_{k,i}$ (i.e., the i-th level overlap with k-th lead) [10]. For identical matrix elements one sharp peak in the local density of states remains, while if one of the four matrix elements has a different sign, no such features are observed.

In this letter we show that in the limit $g_{\rm dot} \to \infty$, the relevant parameter in determining the number of bound states in the dot is the dimensionless conductance g of the leads. Using numerical exact diagonalization and analytical methods for non-interacting systems, and numerical density-matrix renormalization group (DMRG) as well as mean-field techniques for interacting systems, we demonstrate that for N one-dimensional leads coupled to a dot, generically $N_{\rm dot} - N$ states remain bound to the dot, except when the coupling matrix elements between leads and dot are independent of either dot level or channel index. For the latter cases, $N_{\rm dot} - 1$ states remain bound to the dot. Since for a one-dimensional lead the dimensionless conductance is equal to one, we may restate the previous results as $N_{\rm dot} - g$ states remaining bound to a strongly coupled dot, even for infinitely strong coupling. Thus, in order to wash out all discrete features of a dot in the limit of strong coupling, one or more leads of total dimensionless conductance $g > N_{\rm dot}$ must be connected. With increasing coupling strength, a dot coupled to leads will evolve from $N_{\rm dot}$ bound states at very weak coupling, to no bound states at intermediate coupling [3] and finally to $N_{\rm dot} - g$ bound states at strong coupling. Criteria for the different regimes and experimental realizations will be discussed.

We consider a dot-lead system described by the Hamiltonian

$$H = H_{\rm dot} + \sum_{k=1}^{N} \left(H^k_{Lead} + H^k_{Coupling} \right). \qquad (1)$$

Here, the dot is represented by the Hamiltonian

$$H_{\rm dot} = \sum_{i=1}^{N_{\rm dot}} (\epsilon_i - \mu) a_i^\dagger a_i + U \sum_{i>j}^{N_{\rm dot}} a_i^\dagger a_i a_j^\dagger a_j \qquad (2)$$

in terms of the creation operators $a_i^\dagger$ of an electron in the i-th single-particle eigenstate of the dot with energy ϵ_i, charging energy $U = e^2/C$ and chemical potential μ. For disordered dots its eigenstates and eigenvalues are usually obtained from a random matrix ensemble. The Hamiltonian of the k-th lead reads

$$H^k_{Lead} = \mu \sum_{j=1}^{\infty} c_j^{k\dagger} c_j^k - t \sum_{j=1}^{\infty} c_j^{k\dagger} c_{j+1}^k + h.c., \qquad (3)$$

where $c_j^{k\dagger}$ is the creation operator of an electron on the j-th site of the k-th 1D lead, and t is the hopping matrix element in the lead. The coupling between the dot and the lead is contained in

$$H^k_{Coupling} = \sum_{i=1}^{N_{\rm dot}} V_{k,i} a_i^\dagger c_1^k + h.c., \qquad (4)$$

where the dot is assumed to be attached to the edge of the lead, and the coupling amplitude between the i-th orbital in the dot and the k-th lead is given by $V_{k,i}$. The N one-dimensional leads may also be connected by transverse hopping $-t\sum_{k=1}^{N-1}\sum_{j=1}^{\infty} c_j^{k\dagger} c_j^{k+1} + h.c.$ in order to turn them into a quasi-one dimensional lead with N channels.

We shall begin by presenting the exact-diagonalization results for a typical non-interacting ($U = 0$) dot coupled to external 1D leads. Exact diagonalization can only treat finite systems, and therefore cannot deal with infinite leads. Nevertheless, as long as the level broadening in the dot is much larger than the level spacing within the lead, the description of the system is accurate. This requirement translates for a finite lead with M sites to $M \gg (4t/V)$. After diagonalizing the Hamiltonian H, we obtain the eigenvalues ε_m and eigenvectors $|m\rangle$ of the dot-lead system. The number of electrons on the dot at a given chemical potential is $n = \sum_{m=1}^{\varepsilon_m<0}\sum_{i=1}^{N_{\rm dot}} |\langle m|a_i^\dagger a_i|m\rangle|^2$. The change in the occupation of the dot with chemical potential is given by $dn/d\mu$.

In Fig. 1 we present the discrete increases $\Delta n(\mu, N) = \int_{\mu-0.001t}^{\mu+0.001t} (dn/d\mu')\, d\mu'$ in the occupation of a disordered quantum dot with $N_{\rm dot} = 16$ orbitals (generated by a random matrix with a Gaussian distribution of width $0.1t$) as function of the chemical potential μ and the number N of one-dimensional leads connected to the dot. In the absence of dot-lead coupling ($N = 0$), the eigenenergies ϵ_m of the dot follow the random-matrix theory, and all increases $\Delta n(\mu, N) > 0$ occur at $\mu = \epsilon_m$. The integer points on the x-axis correspond to N one-dimensional leads connected to the dot by couplings $V_{k,i}$ drawn from a random Gaussian distribution with a zero mean and variance t. For non-integer values of N, $\lfloor N \rfloor$ leads are fully connected, while the couplings of the last lead are logarithmically increased from $0.007V_{\lfloor N\rfloor+1,i}$ to the full strength $V_{\lfloor N\rfloor+1,i}$ with $N - \lfloor N\rfloor$ going from 0.04 to 1. For integer values of N it can be clearly seen that there

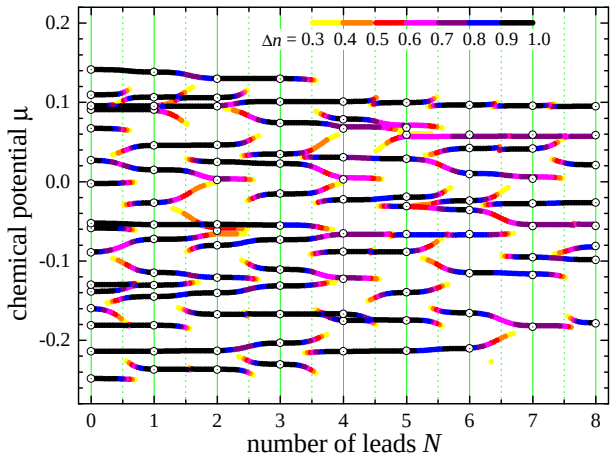

FIG. 1: The increases $\Delta n(\mu, N)$ in the occupation of a quantum dot with $N_{\rm dot} = 16$ orbitals as function of the chemical potential μ and the number N of one-dimensional leads (length $M = 100$) connected to the dot. Non-integer numbers of N correspond to having the connection of the last lead logarithmically increased (see text). The increase in the occupation is color coded as indicated in the figure. The symbols correspond to the derivative in the limit of $V \to \infty$

are $N_{\rm dot} - N$ jumps in the occupation of the dot corresponding to the same number of states bound to the dot. As one couples an additional 1D lead to the dot the energies of these states gradually change, until for some intermediate strength of coupling some of the states move abruptly, split, or disappear. At stronger couplings (i.e., close to the next integer N) the ordered structure of the states reappears, with one less state than for the previous value of N. If $V_{k,i} = t$ independent of i or k (i.e., all the couplings to the same lead or orbital are identical) a loss of a bound state occurs only when connecting the first lead to the dot. Attaching additional leads does not change the number of bound states on the dot.

To understand these numerical results we approach the system within the scattering-matrix formalism. For N propagating channels in the leads, the dot-lead system can be characterized by the $N \times N$ scattering matrix [11]

$$S = \mathbf{1} - 2\pi i \nu V \frac{1}{E - H_{\rm dot} + i\pi\nu V^\dagger V} V^\dagger, \qquad (5)$$

where V is an $N \times N_{\rm dot}$ matrix describing the coupling of the channels to the $N_{\rm dot}$ orbitals of the dot. The local density of states of the dot is given by

$$\frac{dn}{d\mu} = \frac{1}{\pi} {\rm Im\,tr} \frac{1}{\mu - H_{\rm dot} + i\pi\nu V^\dagger V}. \qquad (6)$$

If we take $H_{\rm dot}$ to be diagonal with random-matrix spectrum, the couplings $V_{k,i}$ are essentially independent random Gaussian variables of variance v^2.

When considering tunneling through isolated impurities, we can compute the scattering matrix by first diag-

onalizing the Hamiltonian $H_{\rm dot}$ of the isolated Hamiltonian. The broadening of the levels could then be obtained by treating $i\pi\nu V^\dagger V$ in first-order perturbation theory. To understand the opposite limit of strong coupling, we can first diagonalize $i\pi\nu V^\dagger V$ and subsequently account for $H_{\rm dot}$ perturbatively. We start by writing

$$V^\dagger = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N) \tag{7}$$

where the $\mathbf{v}_i$ are $N_{\rm dot}$-dimensional vectors. In obvious notation, we can then write $\pi\nu V^\dagger V = \pi\nu \sum_{i=1}^{N} |\mathbf{v}_i\rangle\langle\mathbf{v}_i|$ which shows that the $N_{\rm dot} \times N_{\rm dot}$ matrix $\pi\nu V^\dagger V$ has at most rank N and generically only N nonzero eigenvalues $\lambda_\ell \sim \pi\nu N_{\rm dot} v^2$ with $\ell = 1, \ldots, N$.

Including $H_{\rm dot}$ perturbatively, we first need to diagonalize $H_{\rm dot}$ in the $N_{\rm dot} - N$-dimensional degenerate subspace of zero eigenvalues. In the limit $N_{\rm dot} \gg N$, this leads to a random-matrix spectrum of $N_{\rm dot} - N$ real eigenvalues e_i whose width and level spacing Δ equal those of the Hamiltonian $H_{\rm dot}$ of the uncoupled dot. Thus, in first-order perturbation theory we find $N_{\rm dot} - N$ infinitely sharp resonances in addition to N purely imaginary eigenvalues which lead to an extremely broad background (since $\lambda \sim N_{\rm dot}$) in the local density of states.

In second-order perturbation theory, these resonances acquire a width since $H_{\rm dot}$ couples the sharp resonances to the broad background. The resulting width can be easily estimated to be

$$\Delta e_i \simeq \sum_{\ell=1}^{N} \frac{|\langle i|H_{\rm dot}|\ell\rangle|^2}{-i\lambda_\ell} \sim i\frac{N\Delta^2}{\pi^2\nu v^2} \sim i\frac{N^2\Delta^2}{\pi\Gamma}. \tag{8}$$

Here, we used that $H_{\rm dot}$ is a random-matrix Hamiltonian and defined the Fermi-Golden-rule expression for the width $\Gamma = \pi\nu N v^2$ of the eigenstates ϵ_i of the Hamiltonian $H_{\rm dot}$ of the uncoupled dot. We assume strong coupling so that $\pi\nu v^2 \gg \Delta$ which allows us to neglect the unperturbed energy e_i in the denominator. When this width remains small compared to the level spacing, i.e., when $N^2/\pi g_{\rm dot} \ll 1$ we find $N_{\rm dot} - N$ isolated resonances in both conductance and local density of states even though dot and lead are very strongly coupled, in agreement with our numerical results.

By an analogous argument one finds only one imaginary eigenvalue and hence $N_{\rm dot} - 1$ sharp resonances in the non-generic cases in which the coupling $V_{k,i}$ is independent of either channel k or dot level i. These resonances have a width of order $\Delta/\pi g_{\rm dot}$. This width is smaller by a factor N^2 compared to the resonance width in the case of arbitrary dot-lead coupling.

We now turn to the influence of interactions in the dot on the previous result. The ground state for an interacting dot attached to several 1D leads may be calculated as function of μ using an extension of a DMRG method developed for treating a single 1D lead connected to a dot [12] which will be described in detail elsewhere. As in the single lead case, the essence of the method is similar to the regular DMRG for 1D systems [13]. The main difference is that in every iteration a site is added to each of the leads. Fig. 2 shows the occupation number n as function of μ for a $N_{\rm dot} = 3$ dot attached to two leads for different values of the dot-lead coupling.

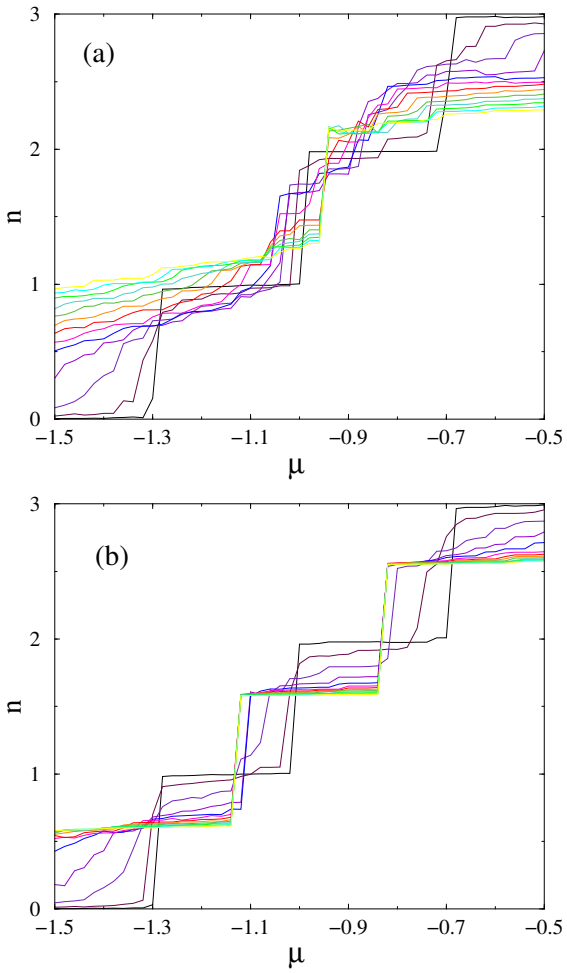

FIG. 2: The occupation n as function of the chemical potential for $N_{\rm dot} = 3$. The levels in the dot have energies $\epsilon_1 = -1.3t$,$\epsilon_2 = -1.2t$, and $\epsilon_3 = -1.1t$. The interaction $U = 0.2t$. In (a) the couplings are ,$V_{11} = 0.05pt$, $V_{12} = 0.09pt$, $V_{13} = 0.01pt$, $V_{21} = 0.09pt$, $V_{22} = 0.01pt$, $V_{23} = 0.01pt$, where $p = 1, 2, 3 \ldots 12$ for the different curves, while in (b) all the couplings are $V = 0.05pt$.

In Fig. 2a, the case of non-identical couplings is presented. The general behavior seen for the non-interacting case is repeated in the interacting case. For weak coupling, there are three discrete jumps in the occupation of the dot separated by $\Delta + U$. As the coupling increases only *one* discrete jump remains. Thus, the interactions in the dot do not eliminate the bound state. Moreover, interactions shift the position of the remaining jump to higher μ relative to the noninteracting case.

If the couplings are symmetric to all leads the number of bound states is $N_{\rm dot} - 1$ no matter how many leads

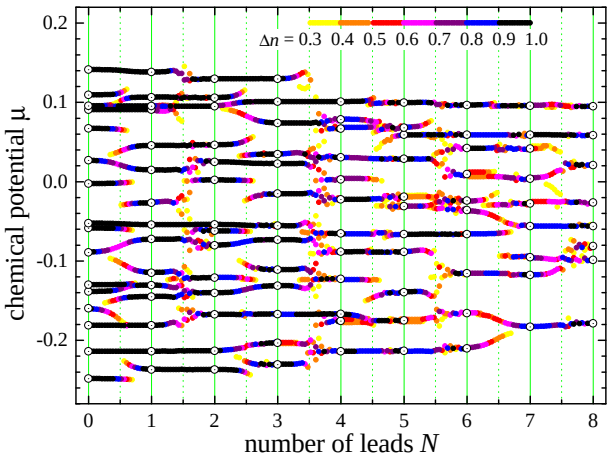

FIG. 3: The increases $\Delta n(\mu, N)$ in the occupation of a quantum dot versus the chemical potential μ and the width N of a quasi-1D lead connected to the dot; for parameters, see Fig. 1.

are attached. This is illustrated in Fig. 2b, where two discrete jumps remain even for strong coupling. These bound states are separated by a distance of $\Delta + U$ as one expects from two bound states on an interacting dot.

This behavior can be explained by a simple extension of the scattering theory developed above which includes the charging energy within the Hartree approximation. Within this approximation, we can account for U by replacing $e_i \to e_i + \sum_{j\neq i}\langle b_j^\dagger b_j\rangle$ where b_j annihilates an electron in the dot state corresponding to the energy e_j. Here we neglect the charging of the broad resonances which is allowed as long as we consider chemical potential changes which are small compared to the bandwidth. With this approximation, one finds that the separation between subsequent resonances is given by $\Delta + U$ in the presence of the charging energy.

In the analytical formulation one may replace the attachment to N 1D leads by an attachment to a single lead with N independent channels, i.e., a lead of dimensionless conductance $g = N$. Of course these channels will not necessarily be identical and therefore the coupling to the dot will be asymmetric. Thus, we expect a dot with $N_{\rm dot}$ orbitals strongly attached to any lead (or set of leads) with a total conductance g to retain $N_{\rm dot} - g$ states bound to it. In order to check this expectation we repeated our exact diagonalization calculation depicted in Fig. 1, for a quasi-1D lead of width N. The behavior of the states bound to the dot as function of the width N of the quasi-1D lead is given in Fig. 3, which can be compared with Fig. 1 for N individual leads. Here the non-integer values of N correspond to increasing logarithmically the values of $V_{\lfloor N\rfloor+1,i}$ and those for the transverse hopping while an additional row is added. It can be seen that the same qualitative behavior as in Fig. 1 is retained.

One remains with the question of how to reconcile these results with the simple intuitive picture (as well as the analytical calculations for interacting dots [3, 4]) that once the dot is well coupled to the leads no bound states remain. To clarify the picture let us consider a quantum wire (1D dot) described by a Hamiltonian akin to Eq. (3). The eigenvalues in the uncoupled dot are $\epsilon_j = -2t\cos(2\pi j/N_{\rm dot})$ and eigenvectors $\sin(2\pi jx/N_{\rm dot})/\sqrt{N_{\rm dot}}$ (x is the site number). If there is no barrier, i.e., the hopping from the last site in the dot to the first site in the lead is equal to t, we obtain $V_{1,j} \sim t/\sqrt{N_{\rm dot}}$, and $\Delta \sim t/N_{\rm dot}$, i.e., $N^2\Delta/\pi\Gamma \sim N \sim 1$, which is not the strong coupling regime. Moreover, there are no almost degenerate states for which $\Delta \ll \Gamma$ and therefore in this case no bound states should be observed. Indeed, in all figures for weak ($N^2/\pi g_{\rm dot} \ll 1$) and strong couplings $N^2/\pi g_{\rm dot} \gg 1$) one sees clear discrete features, while for intermediate couplings $N^2/\pi g_{\rm dot} \sim 1$) these features are washed out.

Finally, we have to ask if strong coupling can occur in a realistic experiment. One approach is to enhance the coupling V between the dot and lead. This might be achieved by a quasi-1D tip inserted into the middle of a molecule or a ring shaped dot so couplings of order $V \sim t$ can be achieved. Another possible approach is to enhance locally the density of states in the dot. One possibility is to use a degeneracy point in a highly symmetric dot. A different way may be to couple the leads to a dot which is also coupled to several other dots controlled by gates. The levels in the dots may then be manipulated to obtain near degeneracy.

In conclusion, contrary to naive expectation, strong dot-lead coupling alone is not sufficient in order to erase all signatures of the original states in a dot strongly coupled to a lead or a set of leads. The conductance (number of channels) g of the attached leads determines the number of states which remain bound to the dot in the limit of strong coupling. We have demonstrated both analytically and numerically that the number of bound states remaining on the dot is $N_{\rm dot} - g$. These states are well bound, and exhibit the usual response to electron-electron interactions in the dot, namely Coulomb blockade.

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