Density matrix renormalization group study of the charging of a quantum dot strongly coupled to a single lead

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A new application of the density matrix renormalization group (DMRG) method to a system composed of an interacting dot coupled to a infinite one dimensional lead is presented. This method enables one to study the influence of the coupling to an external lead on the thermodynamical properties of the dot. It is shown that this method reproduces known results for a non-interacting dot coupled to a lead, i.e., that for strong coupling discrete states remain in the dot. We show that these states are robust and do not disappear once interactions in the dot are considered. Moreover, due to these discrete states, Coulomb blockade affects the charging of the dot even though its strongly coupled to a lead.

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INTRODUCTION

Recently there has been much in the influence of the dot-lead couplings on the properties of a quantum dot. Once the dot is strongly coupled to the lead a suppression of the Coulomb blockade is predicted \[1\], arising from the fact that the number of electrons in the dot is no longer a good quantum number. Nevertheless, a weak remnant of the Coulomb blockade physics persists even for strong coupling \[2\].

Surprisingly, the details of the couplings to the lead play a very important role in determining the properties of the dot. König, Gefen and Schön \[3\] have shown analytically that the tunnelling density of states of a non-interacting two orbital dot strongly coupled to a single lead contains a delta like peak. Such a feature indicates that a well defined localized state remains in the dot although the dot is strongly connected to the lead. Thus, if one measures the number of electrons in the dot as function of the chemical potential or gate voltage, one will observe sharp jumps once the chemical potential crosses the localized state energy. Once two leads are connected to a two orbital dot \[4\], a delta like peak in the density of states of the dot exists if the lead-dot coupling matrix elements are of equal signs, while no such feature is predicted if one of the matrix elements is of opposite sign. When the dot contains \(N_{\text{Dot}}\) orbitals connected to a single lead, \(N_{\text{Dot}} - 1\) delta like peaks appear in the tunnelling density of states \[5\].

The situation for interacting dots has not been studied, although it was argued that the delta like peaks will not be suppressed by interactions \[4\].

Several numerical methods, especially exact diagonalization \[6\], self consistent Hartree-Fock \[7, 8, 9\] and density-functional approaches \[10, 11\], have proven themselves to be a very useful tool in studying the properties of interacting quantum dots \[12\]. Unfortunately, none of these methods is appropriate for the study of the strong lead-dot coupling regime. Exact diagonalization methods are limited by the size of the Hilbert space. Although one may consider a non-interacting lead, due to the coupling with the interacting dot the whole system (dot + lead) must be treated via the full many particle states. This will create an exponentially large Hilbert space even for a moderate sized lead. Taking into account that the density of states in the lead must be much larger than in the dot, its clear that exact diagonalization is not a viable option. The treatment of larger leads using self consistent Hartree-Fock is possible, but at the price of using an uncontrollable approximation which might lose important many body effects. Functional density methods are not suitable for the treatment of steep potential gradients of the type expected close to the dot-lead interface. Thus, a new numerical approach is needed.

In this paper we shall use the density matrix renormalization group method (DMRG) \[13\] in order to treat a single one dimensional lead connected to a dot with \(N_{\text{Dot}}\) orbitals. We shall begin by describing the DMRG treatment of the lead-dot system. We shall first review several features of the occupation of the orbitals as function of the chemical potential for the non-interacting case \[3, 4, 5\]. Finally, we shall establish that for an interacting dot all the \(N_{\text{Dot}} - 1\) states localized on the dot show full Coulomb blockade behavior in the limit of strong coupling.

The paper is organized as follows: The second section contains the definition of the dot-lead model. In the third section we describe the details of the DMRG method developed for the calculation. The orbital occupation as function of the chemical potential for the non-interacting and interacting dots is studied in the forth section. The results are discussed in the last section.

MODEL

The system which is discussed in this paper is a quantum dot connected to a one dimensional lead. The elec-
trons are treated as spinless electrons. The quantum dot is represented by the following Hamiltonian:

$$H_{QD} = \sum_{i=1}^{N_{Dot}} (\varepsilon_i - V_g) a_i^\dagger a_i + U \sum_{i>j} a_i^\dagger a_j^\dagger a_j a_i.$$  \hfill (1)

Here $a_i^\dagger$ depicts the creation operator of an electron on the i-th orbital in the dot, $\varepsilon_i$ corresponds to the energy of the orbital, $N_{Dot}$ is the number of orbitals, and $U = e^2/C$, where $C$ is the capacitance of the dot. The influence of an external gate coupled to the dot is taken into account via $V_g$. The one dimensional lead corresponds to:

$$H_{Lead} = -t \sum_{j=1}^{\infty} c_j^\dagger c_{j+1} + h.c,$$  \hfill (2)

where $c_j^\dagger$ is the creation operator of an electron on the j-th site of the lead, and $t$ is the hopping matrix in the lead. For an infinite lead with no coupling to the dot this will result in a lead with a band width of $4t$. The tunnelling between the dot and the lead is represented by:

$$H_{DL} = \sum_{i=1}^{N_{Dot}} V_i a_i^\dagger c_1 + h.c,$$  \hfill (3)

where the dot is assumed to be attached to the edge of the lead, and the tunnelling amplitude between the i-th orbital in the dot and the lead is given by $V_i$.

Since the lead is assumed to be infinite one can not assign a fixed number of electrons in the system, as is customary in exact diagonalization studies of interacting fermionic systems. The number of electrons in our system is determined by the chemical potential $\mu$. Thus, the Hamiltonian of the dot-lead system is governed by:

$$H = H_{Dot} + H_{Lead} + H_{DL} - \mu \left( \sum_{i=1}^{N_{Dot}} a_i^\dagger a_i + \sum_{j=1}^{\infty} c_j^\dagger c_j \right).$$  \hfill (4)

Since we are interested in the number of electrons residing in the dot at a given chemical potential $\mu$ (or at a particular gate voltage $V_g$ for a given $\mu$) at zero temperature, we must calculate the ground state eigenvector of $H$. In the next section we shall discuss the numerical methods we use to calculate this quantity.

**NUMERICAL METHOD**

As long as there are no interactions in the system (i.e., $U = 0$ in the dot) the main obstacle for obtaining the ground state of $H$ (Eq. 4) is the infinite span of the lead. But since we are really interested in the number of electrons in the dot, one may expect that as long as level broadening of the orbitals in the dot (roughly proportional to $\pi \nu |V_i|^2$ for weak coupling, where $\nu$ is the local density of states in the lead) is much larger than the level spacing within the lead, the finite lead treatment of the system is accurate. Thus, replacing the infinite lead by a finite one with $N$ sites makes sense as long as $N \gg (4t/V_i)^2$ (where $\nu = 1/4t$) taking a finite lead coupled to the dot we can exactly diagonalize $H$ and obtain the ground state for any value of $\mu$ of $V_g$. The situation is much more difficult when interactions in the dot are taken into account. Exact diagonalization is out of questions, since the size of the Hilbert space grows exponentially as function of the number of sites in the lead. We will use the DMRG method [12] to treat the system. This method is usually used for one dimensional interacting system and the resulting ground state is as accurate as the one obtained from exact diagonalization.

In order to incorporate the dot into the DMRG method we propose the following procedure: First we create a block composed of the dot and the first site of the lead,

$$H_B = H_{Dot} + H_{DL} - \mu \left( \sum_{i=1}^{N_{Dot}} a_i^\dagger a_i + c_1^\dagger c_1 \right).$$  \hfill (5)

and exactly diagonalize it. Then we begin an iteration process. An additional site (in the first iteration $j = 2$) is added to the lead, and the Hamiltonian is given by:

$$H_{B\bullet} = H_B + c_{j-1}^\dagger c_j + h.c - \mu c_j^\dagger c_j.$$  \hfill (6)

Then a superblock Hamiltonian $H_{B\bullet\bullet R}$ is formed by joining $H_{B\bullet}$ to its mirror image $H_{B\bullet R}$ (see Fig. 1), resulting in

$$H_{B\bullet\bullet R} = H_{B\bullet} + c_j^\dagger c_j^R + h.c + H_{B\bullet R},$$  \hfill (7)

where $j^R$ is the index of the mirror image lead. The ground state $\Psi(B\bullet\bullet R)$, which is a function of the superblock coordinates is calculated by the Lanczos method. Using this ground state a density matrix, 

$$\rho(B\bullet) = \sum_{B\bullet R} \Psi(B\bullet\bullet R)\Psi^\dagger(B\bullet\bullet R),$$  \hfill (8)

is formed (the trace is over the coordinates of the mirror reflection part of the Hamiltonian $H_{B\bullet\bullet B}$). The density matrix is diagonalized and only half of the states with the largest eigenvalues are retained as a truncated basis. A new block Hamiltonian $H_B$ is formed by projecting $H_{B\bullet}$ onto the truncated basis. Also other relevant operators, such as $a_i^\dagger$, are rewritten in terms of the truncated basis. The new $H_B$ now replaces the one given in Eq. 4 in a new iteration cycle. These iteration continue until a satisfactory accuracy is obtained for the occupation of the orbitals in the dot.
RESULTS

Non interacting dot

We shall begin by considering the behavior of a non-interacting dot coupled to a one dimensional lead. We are interested in the behavior of the orbital occupation in the dot as function of the chemical potential $\mu$ or the gate voltage $V_g$. As discussed in the previous section, we shall use numerical exact diagonalization in order to obtain the single electron eigenvectors $\phi_k$ and eigenvalues $\epsilon_k$ of the finite lead coupled to a dot system, i.e. of $H$ as given in Eq. (4). The dot’s $i$-th orbital occupation, $n_i$, as function of the chemical potential, is defined in the following way:

$$n_i = \sum_k |\langle \phi_k | a_i^\dagger a_i | \phi_k \rangle|^2 \theta(\mu - \epsilon_k).$$ (9)

In Fig. 2, typical results for $n_i(\mu)$ as function of the coupling (a) $V_1 = V_2 = V$ and (b) $V_1 = 2V_2 = V$ for a two orbital dot are presented. As expected, for small values of $V$, $n_i$ shows a jump at $\epsilon_i$, and this jump becomes less sharp as $V$ increases. One might expect that for an increasing $V$, any signature of the original orbitals in the dot will be washed out. Nevertheless, quite surprisingly, that is not the case and as $V$ increases a new jump in both $n_1$ and $n_2$ appears for a value of $\mu$ in between to original orbital energies $\epsilon_1$ and $\epsilon_2$. The sum of the jumps in the occupation of both orbital is equal to one for large $V$, i.e., although the dot is strongly coupled to the lead, a state which contains a single electron remains localized in the dot. Such a behavior was indeed predicted in Ref. 3, where the tunnelling density of states for a non interacting two level system coupled to a lead was calculated. They show that for strong coupling the tunnelling density of states acquires a sharp peak at an energy between the two levels, on the background of a very wide peak. This behavior is reproduced when $\mu$ is kept constant but the gate voltage coupled to the dot $V_g$ is changed.

As can be seen in Fig. 2, the location in $\mu$-space of the localized state depends on the ratio of $V_1$ to $V_2$. This location may be calculated using the following three state
Hamiltonian:

\[ H_{\text{level}} = \begin{pmatrix} \varepsilon_1 & 0 & V_1 \\ 0 & \varepsilon_2 & V_2 \\ V_1 & V_2 & 0 \end{pmatrix}, \]

which takes into account the effect of the lead by a single site that is strongly coupled to both orbitals. At the limit of large coupling, \( H_{\text{level}} \) has two eigenvalues at \( \pm \sqrt{V_1^2 + V_2^2} \), and (assuming \( V_1 > V_2 \)) a third at

\[ \tilde{\varepsilon} = \varepsilon_2 + \frac{\varepsilon_1 - \varepsilon_2}{\left( \frac{V_1}{V_2} \right)^2 + 1}. \]

The eigenvector of this state is composed exclusively from the two dot orbitals, and the eigenvalue \( \tilde{\varepsilon} \) corresponds to the location of the jump in the orbital occupation seen in Fig. 2. Thus, at the limit of strong coupling, the details of the lead are not important in determining the energy of the localized state on the dot, which can be adequately predicted by coupling of all orbitals to a single external orbital [14]. This behavior is not limited to a two orbital dot [5]. For any number of orbitals \( N_{\text{Dot}} \) in a dot that are strongly coupled to the lead, the location of the \( N_{\text{Dot}} - 1 \) jumps in the orbital occupation may be estimated by calculating the eigenvalues of an \( N_{\text{Dot}} + 1 \) matrix:

\[ \begin{pmatrix} \varepsilon_1 & 0 & 0 & V_1 \\ 0 & \varepsilon_2 & 0 & V_2 \\ 0 & 0 & \varepsilon_2 & V_3 \\ \vdots & \vdots & \vdots & \vdots \\ V_1 & V_2 & V_3 & 0 \end{pmatrix}. \]

This is shown in Fig. 3 where the derivative of the total orbital occupation as function of the chemical potential \( \partial n/\partial \mu \) (where \( n = \sum_i n_i \)) for a dot with ten orbitals is compared with the eigenvalues of the matrix given in Eq. (12). An excellent correspondence for the position of the \( N_{\text{Dot}} - 1 \) peaks of \( \partial n/\partial \mu \) and the position of the intermediate \( N_{\text{Dot}} - 1 \) eigenvalues of Eq. (12) is obtained.

In the following section we shall discuss the role of interactions in determining the orbital occupation of the dot. As previously discussed, for the interacting case we must use the DMRG method. It would be interesting nevertheless to compare the results of the DMRG approach to exact diagonalization results. This, of course, is only possible for non-interacting systems. An example of the comparisons we performed are presented in Fig. 4 where the block size \( (H_B) \) was chosen to be 32 states, resulting in the maximum matrix size \( H_{B \bullet B^\mu} \) of 4,096. The iterative process continued until the occupation of the levels in the dot changed by no more than \( 10^{-3} \) for three consecutive iterations. The correspondence between the exact diagonalization results and the DMRG ones at the tails of the jumps is perfect. At the immediate vicinity of the jump there is a slight difference between the two methods. We shall return to the behavior of the DMRG in the immediate vicinity of the jump in the next section.

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**FIG. 3:** The derivative of the total orbital occupation \( \partial n/\partial \mu \) as function of \( \mu \) for a dot with \( N_{\text{Dot}} = 10 \) described by a random matrix Hamiltonian and random coupling \( V_i \) between the dot and lead. The dashed lines correspond to the case where \( V_i = 0 \), the line corresponds to an average value of the coupling \( \langle V_i \rangle = 0.4t \), and the dotted line indicates the position of the eigenvalues of Eq. (12).

**FIG. 4:** The orbital occupation \( n_1 \) (full lines, circles) and \( n_2 \) (dotted lines, squares) of a two orbital dot coupled to a one dimensional lead as function of \( \mu \) for different values of the couplings \( V_1 = V_2 = 0.05t, 0.3t, 0.55t, 0.8t \). The lines correspond to the DMRG results while the symbols correspond to the exact diagonalization results.
Interacting dot

In this section we shall concentrate on the influence of electron-electron interaction in the dot on the occupation of levels in the dot coupled to a lead. For weak interactions we expect the usual Coulomb blockade behavior, i.e., the position of the jump in occupation of the j-th orbital (ordered according to \( \varepsilon_1 < \varepsilon_2 < \ldots < \varepsilon_{N_{\text{dot}}} \)) should occur at \( \mu = \varepsilon_j + (j - 1)U \). Once the coupling with the lead becomes strong enough, it is not clear what influence the interactions will have on the existence of the localized states in the dot discussed in the previous section.

Let us begin by discussing the role of interactions on a two orbital dot \((\varepsilon_1 = -1.1t, \varepsilon_2 = -0.9t)\). The orbital occupations for weak \((U = 0.1t)\), intermediate \((U = 0.2t)\) and strong \((U = 0.4t)\) interactions are presented in Fig. 5. The main feature of the non-interacting behavior, i.e., that at the limit of strong coupling between dot and lead a state which contains a single electron remains localized in the dot (Fig. 2), persists in the interacting case. The energy of the localized state corresponds to \((\varepsilon_2 + \varepsilon_1)/2 + f(U)\), where \(f(U)\) depends on the change in occupation of both orbitals as the localized state is filled. For \(V_1 = V_2\) one can see that \(f(U) \sim U/2\), but we shall analyze \(f(U)\) in detail in the next paragraph. Another interesting feature of interactions can be seen even for moderate values of \(V_i\). The orbital occupation of the second orbital \(n_2\), which is partially filled for low values of \(\mu\) depopulate once a jump occurs in \(n_1\). This is an obvious response to the interaction between the two levels.

Although it is not possible to directly compare the DMRG results for the interacting case to an exact calculation, one can nevertheless gain some insight into the reliability of the method by checking its sensitivity to a change in the block size. In Fig. 6 the DMRG results for a two orbital dot in which a block size of 16 states is compared with a block size of 32 states. Perfect correspondence between both sizes is seen at the at the tails of the jumps, while small deviations are seen in the immediate vicinity of the jump. This is very similar to the situation for the non-interacting case (Fig. 4). Thus, the DMRG seems to be somewhat less accurate in the description of the dot occupation in the immediate vicinity of a steep jump in occupation.

In order to clarify the role played by the interaction and coupling in determining \(f(U)\), we begin by analyzing the case for which \(V_2 = 0\), i.e., the second orbital is disconnected from the lead. Under such conditions the second orbital may acquire only two values \(n_2 = 0\) or \(n_2 = 1\). Naively one expects that the second orbital will be filled once \(Un_1(\mu) < \mu - \varepsilon_2\). This is indeed the case, but as can be seen in Fig. 7, \(n_1(\mu)\) is not a monotonous function of \(\mu\), since once the second orbital is populated, there is a reduction in the occupation of the first orbital.

**FIG. 5:** The orbital occupation \(n_1\) (full lines) and \(n_2\) (dotted lines) of a two orbital interacting dot coupled to a one dimensional lead as function of \(\mu\) for (a) \(U = 0.1t\); (b) \(U = 0.2t\); (c) \(U = 0.4t\). The couplings \(V_1 = V_2 = 0.05t, 0.1t, \ldots t\). Inset: the total orbital occupation \(n = n_1 + n_2\) as function of \(\mu\).
Therefore, the condition for the population of the second must be rewritten as $U n_1(\mu^+) < \mu^+ - \varepsilon_2$, where $\mu^+$ is the chemical potential just above the jump. Of course, once the coupling $V_1$ is strong enough to completely localize the remaining resonance, then $n_1(\mu^+) = n_1(\mu^-) = 1/2$ and the second orbital will populate at $\mu = \varepsilon_2 + U/2$. The situation becomes more complicated once $V_2 \neq 0$. The additional charging energy due to the population of the localized state is proportional to $U(n_1(\mu^+) - n_1(\mu^-))(n_2(\mu^+) - n_2(\mu^-))$, which must be smaller than $\mu - \tilde{\varepsilon}$ in the limit of strong coupling.

As might be expected, the situation is similar for dots with a higher number of orbitals. A three orbital dot is depicted in Fig. 9. The orbitals have energies $\varepsilon_1 = -1.1$, $\varepsilon_2 = -1$, $\varepsilon_3 = -0.9$, and the interaction $U = 0.2$. In Fig. 9 a four orbital dot, with energies $\varepsilon_1 = -1.2$, $\varepsilon_2 = -1.1$, $\varepsilon_3 = -1$, $\varepsilon_4 = -0.9$, and interaction $U = 0.1$ is shown. In both cases there is a transition from $N_{\text{Dot}}$ jumps in the occupation of the dot for weak couplings to $N_{\text{Dot}} - 1$ jumps for strong couplings. The jumps in the strong coupling regime are separated by $U + \Delta$ ($\Delta$ is the orbital spacing) as in the regular Coulomb blockade case [12]. The suppression of the the occupation of higher orbitals as lower ones become occupied is also evident. Thus, the Coulomb blockade behavior between the resonances which remain localized on the dot continues although the dot is well connected to the external lead.

As we have seen in the previous section, the DMRG method enables us to calculate the charging of a dot as function of the chemical potential for the whole span of coupling strength. Contrary to intuition, strong coupling to a single one dimensional lead does not remove all discrete features from the dot, as was discussed in Refs. [3, 4, 5]. This conclusion remains valid also for a dot in which interactions between electrons are taken into account. These interactions manifest themselves as Coulomb blockade steps in the filling of the dot.

This paper concentrated on developing the DMRG numerical method and examining the role of interaction at the strong coupling limit. Several important questions remain open. The crossover from the weak coupling to the strong coupling regime should be quantified, and its dependence on the level spacing in the dot and the interaction studied. This is especially important since Ref. [1], which essentially treats the intermediate values of coupling, sees no pronounced discrete features in the dot. Thus, one may speculate that an intermediate regime of coupling, for which discrete features in the dot are suppressed, exists between the weak and strong coupling regimes in which these features are pronounced. Hints of this intermediate regime might be seen in Figs. 6 and 7 for $V_1 \sim 0.2$, but this warrants further study. The influence of the dimensionality of the lead, the number of channels in the lead and the number of leads should be clarified. The DMRG method presented in this pa-
FIG. 8: The orbital occupation $n_1$ (full lines), $n_2$ (dotted lines), and $n_3$ (dashed lines) of a three orbital interacting dot ($U = 0.2t$) coupled to a one dimensional lead as function of $\mu$. The couplings $V_1 = V_2 = V_3 = 0.05t, 0.1t, \ldots, 0.6t$. Inset: the total orbital occupation $n = n_1 + n_2 + n_3$ as function of $\mu$.

per could, in principal, be expanded to deal with several one-dimensional leads, and probably also to quasi-one dimensional leads. Thus, by expanding the methods introduced here, it may be possible to answer open questions regarding the dot-lead coupling.

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