Single-electron charging and detection in a laterally-coupled quantum dot circuit in the few-electron regime

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(Dated: March 22, 2022)

Abstract

We provide a physical analysis of the charging and detection of the first few electrons in a laterally-coupled GaAs/AlGaAs quantum dot (LCQD) circuit with integrated quantum point contact (QPC) read-out. Our analysis is based on the numerical solution of the Kohn-Sham equation incorporated into a three-dimensional self-consistent scheme for simulating the quantum device. Electronic states and eigenenergy spectra reflecting the particular LCQD confinement shape are obtained as a function of external gate voltages. We also derive the stability diagram for the first few electrons in the device, and obtain excellent agreement with experimental data.

PACS numbers: 73.21.-b, 72.20.My, 73.40.Gk

I. INTRODUCTION

Lateral GaAs/AlGaAs quantum dots (QD’s) are now routinely fabricated with planar technology. Three-dimensional (3D) quantum confinement is achieved, in part, by using the GaAs/AlGaAs semiconductor heterostructures to confine the conduction electrons into a two dimensional electron gas (2DEG) at the interface between the two materials. By placing metal gates on top of such a structure, carrier confinement in other in-plane directions can be realized by energizing the gates that create lateral energy barriers to electrons in the 2DEG. Design of these QD’s, which previously contained tens of electrons, has been improved to operate them in a few-electron regime where the charging of the very first electrons can be observed experimentally. Two quantum dots can be placed adjacent to each other to form a laterally coupled device with both electrostatic and quantum-mechanical coupling between them. Fine variations of the top gate biases change the confinement of each dot, while precise coupling between them through the central gates leads to a fully tunable two-qubit quantum system, which can be used as a building block for quantum computing. Recently, it has been shown that laterally-coupled quantum dots (LCQD) containing a few conduction electrons could be coupled to single charge detectors to form an integrated quantum circuit. The read-out of the charge state in the LCQD is realized by integrating monolithically quantum point contacts (QPC’s) adjacent to each of the QD’s. Each QPC can be calibrated through electrostatic coupling with the dots so that its conductivity changes abruptly once a single-electron charging event occurs in one of the dots. With this sensitive detector, it is then possible to obtain the “stability diagram” that describes the stable charge regimes of the LCQD as a function of the tuning (plunger) gate biases.

This quantum dot circuit has a two-fold advantage: it is possible (i) to scale it to a quantum dot array, (ii) to perform single-quantum sensitivity measurements, both of which are favorable features of a realizable quantum computer.

In this paper we study the properties of the above circuit via numerical simulation that involves the self-consistent solution of coupled Poisson and Kohn-Sham equations discretized on a 3D mesh. In Sec. II we describe the LCQD structure and in Sec. III we present the approach for solving the Kohn-Sham equations in the device environment within the local spin density approximation (LSDA) and express the criterion used to determine the charging events as a function of the applied gate biases. In Sec. IV we present our simulation results of the circuit, including both electrostatic and quantum-mechanical features, the functionality of the QPC’s, and the stability diagram in the few-electron charging regime. Finally, we summarize our work in Sec. V.

II. DOT STRUCTURES

Figure 1(a) shows the top view of the LCQD and QPC gates in the $xy$-plane. Top L-, R-, T- and M-gates are used to define the two coupled-dot region. Among them, the T- and M-gates can also control the cou-
pling between the two dots. The PL- and PR-gates, called the “plungers,” have smaller feature sizes than the other gates and are used for fine tuning the confinement of each dot. The QPC-L and QPC-R gates are associated with the L- and R-gates (via the tips) to form the QPC detectors. Charging paths into the dots (shown by the ovals) from external reservoirs are shown by curved arrows, whereas the QPC currents are shown by straight arrows. Figure 1(b) shows a cross-sectional view of the layer structure in the z-direction. Our model involves four different layers of semiconductor materials (from top to bottom): a 50-Å thick n-type \( (N_D = 1.5 \times 10^{18} \text{ cm}^{-3}) \) GaAs layer, a 650-Å thick n-type \( (N_D = 0.31 \times 10^{18} \text{ cm}^{-3}) \) \( \text{Al}_0.27\text{Ga}_{0.73}\text{As} \) layer, a 200-Å thick undoped \( \text{Al}_0.27\text{Ga}_{0.73}\text{As} \) layer, and a 1610-nm thick p-type \( (N_A = 1.0 \times 10^{15} \text{ cm}^{-3}) \) GaAs layer. The 2DEG is formed at the interface between the undoped \( \text{AlGaAs} \) layer and the lightly p-type doped GaAs layer (900 Å below the top surface).

III. NUMERICAL MODEL

The electron density in the LCQD region is obtained by describing the charge carriers within the density functional theory (DFT) that incorporates many-body effects among particles. In order to take into account the spin dependence of the electron-electron interaction, the Kohn-Sham equations\(^{14}\) for spin-up (\( \uparrow \)) and spin-down (\( \downarrow \)) are solved simultaneously:

\[
H^\uparrow \psi^\uparrow_i(r) = \varepsilon^\uparrow_i \psi^\uparrow_i(r), \\
H^\downarrow \psi^\downarrow_i(r) = \varepsilon^\downarrow_i \psi^\downarrow_i(r).
\]

(1)

Here \( \varepsilon^\uparrow_i \) and \( \varepsilon^\downarrow_i \) are the corresponding eigenenergies and eigenfunctions of the Hamiltonian \( H^\uparrow \);

\[
H^\uparrow = -\frac{\hbar^2}{2m^*} \nabla \left[ \frac{1}{m^*(\mathbf{r})} \nabla \right] - q \phi(r) + \Delta_E + \phi_{xc}^{\uparrow}(n),
\]

(2)

where \( m^*(r) \) is the position dependent effective mass. \( \phi(r) = \phi_{\text{ext}} + \phi_{\text{ion}} + \phi_H \) is the electrostatic potential which consists three parts: \( \phi_{\text{ext}} \) is the potential due to external gate biases, \( \phi_{\text{ion}} \) is the potential resulting from ionized donors and acceptors, and \( \phi_H \) is the Hartree potential accounting for repulsive electron-electron interactions. \( \Delta_E \) is the conduction-band offset between different materials, and \( \phi_{xc}^{\uparrow}(r) \) is the exchange-correlation potential energy for spin-up (\( \uparrow \)) and spin-down (\( \downarrow \)) computed within the local spin density approximation (LSDA) according to Perdew and Wang’s formulation.\(^{15}\) Hence our approach is spin unrestricted by allowing for different orbitals with different spins.

The electron density \( n(r) \) in the LCQD region is

\[
n(r) = n^\uparrow(r) + n^\downarrow(r) = \sum_{i=1}^{N}\left| \psi^\uparrow_i(r) \right|^2 + \sum_{i=1}^{N}\left| \psi^\downarrow_i(r) \right|^2, \]

(3)

where \( N^\uparrow + N^\downarrow = N \) is the total number of electrons in the dots.

The electrostatic potential \( \phi(r) \) is computed by solving Poisson’s equation

\[
\nabla \left[ \varepsilon(r) \nabla \phi(r) \right] = -\rho(r),
\]

(4)

where \( \varepsilon(r) \) is the position-dependent permittivity and \( \rho(r) \) is the total charge density given by

\[
\rho(r) = q \left[ N^+_D(r) - N^-_A(r) + p(r) - n(r) \right].
\]

(5)

Here \( N^+_D(r) \) and \( N^-_A(r) \) are the ionized donor and acceptor concentrations in the relevant device layers, \( p(r) \) is the hole concentration, and \( n(r) \) is the total electron concentration given by Eq. (3) in the QD region, while outside this region the free electron charge is entirely determined by using the semi-classical Thomas-Fermi approximation.\(^{12}\)

We solve Kohn-Sham and Poisson equations self-consistently by finite element method.\(^{11,12}\) Zero normal electric field on lateral and bottom surfaces and Schottky barrier values on the top surface are imposed as boundary conditions for the solution of Poisson equation. Since the quantum dots are much smaller than the physical dimensions of the device, the wavefunctions actually vanish long before reaching the device boundaries. This allows us to embed a local region in the global mesh for solving the Kohn-Sham equations. This local region is chosen large enough to ensure vanishing wavefunctions on its boundaries. A non-uniform 3D grid of 141, 52 and 71 mesh points in the \( x \)-, \( y \)- and \( z \)-directions respectively, is used for solving Poisson equation, while \( 71 \times 45 \times 19 \) grid points are used to discretize the local region where Kohn-Sham wavefunctions are evaluated.

Because the LCQD are weakly coupled to the external reservoirs, we assume that electrons in the dots are completely localized in that region. At equilibrium, and for a given bias, an integer number of electrons \( N \) minimizes the total energy \( E_T \) of the dots. In order to determine \( N \), we use the Slater formula:\(^{10}\)

\[
E_T(N+1) - E_T(N) = \int_0^1 \varepsilon_{\text{LUO}}(n) dn \approx \varepsilon_{\text{LUO}}(1/2) - E_F,
\]

(6)

where \( E_T(N+1), E_T(N) \) are the total energies for \( N+1, N \) electrons in the dots, and \( \varepsilon_{\text{LUO}}(1/2) \) is the eigenenergy of “the lowest unoccupied orbital” with half occupancy. The sign change of the right-hand side of Eq. (6), as a function of the tuning gate voltage, determines the electron occupation in the LCQD. In our simulation, we use a variation of the above rule where charging occurs when \( \varepsilon_{\text{LUO}}(1) - E_F = E_F - \varepsilon_{\text{LUO}}(0) \), which was justified in Ref. 12.

FIG. 1: (a) Layout of the top gates (Light gray areas show the gate pattern for the LCQD and the QPC’s; ovals show the dots; curved arrows show the possible charging current paths; and straight arrows show the QPC currents.). (b) Layers of the heterostructure (not to scale), after Elzerman et al.\(^{2}\)
IV. RESULTS AND DISCUSSIONS

Figures 2 shows the conduction band edge profiles in the $xy$-plane at the 2DEG interface (contour plot, Fig. 2(a)) and in the z-direction (Fig. 2(b)) under the condition $V_L = V_R = V_{\text{QPC-L}} = V_{\text{QPC-R}} = V_m = -0.585$ V, $V_P = -0.9$ V, $V_{PL} = V_{PR} = -0.15$ V (These voltages correspond to point A in Fig. 8.) and zero electrons in the dots. The Fermi level is set at zero throughout the device at the temperature $T = 4$ K. The LCQD region and the QPC region with low equipotential-line density are clearly visible in Fig. 2(a). The outer energy barrier for the LCQD is $\sim 110$ meV whereas the energy barrier between the dots is $\sim 9$ meV. A large negative T gate bias is used to prevent the wavefunctions from leaking into the external reservoirs, which clearly defines the LCQD region. The confinement along the z-direction is achieved by a quasi-triangular shaped well shown in Fig. 2(b), for which the relaxation of the potential to zero-field is not shown at the far end (substrate) of the device. Due to the strong confinement in the triangular well, only the ground state along the z-direction is occupied (the shape of the ground state wavefunction along the z-direction is shown in the inset in Fig. 2(b)). Under the above condition, the wavefunction contour plots in the $xy$-plane at the 2DEG interface are shown in ascending energies for the first eight spin-up ($\uparrow$) eigenstates in Fig. 3. A similar set of wavefunctions is obtained for the spin-down ($\downarrow$) eigenstates (not shown). They are similar to orbitals observed in diatomic molecules: the two columns represent the familiar bonding and anti-bonding state pairs. Notice that the shape of the wavefunctions reflects the shape of the confinement seen in the local minima of the conduction band edge in Fig. 2(a).

In Figure 4(a), we show the variation of the first eight spin-up ($\uparrow$) eigenenergies when the plunger gate bias configuration is changed from the values $V_{PL} = V_{PR} = -0.15$ V to the new values $V_{PL} = -0.15$ V, $V_{PR} = -0.06$ V. The first eight eigenenergies are separated into two groups, one for the right dot (solid lines) and one for the left dot (dashed lines), which are lowered simultaneously as the right plunger gate bias increases. However, the eigenenergies of the right dot decrease more rapidly than those of the left dot because of the proximity of the former to the varying plunger. At $V_{PR} = -0.074$ V, the charging of the first electron (spin-up ($\uparrow$)) occurs in the right dot, which is indicated by a discontinuity of $8.2 \times 10^{-4}$ eV in the variation of the ground state energy level with respect to the right plunger gate bias. At the same gate bias, we also observe a jump of the conduc-

tion band edge in the constriction of the two QPC’s, i.e., $2.6 \times 10^{-6}$ eV for the left QPC and $5.4 \times 10^{-6}$ eV for the right QPC (see Fig. 4(b), where the vertical axis is shifted up by 0.0201 eV for clarity). The up-shift of the conduction band edge in the QPC constriction results from the Coulomb interaction between the electrons in the LCQD and electrons in the QPC’s, which reduces the total charge number in the conduction channel and leads to a discontinuity in the QPC current observed in experiments.[4] Obviously, the right QPC is more sensitive to the single-electron charging because of its proximity with the right dot. On the stability diagram (Fig. 8), this transition is represented by the vertical A to B line with the diamond indicating the charging point for the first electron.

From the eigenenergies variation vs. $V_{PR}$ diagram (Fig. 4(a)), we also observe three “anti-crossing” points between the two different sets of eigenenergy levels, each arising from the distinct QD’s as mentioned above and indicated by arrows in Fig. 4(a), i.e., ($\alpha$) at $V_{PR} \sim -0.09$ V, between the 3rd and 4th excited states; ($\beta$) at $V_{PR} \sim -0.07$ V, between the 3rd and 4th excited states; and ($\gamma$) at $V_{PR} \sim -0.11$ V, between the 5th and 6th excited states. The behavior of the system near the “anti-crossing” points can be further illustrated by examining the evolution of the wavefunctions for the “anti-crossing” levels. “Interchange” of the wavefunctions is clearly observed before and after these points. In Fig. 5, contour plots of the wavefunctions in the $xy$-plane at the 2DEG interface are shown for the three “anti-crossing” points: the 3rd and 4th excited states labeled $\alpha_1$, $\alpha_2$ at $V_{PR} = -0.10$ V and $\alpha'_1$, $\alpha'_2$ at $V_{PR} = -0.08$ V, respectively; the 3rd and 4th excited states labeled $\beta_1$, $\beta_2$ at $V_{PR} = -0.074$ V and $\beta'_1$, $\beta'_2$ at $V_{PR} = -0.06$ V; and the 5th and 6th excited states labeled $\gamma_1$, $\gamma_2$ at $V_{PR} = -0.12$ V and $\gamma'_1$, $\gamma'_2$ at $V_{PR} = -0.10$ V.

The detection of single-electron charging events can also be carried out for the B to C transition in Fig. 8, in which the right plunger gate bias $V_{PR}$ is fixed to be $-0.06$ V while the left plunger gate bias is changed from
charging,
can find another charging path for the first electron
where eigenenergy levels are fully degenerate.
levels for two electrons in the system to a symmetric one
an asymmetric configuration with different eigenenergy
It demonstrates the evolution of the wavefunctions from
charging from one to two electrons, F to G in Fig. 8,
relevant range of plunger gate biases. More interesting
configuration (solid lines) is larger than those in the right
dot (solid lines). In our LSDA approach, the second electron
has the same spin (spin-up (↑)) as the first one as they
are uncorrelated by the height of the coupling barrier.
The corresponding jump of the conduction band edge is
5.6 × 10^{-6} eV for the left QPC and 2.8 × 10^{-6} eV for the
right one. The left QPC is more sensitive to the second
electron charging because it occurs in the left dot. Fig.
7 shows the spin-up (↑) wavefunctions in ascending ener-
gies (from top to bottom) after the charging of the second
electron for two bias conditions, 1) $V_{PL} = -0.08$ V and
2) $V_{PL} = -0.06$ V (for both cases, $V_{PR} = -0.06$ V).
It demonstrates the evolution of the wavefunctions from
an asymmetric configuration with different eigenenergy
levels for two electrons in the system to a symmetric one
where eigenenergy levels are fully degenerate.

Following the same procedure as described above, we
can find another charging path for the first electron
charging, i.e., from point E to F in Fig. 8, and for the
charging from one to two electrons, F to G in Fig. 8,
for distinct stable charge regimes of electrons in the two
dots. On the path E to F ($V_{PL}$ is fixed to $-0.125$ V, $V_{PR}$
is changed from $-0.125$ V to $-0.07$ V), charging hap-
pens for the first electron (spin-up (↑)) in the right dot
at $V_{PR} = -0.082$ V; on the path F to G ($V_{PR}$ is fixed
to $-0.07$ V, $V_{PL}$ is changed from $-0.125$ V to $-0.07$ V),
charging happens for the second electron (spin-up (↑)) in
the left dot at $V_{PL} = -0.092$ V.

We can further interchange the plunger gate biases and
obtain different transitions, i.e., from A to D to C and E
to H to G, as shown in Fig. 8 to realize closed cycles of
charging and discharging paths. These two closed paths
(dashed and dotted lines) are shown in Fig. 8. Each
corner of the two squares is in a different stable charge
state with numbers in the parentheses showing the elec-
tron number in the left and right dots, respectively, e.g.,
(0,1) means zero electron in the left dot and one in the
right dot. On each path, we record the charging points
(diamonds in Fig. 8) and make linear extrapolations be-
tween the two charging points on each two parallel paths,

which leads to four lines crossing at two points (circles in
Fig. 8).

The two crossing points are linked afterwards. Now,
five segments (solid lines in Fig. 8) separate the dia-
gram into four regions to define the stability diagram for
the LCQD system in the few-electron charging regime.
Each region, separated by the solid lines, indicates a sta-
ble charge configuration assumed by the LCQD under a
particular range of plunger gate biases. More interesting
are the two crossing points (circles), called the double-
triple point, occurring at $V_{PL} = V_{PR} = -0.0924$ V
for the three charging states (0,0), (0,1) and (1,0) and
at $V_{PL} = V_{PR} = -0.0847$ V for (0,1), (1,0) and (1,1)
states. We then determine the voltage range of the right
plunger that spans the distance between the double-triple
point to be $\Delta V_{PR} = 7.7$ mV, which is comparable to the
experimental result $\sim 7.4$ mV.

Finally, from the charging diagrams in the few-electron
regime we extract the addition energy for the second
electron charging in the right dot: we determine the $V_{PR}$-
voltage interval on the stability diagram for the (0,1)
configuration (i.e., between the (0,0) configuration and
the (0,2) configuration in the singlet state) to be 0.1 V,
which is in excellent agreement with the experimental re-
sult $\sim 0.1$ V. By linear projection of this $V_{PR}$ interval
from the energy scale, we obtain the addition energy
for charging the second electron, which is 2.5 meV.
By comparing this value to the experimental result of 3.7
meV, we attribute the difference to the fact that our
simulation is performed on a coupled-dot system, while
the experimental result is obtained by grounding one of
the dots where the confinement is stronger in an individ-
ual dot compared to our simulation case.

\textbf{V. CONCLUSION}

We performed numerical simulations of the electro-
static and quantum-mechanical characteristics of a novel
laterally-coupled quantum dot circuit with integrated
quantum point contact read-out. We were able to repro-
duce detailed single-electron charging behavior of the el-
ementary quantum circuit and demonstrate the function-
ality of the QPC’s as single-electron charging detectors.
In particular, we obtained excellent agreement with the

\textbf{FIG. 6:} (a) Eigenenergy spectrum (spin-up (↑) states) (solid
lines: right dot; dashed lines: left dot) and (b) variation of
the conduction band edge in the constriction of the left
and right QPC’s as a function of the left plunger gate bias from
point B to C in Fig. 8 ($V_{PR}$ is fixed to $-0.06$ V; the vertical
axis of Fig. 6(b) is shifted up by 0.0201 eV).

\textbf{FIG. 7:} Evolution of the first eight spin-up (↑) wavefunc-
tions from bias condition 1) $V_{PL} = -0.08$ V to 2) $V_{PL} = -0.06$ V
(for both cases, $V_{PR} = -0.06$ V).

\textbf{FIG. 5:} Wavefunction (for spin-up (↑) states) “interchanges”
at the “anti-crossing” points corresponding to (a) point $\alpha$, (b)
point $\beta$ and (c) point $\gamma$ in Fig. 4(a).
FIG. 8: Stability diagram for the first two charging electrons characterizing the double-triple point (shown by circles).

experiment for the voltage range of the extension of the double-triple point at the (0,0) to (1,1) transition and the addition energy for single-electron charging in the dots, which validates our quantum device modeling approach for simulating efficiently nanoscale qubit circuits.

Acknowledgments

This work is supported by DARPA QUIST program through ARO Grant DAAD 19-01-1-0659. The authors thank D. Melnikov for constructive discussions. L.-X. Zhang thanks R. Ravishankar, S. Barraza-Lopez for their technical assistance.

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