Nonlinear Transport through Coupled Double Quantum Dot Systems

R. KOTLYAR and S. DAS SARMA
Department of Physics, University of Maryland, College Park, Maryland 20742-4111
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Abstract

We investigate sequential tunneling transport through a semiconductor double quantum dot structure by combining a simple microscopic quantum confinement model with a Mott-Hubbard type correlation model. We calculate nonperturbatively the evolution of the Coulomb blockade oscillations as a function of the interdot barrier conductance, obtaining good qualitative agreement with the experimental data over the whole tunneling regime from the weak-coupling individual dot to the strong-coupling coherent double-dot molecular system.

73.20.Dx, 71.45.-d, 73.40.Gk
By tuning the tunnel barrier between the individual dots of a voltage-biased semiconductor double quantum dot system, it has recently been possible\textsuperscript{1} to observe the formation of an artificial double-dot molecule (with each dot as its atomic constituents) in Coulomb blockade transport experiments.\textsuperscript{2–3} As the interdot tunneling is increased, the series of linear conductance peaks of the two individual near-identical dots\textsuperscript{1–3} changes continuously to a series of split peaks which then form a well-defined Coulomb blockade oscillation series with twice the individual Coulomb blockade period. This period doubling transition in the Coulomb blockade oscillations closely follows the energetics of the transition of two fully isolated dots into a single composite dot due to enhanced interdot tunneling. This transition raises important general questions on how the parameters which can be uniquely defined for the isolated system would renormalize in the transparent composite system. For example, to add an electron to a single dot requires energy in excess of the intradot interaction energy $u_{11}$. For two isolated dots in series in a double-dot system, supplying the required energy $u_{11}$ corresponds to the addition of one electron to each of the dots. With the increased ‘transparency’ of the system due to enhanced tunneling, the energy $u_{11}$ required to add an electron changes as the doubling in the periodicity of the linear conductance Coulomb peaks demonstrates. The pertinent theoretical question is how to characterize the increase of the ‘transparency’ of the composite system. The classical capacitive charging model attributes this transition to the interdot electrostatic coupling energy $u_{12}$. In this model each dot is considered to contain an integer number of electrons. The splitting of the individual Coulomb blockade peak is proportional to the interdot coupling $u_{12}$. The saturation of the splitting in the strong coupling limit is explained by the increase of $u_{12}$ to the value of $u_{11}/2$ with all the other system parameters assumed to be constant.\textsuperscript{4} The energy $u_{12}$ is taken to arise from the capacitive coupling between the two dots, which is classically determined by the fixed geometrical arrangement of the dots. Thus, within the classical capacitive charging model the fixed geometrical arrangement of the two dots in the experimental system provides no physical reason for the increase of $u_{12}$ necessary to account for the saturation of the observed peak splitting. It has also been noted\textsuperscript{5} that the classical capacitance values needed to quantitatively explain the observed peak splitting are unphysically high.

A recent fully quantum theory\textsuperscript{6,7} of charge fluctuations between the two dots formulates the double-dot problem in terms of the dimensionless interdot conductance
per tunneling channel \( g = G_{\text{int}}/(N_{\text{ch}}e^2/h) \) and the number of interdot tunneling channels \( N_{\text{ch}} \). In the limit of the tunneling bandwidth being much larger than the intradot charging energy, each dot is treated as an infinite charge reservoir for the other dot. A perturbation analysis in \( g \) or in \((1 - g)\) reproduces the weak and strong interdot coupling limits of the peak splitting. This elegant perturbative analysis does not apply in the intermediate regime where \( 0 \ll g \ll 1 \). The charge fluctuation perturbation analysis has not yet been extended to the nonlinear transport regime, which is one focus of our work.

In this paper we study the transition from degenerate one dot Coulomb blockade oscillation to the coherent molecular double-dot oscillation by using a 2-site generalized Mott-Hubbard model within an extremely simple physically motivated microscopic confinement potential describing the double-dot system. A Hubbard-type model of linear transport through the single-particle states of quantum dots\(^6\) predicts the distinct phases in the conductance pattern characterized by an increase of the interdot tunneling strength \( t \). In the strong tunneling limit the Mott-Hubbard insulator-metal transition opens a transmission channel through an array of quantum dots\(^6\). This transition is equivalent to the formation of a single composite coherent molecular system with a concomitant doubling of Coulomb blockade periodicity. To characterize the dependence of the Hubbard model parameters on the value of the interdot conductance \( g \), we use a simple phenomenological step-well model for the confinement potential profile of the double-dot system. We obtain the exact Hubbard model predictions for the zero-bias voltage limit current peak splitting and the threshold voltage for the onset of conduction through the double-dot with 1 and 2 excess electrons.

The capacitive model of the experimental circuit configuration for the double-dot system\(^1\) is shown in Fig. 1. We consider a symmetrical configuration of two identical GaAs dots with the same electrostatic couplings to the common back gate and to the bias leads, i.e. \( C_{g1} = C_{g2} = C_g \), \( C_1 = C_2 = C \), \( V_{g1} = V_{g2} = V_g \), and common self-capacitances \( C_0 \). The interdot capacitor with the capacitance \( C_{\text{int}} \) provides the electrostatic coupling between the two dots. Following the experiments, we set an asymmetric bias across the system, i.e. \( V_1 = V, V_2 = 0 \). We express the electrostatic part of the free energy of the system using the classical capacitance matrix\(^9\) formalism. In the usual final step of going into the quantum-mechanical description we replace the classical excess charge on a dot by the charge density operator. Then the operator
of the electrostatic free energy of the coupled system of the double-dot and leads is
\[ F^e = u_{11}(\hat{N}_1^2 + \hat{N}_2^2) + u_{12}\hat{N}_1\hat{N}_2 + eV(x_{b1}\hat{N}_1 + x_{b2}\hat{N}_2) + eV_g(x_g\hat{N}_1 + \hat{N}_2). \] (1)

In Eq. (1) the Hubbard parameters are expressed through the elements of the capacitance matrix, i.e.
\[ u_{11} = e^2 C_{\Sigma} \delta, \quad u_{12} = e^2 C_{\text{int}} \delta, \quad x_g = \frac{C_g}{e^2} (2u_{11} + u_{12}), \quad x_{b1} = \frac{C}{e^2} (2u_{11}), \quad x_{b2} = \frac{C}{e^2} (u_{12}), \]
where \( C_{\Sigma} = C_0 + C_g + C \), and \( \delta = C_{\Sigma}^2 - C_{\text{int}}^2 \). The bottom of the conduction band, considered to be the same in all GaAs electrodes in the system, is taken as the reference. Due to quantum confinement in the dot the continuous conduction band for an excess quasiparticle becomes a discrete series of single-particle energy levels \( \varepsilon_\alpha \) where \( \alpha \) denotes the single-particle state including spin. We consider spin-degenerate single-particle levels in the dot. The quasiparticles are allowed to tunnel between the single-particle states in the two dots with the tunneling amplitude \( t_\alpha \). By including the kinetic energy in each dot and the tunneling energy, we write the total free energy operator as
\[ F_0 = F^e + \sum_{i=1,2, \alpha} \varepsilon_{i\alpha} c_{i\alpha}^\dagger c_{i\alpha} - \sum_\alpha (t_\alpha c_{1\alpha}^\dagger c_{2\alpha} + \text{h.c.}). \] (2)

The indices 1, 2 denote the spatial positions of dots, \( \hat{N}_i = \sum_\alpha c_{i\alpha}^\dagger c_{i\alpha} \) is the density operator, where \( c_{i\alpha}^\dagger (c_{i\alpha}) \) is a creation (annihilation) operator for a quasiparticle on the i-th dot in a state \( \alpha \).

The double-dot is isolated from the leads so that it is coupled to them only electrostatically and through (very weak) tunneling matrix elements \( t_{1,2}^{\alpha} \). The conductance of the dot to the leads \( G_{\text{lead}} = 0.02 e^2/h \) (\( << e^2/h \)) is kept constant throughout. (The lead-dot tunneling strengths \( t_{1,2}^{\alpha} \) are estimated to be \( 3 \mu eV \).) The tunneling hybridization energy between the double-dot and the bias leads is treated as a weak perturbation \( H_T \):
\[ H_T^{1,2} = \sum_{k\alpha} (t_{1,2}^{\alpha} c_k^\dagger c_{1,2\alpha} + \text{h.c.}), \] (3)
where the index \( k \) denotes a quasiparticle state in the leads.

Using Eqs. (1)-(3) it is possible to calculate the current through the double-dot system under the assumptions of sequential tunneling and weak coupling to the outside leads, provided that the level separation in the double-dot system is much less than the width of the transmission resonance. We skip the calculational details which follow the corresponding single dot Coulomb blockade formalism (suitably
generalized to the double-dot system). In particular, the Coulomb gap $\Delta V_{\text{gap}}$ and the normalized peak splitting $f$, defined as the ratio of the additional energy needed to increase the number of quasiparticles by one to its maximum (saturation) value are respectively given by (with the total number of particles being 1 or 2)

$$\Delta V_{\text{gap}} = 4 \left[ \frac{(2 - b_2)(u_{11} + \varepsilon_1) - \sqrt{b_1^2(u_{11} + \varepsilon_1)^2 + [(2 - b_2)^2 - b_1^2]t^2}}{[(2 - b_2)^2 - b_1^2]} \right], \quad (4)$$

$$f = \left( u_{11} + u_{12}/2 + 2t - \sqrt{(u_{11} - u_{12}/2)^2 + 2t^2} \right) / (U/2), \quad (5)$$

where $u$ and $t$ are those appearing in the Mott-Hubbard model defined through Eqs. (1) - (3), $U$ is the intradot interaction energy of the isolated dot, $b_1 = x_{b1} - x_{b2}$ and $b_2 = x_{b1} + x_{b2}$. Thus a knowledge of the Mott-Hubbard parameters $u_{11}, u_{12}, t$ etc. allow us to obtain the complete current-voltage characteristics of the double-dot system.

We construct a simple microscopic quantum mechanical model to phenomenologically describe the double-dot system depicted in Fig. 1. Our microscopic confinement model is shown as an inset of Fig. 2. The model uses two identical one dimensional infinite hard wall potential wells to describe the two isolated dots. Each dot is represented by a two-step well (as shown in Fig. 2) with the lower step well of width $a$ representing the intradot interaction energy of the individual dot and the rectangular barrier of potential height $V_b$ and width $d$ representing the (variable) tunnel barrier separating the two dots. When the barrier $V_b$ is large (e.g. $V_b \to \infty$) the tunnel conductance is vanishingly small and the two dot system is in the uncoupled ‘atomic’ limit whereas for small $V_b$ (e.g. $V_b \to 0$) the dimensionless ‘tunnel’ conductance approaches unity and the system is in the composite ‘molecular’ limit. Within our one dimensional confinement model the barrier of height $V_b$ and width $d$ approximates the intradot constriction. Such simple one dimensional potential confinement models have earlier been used to study quantum tunneling characteristics in three dimensional systems. Without any loss of generality we choose $d/a = 0.1$ throughout our calculation – the exact values of $d$ and $a$ are, of course, unknown but the only relevant point for our simple model to be qualitatively meaningful is for $d << a$.

We evaluate the Mott-Hubbard interaction parameters $u_{11}$ and $u_{12}$ by taking the appropriate expectation values of the screened Coulomb interaction using the potential confinement model. (We take the screening length as $220\text{Å}$. ) The short-ranged
part of the Coulomb interaction is assumed unscreened and is approximated by a
delta function potential. This particular way of calculating the intra- and inter-
dot Coulomb interaction energies is obviously not unique, and one can use alternative
definitions for $u_{11}$ and $u_{12}$, which would give somewhat different numerical values.
We feel, however, that within our simple confinement model our physically motivated
definitions for the Mott-Hubbard parameters is reasonable. Similarly, the hopping pa-
parameter $t$ can be defined in several alternative ways within our microscopic model. We
evaluate $t$ as $t = \Delta_{sas}/2$ where $\Delta_{sas}$ is the so-called symmetric-antisymmetric energy
gap between the two lowest single particle energy levels in our model double-well po-
tential. Conduction in the coupled dot system occurs through a single spin-degenerate
quasiparticle state at the ground state energy $\varepsilon_1$ of the potential well. Finally, we need
to evaluate the interdot conductance $g$ within our microscopic model in order to make
direct contact between the experimental and earlier theoretical results and our
model calculations. The interdot conductance $g$ can of course be exactly evaluated for
our simple one dimensional rectangular barrier model of the point contact separating
the two dots. Because of our hard wall potential confinement model, however, the ex-
actly calculated (‘hard’) conductance for a tunnel barrier of height $V_b$ and width $d$ is a
rather poor approximation (even on a qualitative level) for the experimental interdot
point contact conductance. We have, therefore, also employed a ‘soft’ conductance
approximation using a WKB expression, $g \approx \exp\{-2\frac{md^2}{\hbar^2}(V_b - \varepsilon_1)\}^{1/2}$, which we
believe better represents (on a qualitative level) the adiabatic confinement potential
expected in the experimental double-dot system. We find much better qualitative
agreement between our theory and experiment using the ‘soft’ (as against the ‘hard’)
conductance model, which is what we will mostly present in this paper.

Within our highly simplified microscopic model for the double-dot system, the
gate voltage induced lowering of the interdot barrier $V_b$ causes the crossover from
two isolated dots (for large $V_b$) of size ‘$a$’ each separated by a distance ‘$d$’ to a single
composite coherent double-dot of size $2a + d$. Thus a single tunable parameter, $V_b$,
controls the ‘transparency’ of the system and causes the transition. Instead of using
$V_b$ as the control parameter, however, we follow the experimental procedure of using
the interdot tunnel conductance $g$ (determined completely by $V_b$ in the ‘soft’ and
‘hard’ approximations as described above) as the control parameter in depicting our
results. As $V_b$ is tuned all the parameters of our model (e.g. $t$, $\varepsilon_1$, $u_{11}$, $u_{12}$, $g$) vary
as known functions of $V_b$. We fix the individual dot size $a$ ($\approx 350$ nm) using the
value of the intradot interaction energy $u_{11} \approx 230 \mu$eV for the isolated dot.

Our calculated Hubbard model parameters (e.g. $\varepsilon_1$, $t$, $u_{11}$, $u_{12}$) are shown as functions of the corresponding interdot ‘soft’ conductance $g$ in Fig. 2. Although $u_{11}$ and $u_{12}$ approach each other as $g$ increases, the simplicity and the inadequacy of our microscopic model does not produce $u_{11} = u_{12}$ for $g = 1$. This is mainly due to the various approximations used in calculating the overlap integrals for the Coulomb energy. This discrepancy is the most severe quantitative limitation of our model.

In Fig. 3 we show our calculated Coulomb Blockade oscillations for the double-dot system (in the linear regime) for four values of the ‘soft’ interdot conductance $g = .16, .52, .8, \text{ and } .99$ at $T = 87 \text{ mK} (k_B T << u_{11})$. Note that for the sequential tunneling situation considered here, the width of the Coulomb blockade peaks arises entirely from thermal broadening. Our calculated evolution of the Coulomb blockade oscillations from the degenerate single-dot oscillations (at low $g$) through peak splitting (intermediate $g$) to the eventual period doubling (at large $g$) of the Coulomb blockade oscillations is qualitatively similar to experimental observations (cf. Fig. 5 of Ref. 1). To further quantify our results we show in Fig. 4 our calculated normalized peak splitting $f$ (Eq. 5) and the Coulomb gap $\Delta V_{gap}$ (Eq. 4) as functions of the interdot tunnel conductance $g$, both for ‘soft’ and ‘hard’ conductance models. The corresponding experimental data for $f$ show considerable scatter and our results (for the soft model) agree with experiment. The ‘hard’ model, however, disagrees with the experimental results for reasons discussed above. We point out (and this has been alluded to above) that the main quantitative limitation of our model seems to be a weaker (stronger) dependence of both $f$ and $\Delta V_{gap}$ on the tunnel conductance $g$ for small (large) values of $g$ than seen in experiments.

Finally, in Fig. 5 we show for $g = .16, .8 \text{ and } .99$ our calculated nonlinear Coulomb blockade transport characteristics for the double-dot system by plotting the calculated current (in gray scales) as a function of both the source-drain voltage and the gate voltage. Again, our results are in good qualitative agreement with the experimental data with the main quantitative discrepancy arising from the inadequacy in our tunnel conductance value $g$ which is higher than the corresponding experimental result.

In conclusion, using a simple single-parameter ($V_b$) one dimensional microscopic confinement model we calculate nonperturbatively the linear and nonlinear Coulomb
blockade characteristics of a double-dot system as a function of the interdot tunnel conductance. Our results are in reasonable qualitative agreement with the experimental results which is really the best we can hope for given the great simplicity of our model. We can obtain better quantitative agreement with experiment by using additional (e.g. \( d \) and \( a \)) adjustable parameters, but we feel that to be not particularly meaningful within our simple model.

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FIGURES

FIG. 1. The equivalent circuit of the double-dot system under study. The values of the capacitances $C_1 = C_2 = 38 \ aF$. The other parameters are defined in the text.

FIG. 2. Variation of the Hubbard model parameters $u_{11}$, $u_{12}$, $t$, and $\varepsilon_1$ with ‘soft’ interdot conductance $g$. The conductance $g$ is in units of $2e^2/h$. Inset: The step-well model as defined in the text.

FIG. 3. The conductance $g_{dd}$ in units of $e^2/h$ through the double quantum dot system versus the gate voltage $V_g$ for four values of the ‘soft’ interdot conductance $g = .16$, .52, .8, and .99 at $T = 87 \ mK$ in the linear regime ($V_{sd} = 10 \ \mu eV$). The full thermal equilibration in the double dot system is assumed before and after each tunneling event. We use $\varepsilon_2/\varepsilon_1 = 2$, $t_2/t_1 = 1.2$ and $t_2^{12}/t_2^{12} = 1.2$ for the single-particle spin degenerate levels.

FIG. 4. Calculated normalized peak splitting $f$ (Eq. 5) and the Coulomb gap $\Delta V_{gap}$ (Eq. 4) as functions of the interdot tunnel conductance $g$ (top and bottom panels) for ‘soft’ and ‘hard’ (thick lines) conductance models. The dashed lines show the boundaries for the scatter of the experimental data (taken from Fig. 5 of the second paper in Ref.1). The top thin line in the bottom panel shows the Coulomb gap for fixed values of $\Delta V_{gap}$ with $u_{11} = 227 \ \mu eV$ and $u_{12} = .11 \ \mu eV$.

FIG. 5. The nonlinear current $I$ through the double-dot system (at $T = 87 \ mK$) is plotted versus the values of the gate voltage $V_g$ and the bias voltage $V_{sd}$ for three values of the interdot ‘soft’ conductance $g = 0.16$, 0.8, 0.99. The brightest shades in the plots correspond to $I = 59$, 76, 78 pA for the graphs from top to bottom. The states with $N = 0$ to $N = 8$ electrons in the double dot system contribute to $I$ in the shown parameter space.
Figure 1. R. Kotlyar and S. Das Sarma, *Nonlinear Transport through Coupled ...*
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R. KOTLYAR and S. DAS SARMA

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A recent fully quantum theory\textsuperscript{4,5} of charge fluctuations between the two dots formulates the double-dot problem in terms of the dimensionless interdot conductance
per tunneling channel \( g = G_{\text{int}}/(N_{\text{ch}}e^2/h) \) and the number of interdot tunneling channels \( N_{\text{ch}} \). In the limit of the tunneling bandwidth being much larger than the intradot charging energy, each dot is treated as an infinite charge reservoir for the other dot. A perturbation analysis in \( g \) or in \((1-g)\) reproduces the weak and strong interdot coupling limits of the peak splitting. This elegant perturbative analysis does not apply in the intermediate regime where \( 0 << g << 1 \). The charge fluctuation perturbation analysis has not yet been extended to the nonlinear transport regime, which is one focus of our work.

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In Eq. (1) the Hubbard parameters are expressed through the elements of the capacitance matrix, i.e.,

\[ u_{11} = e^2 C_{x_1} / 2, \quad u_{12} = e^2 C_{x_2} / 2, \quad x_g = C_g / e^2 (2u_{11} + u_{12}), \quad x_{b1} = C_g / e^2 (2u_{11}), \quad x_{b2} = C_g / e^2 (u_{12}), \]

where \( C_\Sigma = C_0 + C_g + C \), and \( \delta = C_\Sigma^2 - C_{\text{int}}^2 \). The bottom of the conduction band, considered to be the same in all GaAs electrodes in the system, is taken as the reference. Due to quantum confinement in the dot the continuous conduction band for an excess quasiparticle becomes a discrete series of single-particle energy levels \( \varepsilon_\alpha \) where \( \alpha \) denotes the single-particle state including spin. We consider spin-degenerate single-particle levels in the dot. The quasiparticles are allowed to tunnel between the single-particle states in the two dots with the tunneling amplitude \( t_\alpha \). By including the kinetic energy in each dot and the tunneling energy, we write the total free energy operator as

\[ F_0 = F^e + \sum_{i=1,2} \varepsilon_{i\alpha} c_{i\alpha}^\dagger c_{i\alpha} - \sum_\alpha (t_\alpha c_{1\alpha}^\dagger c_{2\alpha} + h.c.). \] (2)

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\[ H_T^{1,2} = \sum_{k\alpha} (t_{1,2}^{1,2} c_{k1,2\alpha}^\dagger c_{1,2\alpha} + h.c.), \] (3)

where the index \( k \) denotes a quasiparticle state in the leads.

Using Eqs. (1)-(3) it is possible to calculate the current through the double-dot system under the assumptions of sequential tunneling and weak coupling to the outside leads, provided that the level separation in the double-dot system is much less than the width of the transmission resonance. We skip the calculational details which follow the corresponding single dot Coulomb blockade formalism\(^8-10\) (suitably
generalized to the double-dot system). In particular, the Coulomb gap $\Delta V_{\text{gap}}$ and the normalized peak splitting $f$, defined as the ratio of the additional energy needed to increase the number of quasiparticles by one to its maximum (saturation) value are respectively given by (with the total number of particles being 1 or 2)

$$\Delta V_{\text{gap}} = 4 \left[ \frac{(2 - b_2)(u_{11} + \varepsilon_1)}{(2 - b_2)^2} - \sqrt{b_1^2(u_{11} + \varepsilon_1)^2 + [(2 - b_2)^2 - b_1^2]t^2} \right],$$

where $u$ and $t$ are those appearing in the Mott-Hubbard model defined through Eqs. (1) - (3), $U$ is the intradot interaction energy of the isolated dot, $b_1 = x_{b1} - x_{b2}$ and $b_2 = x_{b1} + x_{b2}$. Thus a knowledge of the Mott-Hubbard parameters $u_{11}$, $u_{12}$, $t$ etc. allow us to obtain the complete current-voltage characteristics of the double-dot system.

We construct a simple microscopic quantum mechanical model to phenomenologically describe the double-dot system depicted in Fig. 1. Our microscopic confinement model is shown as an inset of Fig. 2. The model uses two identical one dimensional infinite hard wall potential wells to describe the two isolated dots. Each dot is represented by a two-step well (as shown in Fig. 2) with the lower step well of width $a$ representing the intradot interaction energy of the individual dot and the rectangular barrier of potential height $V_b$ and width $d$ representing the (variable) tunnel barrier separating the two dots. When the barrier $V_b$ is large (e.g. $V_b \to \infty$) the tunnel conductance is vanishingly small and the two dot system is in the uncoupled ‘atomic’ limit whereas for small $V_b$ (e.g. $V_b \to 0$) the dimensionless ‘tunnel’ conductance approaches unity and the system is in the composite ‘molecular’ limit. Within our one dimensional confinement model the barrier of height $V_b$ and width $d$ approximates the intradot constriction. Such simple one dimensional potential confinement models have earlier been used\textsuperscript{11} to study quantum tunneling characteristics in three dimensional systems. Without any loss of generality we choose $d/a = 0.1$ throughout our calculation – the exact values of $d$ and $a$ are, of course, unknown but the only relevant point for our simple model to be qualitatively meaningful is for $d \ll a$.

We evaluate the Mott-Hubbard interaction parameters $u_{11}$ and $u_{12}$ by taking the appropriate expectation values of the screened Coulomb interaction using the potential confinement model. (We take the screening length as $220\text{A}^\circ$.) The short-ranged
part of the Coulomb interaction is assumed unscreened and is approximated by a delta function potential. This particular way of calculating the intra- and inter-dot Coulomb interaction energies is obviously not unique, and one can use alternative definitions for \( u_{11} \) and \( u_{12} \), which would give somewhat different numerical values. We feel, however, that within our simple confinement model our physically motivated definitions for the Mott-Hubbard parameters is reasonable. Similarly, the hopping parameter \( t \) can be defined in several alternative ways within our microscopic model. We evaluate \( t \) as \( t = \Delta_{sas}/2 \) where \( \Delta_{sas} \) is the so-called symmetric-antisymmetric energy gap between the two lowest single particle energy levels in our model double-well potential. Conduction in the coupled dot system occurs through a single spin-degenerate quasiparticle state at the ground state energy \( \varepsilon_1 \) of the potential well. Finally, we need to evaluate the interdot conductance \( g \) within our microscopic model in order to make direct contact between the experimental \(^1\)-\(^3\) (and earlier theoretical \(^4\),\(^5\)) results and our model calculations. The interdot conductance \( g \) can of course be exactly evaluated for our simple one dimensional rectangular barrier model of the point contact separating the two dots. Because of our hard wall potential confinement model, however, the exactly calculated (‘hard’) conductance for a tunnel barrier of height \( V_b \) and width \( d \) is a rather poor approximation (even on a qualitative level) for the experimental interdot point contact conductance. We have, therefore, also employed a ‘soft’ conductance approximation using a WKB expression, \( g \approx \exp\{-2\left[\frac{2a_d^2}{\pi}\left(V_b - \varepsilon_1\right)\right]^{1/2}\} \), which we believe better represents (on a qualitative level) the adiabatic confinement potential expected in the experimental double-dot system. We find much better qualitative agreement between our theory and experiment using the ‘soft’ (as against the ‘hard’) conductance model, which is what we will mostly present in this paper.

Within our highly simplified microscopic model for the double-dot system, the gate voltage induced lowering of the interdot barrier \( V_b \) causes the crossover from two isolated dots (for large \( V_b \)) of size ‘\( a \)’ each separated by a distance ‘\( d \)’ to a single composite coherent double-dot of size \( 2a + d \). Thus a single tunable parameter, \( V_b \), controls the ‘transparency’ of the system and causes the transition. Instead of using \( V_b \) as the control parameter, however, we follow the experimental procedure of using the interdot tunnel conductance \( g \) (determined completely by \( V_b \) in the ‘soft’ and ‘hard’ approximations as described above) as the control parameter in depicting our results. As \( V_b \) is tuned all the parameters of our model (e.g. \( t, \varepsilon_1, u_{11}, u_{12}, g \)) vary as known functions of \( V_b \). We fix the individual dot size \( a \) (\( \approx 350 \) nm) using the
The experimental value of the intradot interaction energy $u_{11} \approx 230 \mu$eV for the isolated dot.

Our calculated Hubbard model parameters (e.g. $\varepsilon_1$, $t$, $u_{11}$, $u_{12}$) are shown as functions of the corresponding interdot ‘soft’ conductance $g$ in Fig. 2. Although $u_{11}$ and $u_{12}$ approach each other as $g$ increases, the simplicity and the inadequacy of our microscopic model does not produce $u_{11} = u_{12}$ for $g = 1$. This is mainly due to the various approximations used in calculating the overlap integrals for the Coulomb energy. This discrepancy is the most severe quantitative limitation of our model.

In Fig. 3 we show our calculated Coulomb Blockade oscillations for the double-dot system (in the linear regime) for four values of the ‘soft’ interdot conductance $g = .16, .52, .8$, and $.99$ at $T = 87$ mK ($k_B T << u_{11}$). Note that for the sequential tunneling situation considered here, the width of the Coulomb blockade peaks arises entirely from thermal broadening. Our calculated evolution of the Coulomb blockade oscillations from the degenerate single-dot oscillations (at low $g$) through peak splitting (intermediate $g$) to the eventual period doubling (at large $g$) of the Coulomb blockade oscillations is qualitatively similar to experimental observations (cf. Fig. 5 of Ref. 1). To further quantify our results we show in Fig. 4 our calculated normalized peak splitting $f$ (Eq. 5) and the Coulomb gap $\Delta V_{\text{gap}}$ (Eq. 4) as functions of the interdot tunnel conductance $g$, both for ‘soft’ and ‘hard’ conductance models. The corresponding experimental data$^1$ for $f$ show considerable scatter and our results (for the soft model) agree with experiment. The ‘hard’ model, however, disagrees with the experimental results for reasons discussed above. We point out (and this has been alluded to above) that the main quantitative limitation of our model seems to be a weaker (stronger) dependence of both $f$ and $\Delta V_{\text{gap}}$ on the tunnel conductance $g$ for small (large) values of $g$ than seen in experiments.

Finally, in Fig. 5 we show for $g = .16, .8$ and $.99$ our calculated nonlinear Coulomb blockade transport characteristics for the double-dot system by plotting the calculated current (in gray scales) as a function of both the source-drain voltage and the gate voltage. Again, our results are in good qualitative agreement with the experimental data$^2$ with the main quantitative discrepancy arising from the inadequacy in our tunnel conductance value $g$ which is higher than the corresponding experimental result.

In conclusion, using a simple single-parameter ($V_b$) one dimensional microscopic confinement model we calculate nonperturbatively the linear and nonlinear Coulomb
blockade characteristics of a double-dot system as a function of the interdot tunnel conductance. Our results are in reasonable qualitative agreement with the experimental results which is really the best we can hope for given the great simplicity of our model. We can obtain better quantitative agreement with experiment by using additional (e.g. $d$ and $a$) adjustable parameters, but we feel that to be not particularly meaningful within our simple model.

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FIGURES

FIG. 1. The equivalent circuit of the double-dot system under study. The values of the capacitances $C_1 = C_2 = 38 \ aF$. The other parameters are defined in the text.

FIG. 2. Variation of the Hubbard model parameters $u_{11}$, $u_{12}$, $t$, and $\varepsilon_1$ with ‘soft’ interdot conductance $g$. The conductance $g$ is in units of $2e^2/h$. Inset: The step-well model as defined in the text.

FIG. 3. The conductance $g_{dd}$ in units of $e^2/h$ through the double quantum dot system versus the gate voltage $V_g$ for four values of the ‘soft’ interdot conductance $g = .16$, .52, .8, and .99 at $T = 87 \ \mu K$ in the linear regime ($V_{sd} = 10 \ \mu eV$). The full thermal equilibration in the double dot system is assumed before and after each tunneling event. We use $\varepsilon_2/\varepsilon_1 = 2$, $t_2/t_1 = 1.2$ and $t_2^{12}/t_1^{12} = 1.2$ for the single-particle spin degenerate levels.

FIG. 4. Calculated normalized peak splitting $f$ (Eq. 5) and the Coulomb gap $\Delta V_{gap}$ (Eq. 4) as functions of the interdot tunnel conductance $g$ (top and bottom panels) for ‘soft’ and ‘hard’ (thick lines) conductance models. The dashed lines show the boundaries for the scatter of the experimental data (taken from Fig. 5 of the second paper in Ref.1). The top thin line in the bottom panel shows the Coulomb gap for fixed values of $\Delta V_{gap}$ with $u_{11} = 227 \ \mu eV$ and $u_{12} = .11 \ \mu eV$.

FIG. 5. The nonlinear current $I$ through the double-dot system (at $T = 87 \ \mu K$) is plotted versus the values of the gate voltage $V_g$ and the bias voltage $V_{SD}$ for three values of the interdot ‘soft’ conductance $g = 0.16$, 0.8, 0.99. The brightest shades in the plots correspond to $I = 59$, 76, 78 pA for the graphs from top to bottom. The states with $N = 0$ to $N = 8$ electrons in the double dot system contribute to $I$ in the shown parameter space.