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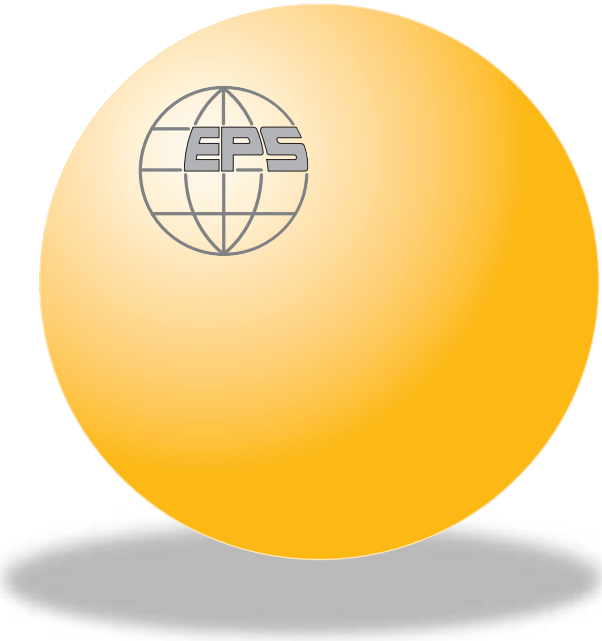

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Discrete charging of a quantum dot strongly coupled to external leads

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Abstract. – We examine a quantum dot with $N_{\rm dot}$ levels which is strongly coupled to leads for varying number of channels N in the leads. It is shown both analytically and numerically that for strong couplings between the dot and the leads, at least $N_{\rm dot} - N$ bound states (akin to subradiant states in optics) remain on the dot. These bound states exhibit discrete charging and, for a significant range of charging energies, strong Coulomb blockade behavior as a function of the chemical potential. The physics changes for large charging energy, where the same (superradiant) state is repeatedly charged.

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]. When 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 states of the uncoupled dot. (ν is the density of states (DOS) 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 condition for the appearance of discrete features in the dot is $g_{\rm dot} < 1$. Nevertheless, one may extrapolate from the Dicke effect [5,6] that a quantum dot strongly coupled to a lead will also show sharp resonances. In an extreme strong-coupling limit, we can think of the dot levels as degenerate, analogous to the identical resonances of the atoms in the Dicke effect. These degenerate levels are coupled via the continuum of lead states which is akin to the coupling of the atoms by the radiation field. Indeed, a resonance in a two-orbital dot strongly coupled to two leads was seen in ref. [7]. The tunneling DOS 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 DOS 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 the 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 for generic dot-lead coupling is the number of channels N of the leads, or, equivalently, the dimensionless conductance g of the leads. We demonstrate that for N channels coupled to a dot, $N_{\rm dot} - N$ 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. Using numerical density-matrix renormalization group (DMRG) as well as analytical arguments, we show that these bound states exhibit discrete charging as well as Coulomb blockade except for very large charging energies. 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. It is interesting to note that the physics discussed here for quantum dots is also closely related to the concept of doorway states in nuclear physics [11].

We consider a dot-lead system described by the Hamiltonian

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

Here, the dot is represented by the Hamiltonian

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

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

$$H^k_{\rm Lead} = \mu \sum_{j=1}^{\infty} c_j^{k\dagger} c_j^k - t \sum_{j=1}^{\infty} c_j^{k\dagger} c_{j+1}^k + \text{H.c.}, \tag{3}$$

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

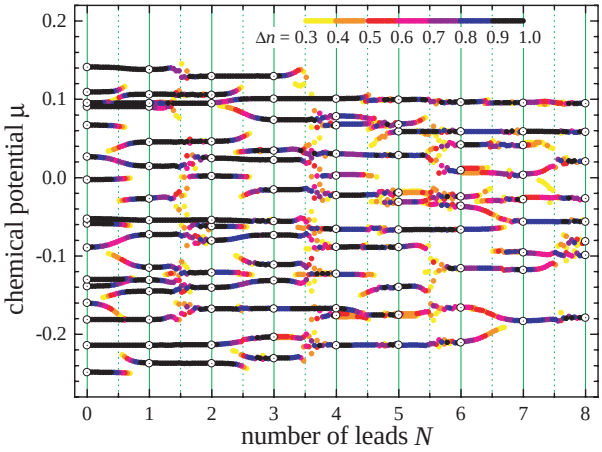

Fig. 1 – The increases $\Delta n(\mu, N)$ in the occupation of a quantum dot with $N_{\rm dot} = 16$ orbitals as a function of the chemical potential μ and the width N of the quasi–one-dimensional lead (length $M = 100$) connected to the dot. Non-integer numbers of N correspond to having the connection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

contained in

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

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 $-t\sum_{k=1}^{N-1}\sum_{j=1}^{\infty} c_j^{k\dagger} c_j^{k+1} + \text{H.c.}$ in order to turn them into a quasi–one-dimensional lead with N channels.

We begin with exact-diagonalization results for a non-interacting ($U = 0$) dot coupled to an external quasi-1D lead of varying width (*i.e.*, number of channels N). 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 in the lead, the description of the system is accurate. Diagonalizing the Hamiltonian H gives 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 $n = \sum_{m=1}^{\varepsilon_m<0}\sum_{i=1}^{N_{\rm dot}} |\langle m|a_i^\dagger a_i|m\rangle|^2$.

In fig. 1 we present the discrete increases $\Delta n(\mu, N) = \int_{\mu-0.001t}^{\mu+0.001t} (\mathrm{d}n/\mathrm{d}\mu')\,\mathrm{d}\mu'$ 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 a function of the chemical potential μ and N, the number of channels connected to the dot. In the absence of dot-lead coupling ($N = 0$), all increases $\Delta n(\mu, N) > 0$ occur at $\mu = \epsilon_m$. The integer points on the x-axis correspond to N channels connected to the dot by couplings $V_{k,i}$ drawn from a random Gaussian distribution with a zero mean and variance t. The non-integer values of N correspond to increasing logarithmically the values of the coupling of the $N + 1$ channel to the dot and its transverse hopping to the neighboring channel up to the full strength $V_{\lfloor N\rfloor+1,i}$ and t at integer N. For integer values of N it can be clearly seen that there 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 channel 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. Similar behavior is seen when there is no transverse hopping between the channels (*i.e.*, N independent 1D leads). If $V_{k,i} = t$ is 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 [12]

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

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 DOS of the dot is given by $\mathrm{d}n/\mathrm{d}\mu = (1/\pi)\,\mathrm{Im\,tr}[\mu - H_{\rm dot} + i\pi\nu V^\dagger V]^{-1}$. If, to be specific, 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. We emphasize, however, that our results are not specific to a random-matrix spectrum.

For a weakly coupled dot, we can compute the S-matrix by first diagonalizing the dot Hamiltonian $H_{\rm dot}$. The broadening of the levels can 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 first diagonalize $i\pi\nu V^\dagger V$ and subsequently account for $H_{\rm dot}$ perturbatively. We start by writing $V^\dagger = (\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_N)$ where the $\boldsymbol{v}_i$ are $N_{\rm dot}$-dimensional vectors. In obvious notation, we can then write $\pi\nu V^\dagger V = \pi\nu \sum_{i=1}^N |\boldsymbol{v}_i\rangle\langle\boldsymbol{v}_i|$ 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 non-zero 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 imaginary eigenvalues which lead to an extremely broad background (since $\lambda \sim N_{\rm dot}$) in the local DOS.

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

$$\Delta e_i \simeq \sum_{\ell=1}^{N} \frac{|\langle i|H_{\rm dot}|\ell\rangle|^2}{-i\lambda_\ell} \sim i\frac{N\Delta^2}{\pi^2\nu v^2} \sim i\frac{N^2\Delta^2}{\pi\Gamma}\,. \tag{6}$$

Here, we used that $H_{\rm dot}$ is a random-matrix Hamiltonian and defined the golden-rule width $\Gamma = \pi\nu N v^2$ of the eigenstates ϵ_i 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 DOS 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.

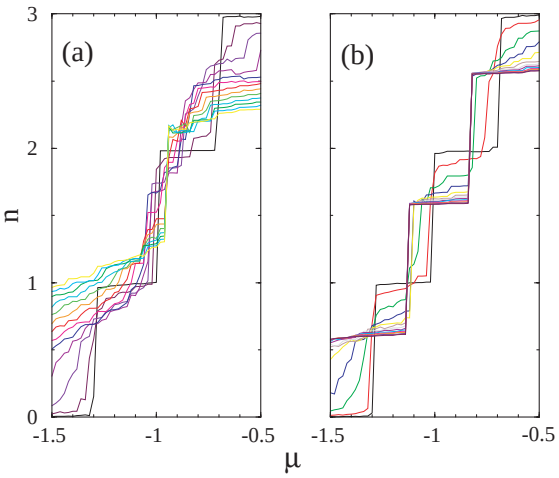

Fig. 2 – The occupation n as a function of the chemical potential for $N_{\rm dot} = 3$ and $N = 2$. The dot levels have energies $\epsilon_1 = -1.3t$, $\epsilon_2 = -1.2t$, and $\epsilon_3 = -1.1t$. The interaction $U = 0.2t$. In (a) the couplings are $V_{11} = 0.05pt$, $V_{12} = 0.09pt$, $V_{13} =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

We now turn to the influence of the charging energy U. We compute the ground state for an interacting dot attached to several 1D leads using an extension of a DMRG method developed for a single 1D lead connected to a dot [13] 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 [14]. The main difference is that in every iteration a site is added to each of the leads. Figure 2 shows the occupation number n as a function of μ for a $N_{\rm dot} = 3$ dot attached to two leads for different values of the dot-lead coupling.

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 non-interacting case.

If the couplings are symmetric to all leads, the number of bound states is $N_{\rm dot} - 1$ no matter how many leads 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. Similar Coulomb-blockade behavior at strong coupling has recently been seen for the Kondo system [15].

This behavior can be explained by extending the scattering theory above to include U within the Hartree approximation. This approximation accounts for U by replacing $e_i \to e_i + U \sum_{j \neq i} \langle b_j^\dagger b_j \rangle$, where b_j annihilates an electron in the dot state e_j. The charging of the broad resonances can be neglected as long as we consider chemical potential changes which are small compared to the bandwidth. With this approximation, subsequent resonances are separated by $\Delta + U$.

Remarkably, the behavior changes for very large charging energy $U \gg \pi \nu N_{\rm dot} v^2$, where the superradiant state becomes Coulomb-blockaded. In this regime, we observe numerically that the number of Coulomb-blockade steps equals the number of dot states $N_{\rm dot}$, cf. fig. 3(a). The

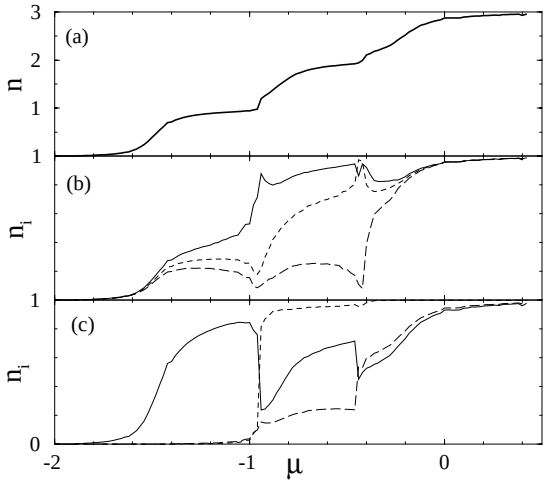

Fig. 3 – Occupations *vs.* μ for $N_{\rm dot} = 3$ ($\epsilon_1 = -1.41t$, $\epsilon_2 = -1.4t$, $\epsilon_3 = -1.39t$) coupled to one lead (all couplings $V = 0.2t$) with strong charging energy $U = 0.6t$. (a) Dot occupation $n = n_1 + n_2 + n_3$. (b) Individual dot-orbital occupations n_1 (full line), n_2 (dashed line), n_3 (long-dashed line). (c) Occupation in the strong-coupling basis: superradiant (full line) and subradiant states (dashed and long-dashed lines).

width of the steps is of order $\pi\nu N_{\rm dot}v^2$, large compared to the step widths of subradiant states at weaker charging energy. Figure 3(b) shows that the charging steps are due to simultaneous charging of all three dot orbitals which leads to an oscillatory structure in the occupations of the dot states. The origin of these oscillations can be traced by considering the occupations of the strong-coupling super- and subradiant states (*i.e.*, the eigenstates of $i\pi\nu V^\dagger V$), as shown in fig. 3(c). Clearly, the origin lies in oscillations in the occupation of the superradiant state which, in this case, is a symmetric superposition of all dot orbitals. At the conductance step, one predominantly charges the superradiant state, while in between steps there is a tendency to exchange occupations between the superradiant and a subradiant state.

To understand this behavior, consider the configuration of the dot when μ takes a value on the charging plateau $n = 1$. In this case, the dot could either charge the superradiant or a subradiant state. In perturbation theory, the dot-lead coupling changes the (many-body) energy of these configurations ($E_{\rm super}$ and $E_{\rm sub}$, respectively) due to virtually exciting an electron from the lead to the superradiant state, if the latter is unoccupied, or by virtually exciting an electron from the dot to the leads, if the superradiant state is occupied. (We neglect virtual processes involving subradiant states since their coupling to the leads is much weaker.) This gives an energy difference $\Delta E = E_{\rm super} - E_{\rm sub} = \frac{W}{2\pi}[\ln(t/|\epsilon + U|) - \ln(t/|\epsilon|)]$ between the two configurations, where ϵ is the energy of the dot state relative to μ and W is the width of the superradiant state. (The single-particle level spacing is neglected here.) Thus, for $|\epsilon| < U/2$ ($|\epsilon| > U/2$) occupying the superradiant (subradiant) state gives the lower energy so that the charging steps are due to charging of the superradiant state, while somewhere on the plateau the occupations of the superradiant and subradiant states are exchanged. The precise location of this switch is affected by the single-particle level spacing of the dot. This mechanism was considered by Silvestrov and Imry in a different context [16].

We close with a discussion of possible experimental realizations. Generically, for a semiconductor quantum dot perfectly coupled to leads by quantum point contacts, in the sense that

there are N perfectly transmitting channels, one finds that $\Gamma \sim N\Delta$, leading to $N^2\Delta/\pi\Gamma \sim N$. This shows that this situation is not in the strong-coupling limit and thus there are no sharp resonances, in agreement with the description of this regime, *e.g.*, in refs. [3, 4].

One situation in which the effect discussed here can be observed is when, by a mesoscopic fluctuation or by symmetry, several dot levels bunch together so that their effective level spacing is much smaller than the average Δ. Alternatively, a situation with an anomalously small Δ can be engineered by a judicious choice of the device. *E.g.*, one can think of a set of n quantum dots with weak interdot tunneling whose energy levels can be manipulated into almost degeneracy by a set of external gates. This realizes a situation with $N_{\rm dot} = n$ and strong coupling $\Gamma \gg N^2\Delta$ to the leads. Finally, one may also think of cases in which leads and "dot" are made from different materials, allowing for an independent manipulation of Γ and Δ. For example, when tunneling through a series of identical impurities or a suitable molecule between metallic electrodes, one expects Γ to be enhanced by the large DOS in the metallic leads.

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