Automatic virtual voltage extraction of a 2×2 array of quantum dots with machine learning

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Spin qubits in quantum dots are a compelling platform for fault-tolerant quantum computing due to the potential to fabricate dense two-dimensional arrays with nearest neighbour couplings, a requirement to implement the surface code. However, due to the proximity of the surface gate electrodes, cross-coupling capacitances can be substantial, making it difficult to control each quantum dot independently. Increasing the number of quantum dots increases the complexity of the calibration process, which becomes impractical to do heuristically. Inspired by recent demonstrations of industrial-grade silicon quantum dot bilinear arrays, we develop a theoretical framework to mitigate the effect of cross-capacitances in 2×2 arrays of quantum dots, that can be directly extended to 2×N arrays. The method is based on extracting the gradients in gate voltage space of different charge transitions in multiple two-dimensional charge stability diagrams to determine the system’s virtual voltages. To automate the process, we train an ensemble of regression models to extract the gradients from a Hough transformation of a stability diagram and validate the algorithm on simulated and experimental data of a 2×2 quantum dot array. Our method provides a completely automated tool to mitigate the effect of cross capacitances, which could be used to study cross capacitance variability across QDs in large bilinear arrays.

I. INTRODUCTION

Spins in semiconductor quantum dots (QDs) such as those in silicon [1, 2] and most recently germanium [3] are potential platforms to build a large-scale quantum computer due to their high qubit density and ease of integration with current semiconductor fabrication lines [4]. Standard quantum computers will be subject to physical errors that will require quantum error correction protocols to be adopted. The most promising implementation, the surface code [5], enables quantum error correction by distributing logical information over a two-dimensional array of physical qubits with nearest neighbour interactions as long as the individual operations reach a fidelity threshold. The surface code achieves topological protection by increasing the number of physical qubits making scaling up an even greater and pressing challenge. An issue with scaling up is the ability to independently control each QD, due to the presence of mutual and cross capacitances, making it non-trivial to independently control each QD, especially given the variability between devices [6]. A way around this is to apply a combination of voltages that correspond to the eigenvectors perpendicular to electronic transitions, that set the virtual gate space. This method has already been implemented to heuristically tune a linear array of eight GaAs QDs [7] and nine QDs in silicon [8]. However, as the size of the arrays increase, automatic methods to compensate for capacitive cross-coupling will be necessary.

Machine learning has gained popularity to automate different aspects of the tuning protocols in double quantum dots (DQDs). Black box type approaches to coarse tune plunger, barrier and gate voltages to a DQD regime have been developed [9][12], allowing tuning devices using direct current measurements faster than a human expert [13]. Furthermore, convolutional neural networks (CNNs) have been trained to determine the charge state of the device at a particular set of gate voltages [11][14][10]. To extract the gradients, Hough transforms have been implemented on a DQD stability diagram in a known charge state [17], allowing to measure the device in virtual voltage space. The protocols developed thus far have proved that automated tuning of such complex systems via machine learning is possible. However, as
the size of the quantum dot arrays increases, redefined methods that can cope with the increasing parameter complexity need to be developed.

Looking at near-term devices, one-dimensional QD arrays are easier to fabricate \[8\] and should enable the implementation of a logical qubit in a chain of 14 QDs each hosting a spin qubit \[18\]. The performance of such a logical qubit can be improved by using spins in silicon due to their long-coherence time \[19\] \[20\] and high-fidelity gate set \[21\] \[22\]. Furthermore, silicon qubits can be manufactured in industry environments allowing for minimised variability \[23\], integrated with local electronics \[4\] \[24\] \[25\] \[26\] \[27\] \[28\] and operated above 1K \[29\] \[30\]: allowing for larger cooling power. More recently, bilinear arrays of silicon quantum dots based on industry-fabricated split-gate transistors \[31\] \[32\] \[33\] have been produced which should provide additional resources for computing due to their increased connectivity \[23\]. Specifically, by using one chain of the array for local radiofrequency (RF) readout via spin projection of the mirror chain \[36\] \[37\] \[38\], the required depth of the algorithms in Ref. \[18\] should be reduced. For this reason, the problem of accurately controlling and managing cross-couplings in bilinear QD arrays becomes technologically relevant.

In this work, we present an automated method to mitigate gate cross-coupling in 2×2 QD arrays that is extendable to 2×N arrays. We derive an analytical solution of the transformation matrix between real and virtual voltages for the increased connectivity space of a 2×N array of QDs. The equations depend on the gradients in gate voltage space of regions of charge bistability that can be effectively measured using radio-frequency reflectometry \[40\]. We outline a series of measurements to obtain all the required gradients (assuming tunnel rates faster or comparable to the probing radio-frequency). To automate the process, we have developed an algorithm based on Hough transforms that extracts the required gradients from a stability diagram when sweeping two gate voltages at a time. To manage the effect of non-idealities in real data-sets, we train an ensemble of regression models to correctly extract the gradients from the \(\theta\) histogram (where \(\theta\) is the set of angles between the x-axis and the normal to the charge transitions) acquired from the Hough transform of the data-set. Finally, we test the trained model on experimental data of a 2×2 QD array and extract partial virtual voltages.

II. DEVICE ARCHITECTURE

The electrostatic interaction between dots can be modelled in the constant interaction approximation as a network of capacitors consisting of gate \(C_{gi}\) and cross \(C_{ij}\) capacitors, as well as mutual capacitors \(C_{ij}\) that are part of the tunnel barriers. In this work, we concentrate on the 2×2 QD array (see Fig. 1b), since it acts as the basic unit for our virtual voltage extraction in a 2×N array. A device with such characteristics can be found in a silicon nanowire wrapped by split-gates \[33\], as shown in Fig. 1b. QDs are formed on the topmost corners of the nanowire by applying a voltage on the top gates (depicted in blue). In this architecture, there are no barrier gates, which are typically used to control the tunnel barriers. Instead, the cross and mutual capacitances are predetermined by the separation between the gates and the width of the nanowire. If barrier gates were physically present, they would need to be tuned beforehand, for which automatic tuning protocols have been developed \[13\] \[31\]. Such device architecture results in higher connectivity than for a 1D array, giving rise to a complex stability diagram, as highlighted for a 2×2 array in Fig. 1c.

The virtual voltage extraction procedure that we propose relies on being able to detect dot to reservoir charge transitions for different two-dimensional stability diagrams. To read every charge transition efficiently, we envisage that LC resonators are connected along one chain of QDs for dispersive readout \[36\] \[38\] \[39\] \[42\], see Fig. 1. Then the resonators can be measured simultaneously using frequency multiplexing \[43\]. To further increase the signal-to-noise ratio, the signals from adjacent resonators can be added together. In the case where the charge tunnel rates are comparable or faster that the resonator frequencies, all electronic transition will be measurable. Due to the fast readout of RF reflectometry, it is possible to measure multiple 2D projections of such a hyper-dimensional voltage space of 300×300 data points in approximately 30 ms \[42\] \[44\]. Thus, by probing two QDs \(i\) and \(j\) at a time (which we indicate as a superscript), and correctly extracting the gradients \(r_{ij}\) and \(r_{ji}\) of dot to reservoir transitions of QDs \(i\) and \(j\) (subscript), it is possible to construct the transformation matrix \(G\) to move from gate voltage space \(\tilde{V}_g\) to virtual voltage space \(\tilde{U}\).

In Section III, we derive the analytical solution for \(G\) in terms of the different gradients. To automate the process, we develop a protocol to extract the gradients from a stability diagram when sweeping two gate voltages at a time, as outlined in Section IV.

III. 2×N VIRTUAL VOLTAGE SPACE

To model the QD array and gain deeper insight in the effect of cross capacitive coupling in bilinear arrays, we use the Coulomb blockade model outlined by Van der Wiel et all. \[15\]. Treating the array as a network of capacitors the energy \(E\) of a particular charge state is given by:

\[
E = \frac{1}{2} \bar{Q} \cdot C^{-1} \bar{Q}
\]

where \(C\) is the capacitance matrix, which as main diagonal elements has the total capacitance and off-diagonal it has the negative mutual capacitances. \(\bar{Q}\) is the charge on each quantum dot given by:

\[
\bar{Q} = C_c \cdot \bar{V} - \bar{N} e
\]


FIG. 1. a) Network of capacitors of a $2 \times 2$ QD device consisting of gate capacitors $C_{g i}$ and cross capacitors $C_{c i j}$ and mutual capacitors $C_{ij}$ that are part of the tunnel barriers ( ). To simplify the diagram, the cross capacitors between dots that are diagonally across, as well as the tunnel barriers to reservoir have been omitted, but are considered within the model. b) Schematic of a $2 \times 2$ QD device consisting of a nanowire with two pairs of split gates. The QDs form at the topmost corners of the nanowire and are defined by the field effect produced by the top gates (depicted in blue). As a result the gate, cross and mutual capacitors are predefined by the geometry of the device. The source (S) and drain (D) on the nanowire act as the reservoirs. Resonators are placed on QDs two and four for RF reflectometry. c) Theoretical stability diagram whilst applying voltages on QDs two and four ($V_{g1}$ and $V_{g3}$ are set to zero), which are expressed in dimensionless units. The z-axis represents the change in probability for a transition to occur due to a change in gate voltage. The capacitances used to model the stability diagram can be found in Appendix C. The reference charge * on the bottom left of the stability diagram corresponds to $\left( \begin{array}{c} 0 \\ 0 \end{array} \right)$ ≡ $\left( \begin{array}{c} 0 \\ 8 \end{array} \right)$,
which to the addition of a single electron to the corresponding QD is denoted as .

Where $C_i$ is the cross capacitance matrix, with the gate capacitance along the main diagonal and the cross capacitance elsewhere. $\vec{V}$ is the voltage applied onto each QD and $\vec{N}$ is the number of electrons. As a result, an analytical solution for any transition between two QDs can be found by equating the two energy states of interest. Possible transitions are from dot to reservoir (DTR), which tend to have a negative slope or inter-dot charge transition (ICT), which have a positive gradient. By only applying voltages onto two of the QDs ($i$ and $j$) at a time, we take a two-dimensional projection of a hyper-dimensional gate voltage space. For this specific regime, the gradients $r_{ij}^k$ for a particular transition between two QDs ($k$ and $l$) is given using Einstein summation convention as:

DTR gradient: $r_{ij}^k = \frac{a_{km}C_{mi}}{a_{km}C_{mj}}$  \hspace{1cm} (3)

ICT gradient: $r_{ij}^k = \frac{(a_{km} - a_{lm})C_{mi}}{(a_{km} - a_{lm})C_{mj}}$  \hspace{1cm} (3)

Where $a_{ij}$ is the $i,j$ element of $C^(-1)$. In order for the DTR transitions to become orthogonal, we adopt an anticlockwise rotation matrix to get $r_{ij}^k$ horizontal, followed by a horizontal shear in order to get $r_{ij}^k$ vertical, as shown in Fig. 2.

If we define $\phi_{ij}^k = tan^{-1}(r_{ij}^k)$, then for a DQD, this transformation matrix $G$ is:

$$G = \frac{1}{-sin(\phi_1)} \begin{pmatrix} -sin(\phi_1) & cos(\phi_1) \\ -sin(\phi_2) & cos(\phi_2) \end{pmatrix}$$  \hspace{1cm} (4)

We divide the whole matrix by $-sin(\phi_1)$ as a scaling factor that allows us to easily extend the model to a $2 \times N$ array. For a $2 \times 2$ QD array, $G$ is given by:

$$G = \begin{pmatrix} 1 & -\frac{tan(\phi_1^2)}{tan(\phi_1)} \cdot G_{11} & -\frac{tan(\phi_1^2)}{tan(\phi_1)} \cdot G_{11} & -\frac{tan(\phi_1^2)}{tan(\phi_1)} \cdot G_{11} \\ \frac{tan(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{11} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{11} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{11} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{22} \\ \frac{tan(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{22} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{22} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{22} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{33} \\ \frac{tan(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{33} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{33} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{33} & -\frac{cos(\phi_1^2)}{sin(\phi_1^2)} \cdot G_{33} \end{pmatrix}$$

Since certain terms within $G$ depend on previous entries, this poses the restriction of having to build up the matrix from the top left and work our way down the main diagonal. In general, for a $2 \times N$ array of QDs, the $G$ matrix is:
can be constructed as follows:

\[ G_{11} = 1 \]
\[ G_{i+1,i+1} = \frac{\cos(\phi_{i+1}^{i+1})}{\sin(\phi_{i+1}^{i+1})} \cdot G_{ii} \]
\[ G_{i,i+n} = -\frac{1}{\tan(\phi_{i}^{i+n})} \cdot G_{ii} \]
\[ G_{i+n,i} = \frac{\sin(\phi_{i+n}^{i+n})}{\sin(\phi_{i}^{i+n})} \cdot G_{ii} \]

Where \( n \) is an integer, which if only nearest neighbours are taken into account will have values between 1 and 3.

IV. AUTOMATIC GRADIENT EXTRACTION

We present an algorithm to automatically extract the gradients, and thus acquire the virtual voltages, from a charge stability diagram when sweeping two gate voltages at a time. The protocol is described in Fig. 3 and the code can be found here [40]. Hough transforms are commonly used in image processing to extract gradients and have already been applied to experimental stability diagrams of DQDs [17, 47]. We modify the algorithm to work with data points, rather than images, to speed up the analysis. Only data points that represent a signal undergo the Hough transform, so the first step is to threshold the data, as outlined in Appendix A. The threshold data points \((x, y)\) are then converted into Hough space:

\[ \rho = x \cdot \cos(\theta) + y \cdot \sin(\theta) \] (6)

Since we are only interested in the two main dot to reservoir transitions, only negative slopes are taken into account by restricting the \( \theta \) values between zero and \( \pi/2 \). The points in which multiple sinusoidal lines intersect are directly related to the gradient \( m \) and y-intercept \( c \) of the best fit lines in polar coordinates \((m = -\frac{\rho}{\sin(\theta)}, \text{ and } c = \frac{\rho}{\sin(\theta)})\).

Due to the presence of multiple honeycomb-like structures in the stability diagram of a \( 2 \times 2 \) array, the intensity histogram of the \( \theta \) values (step 4 in Fig. 3) will generally be constituted by more angles than the target 2 per stability map. There can be potentially ten different gradients (four DTR and six ICT transitions) for a \( 2 \times 2 \) array and often prominent additional peaks appear corresponding to lines that combine different transitions, such as the lines that pass through the centre of the ICT with a constant electron number in one of the dots (rather than following the DTR lines). Additional peaks can also appear due to systematic noise in the data, such as aliasing effects. However, these histograms act as a unique fingerprint to a particular combination of gradients, which we could train a regression model to correctly identify. The trained models are determinant in the identification of relevant angles in the \( \theta \) histogram that generally present comparatively lower intensity.

We generated a database of 64,000 theoretical \( \theta \) histograms, with the corresponding gradients from a simulated stability diagram of a \( 2 \times 2 \) array of QDs (calculated according to Eq. 3). This data was then split 76.5/13.5/10 as train, validation and test data to train an ensemble of four regression models (neural networks and decision trees) to predict the two main DTR gradients present. We use the average prediction of the difference models, and their standard deviation is an estimate of the confidence of the predicted values. From the predicted gradients, we can perform a partial transformation, in which the transition lines from the probed QDs become perpendicular to each other, as highlighted in the final step of Fig. 3.

V. TESTING THE ALGORITHM ON EXPERIMENTAL DATA

The regression models presented here have been trained on theoretical data generated using the constant interaction model, which does not consider quantum effects, such as orbital level spacing or voltage and charge occupation dependent capacitances. To test how it would
perform on experimental data, we use the charge stability diagram of the left silicon double split-gate nanowire transistors measured in Fig. 1d of Ref. [48]. We present the data in Fig. 4 where two gate voltage potentials on the same side of the nanowire ($V_{g2}, V_{g4}$) are varied while the phase response of the resonator is recorded. We observe quasi-vertical (horizontal) lines of enhanced intensity associated to charge transitions between the dot under gate 2(4) and the reservoirs. Additionally, we observe a line with a different gradient, highlighted by the dashed white line, that could be originated from charge transitions in the quantum dots on the opposite side of the nanowire (QD one or three) or from a dopant inside the channel. Either way, the algorithm correctly predicts the main two gradients resulting in the partial rotation matrix $g$:

$$
g = \begin{pmatrix}
1 & 0.2690 \\
0.4477 & 0.9337
\end{pmatrix}$$

As highlighted in Fig. 4, the partial rotation predicted by the algorithm results in the DTR transitions of QDs 2 and 4 to be perpendicular to each other. To benchmark the accuracy of the transformation, we measure the angles in virtual voltage space and obtain an average angle between DTR transitions of $88.31 \pm 7.62^\circ$ approaching the desired $90^\circ$. We note there is a distribution in the original gradients in Fig. 4 due to a voltage dependence of the capacitance matrix, highlighting a deviation from the constant interaction model at large voltage amplitudes. This leads to an average angle between the two DTR transition in real gate voltage space of $123.70 \pm 5.74^\circ$ whose standard deviation accounts for the major part of the error in the transformation. We note that the algorithm can be used to predict virtual voltages locally as well as to provide average values over wide voltage areas as described in the next section.

![Charge stability map of a 2×2 QD device measured using radiofrequency reflectometry.](image)

A. Performance at different voltage amplitudes:

The algorithm is designed to provide the virtual voltages in the voltage range designated by the user. For small amplitudes, the constant interaction model holds and the algorithm predicts the constant values across the window. At larger voltage scales, due to the effect of voltage varying capacitances in semiconductor quantum dots, the algorithm will provide average values across the desired voltage space. To assess the accuracy of the algorithm at different voltages scales, we subdivided the data-set shown in Fig. 4 into increasingly smaller regions and then run the model on each one. The distribution of the predicted gradients are then plotted in Fig. 5a. The data was then transformed into the corresponding virtual voltage space according to the predicted gradients and the angles of the dot to reservoir lines were manually measured using ImageJ to obtain a statistical analysis of how the model performs (Fig 5b). The process consisted in drawing best fit lines for all the DTR transitions present on each data-set and then the average gradients and standard deviation measured were recorded. The mean squared error (MSE) of the model with the increasing number of subdivisions is summarised in Table 1. The algorithm accurately predicts the gradients at the different voltages scales studied showing that it can be used for different levels of resolution depending on the user’s needs.

| Subdivisions | MSE $\theta_1$ | MSE $\theta_2$ |
|--------------|----------------|----------------|
| 1            | $0.017 \times 10^{-2}$ | $0.008 \times 10^{-2}$ |
| 4            | $0.158 \times 10^{-2}$ | $0.497 \times 10^{-2}$ |
| 9            | $0.082 \times 10^{-2}$ | $0.129 \times 10^{-2}$ |
| 16           | $0.298 \times 10^{-2}$ | $0.757 \times 10^{-2}$ |
| 25           | $0.455 \times 10^{-2}$ | $0.788 \times 10^{-2}$ |
| 36           | $0.237 \times 10^{-2}$ | $0.727 \times 10^{-2}$ |
| 49           | $0.485 \times 10^{-2}$ | $0.755 \times 10^{-2}$ |
| 64           | $0.567 \times 10^{-2}$ | $1.614 \times 10^{-2}$ |
| 81           | $1.164 \times 10^{-2}$ | $1.411 \times 10^{-2}$ |
| 100          | $0.484 \times 10^{-2}$ | $1.446 \times 10^{-2}$ |

VI. EXTRACTING VIRTUAL VOLTAGES FOR A 2×2 ARRAY OF QDs

Theoretically, for a 2×2 QD array, ten transitions are possible, resulting in ten different gradients that could be experimentally measured when applying voltages to two gates at a time. Several of which will be related to each other, as:

$$r_{ij}^{kl} = r_{kl}^{im} \cdot r_{kl}^{mj}$$

thus, reducing the number of measurements required to define $G$ to $2N - 1$. However, it is not trivial to correctly
FIG. 5. Statistical analysis of how the algorithm performs at varying voltage amplitudes by subdividing the experimental data in Fig. 4 into equally sized parts. (a) Distribution of the predicted \( \theta \) values from the algorithm (black data points) and the error bars are the standard deviation from the different models used. (b) Average measured angles in virtual voltages, with the error bars corresponding to their standard deviation. The red dotted line is the desired values of 0 and \( \pi/2 \) degrees. (c) Box plot of the difference between the observed and expected values of \( \theta_1 \) and \( \theta_2 \) in virtual voltage space.

label each measured gradient to its corresponding transition. Also, many of these transitions will only appear at particular gate voltage combinations, requiring large gate voltage maps in order to be detected. A more robust solution is to take 5\( N - 4 \) stability diagrams whilst applying relatively small gate voltages. The system will behave similar to a DQD, as transitions will mostly occur between the QDs being probed. Although more measurements are taken, they can be smaller voltage maps, minimising the impact on total measurement time whilst guaranteeing that all the transitions are measured. Another advantage of this approach is that we can implement the automatic gradient extraction protocol introduced in Section VI for each two-dimensional projection. We carried out the virtual voltage extraction protocol on a simulated 2\( \times \)2 QD array by first simulating the six different 2D gate voltage projections to extract all the relevant gradients. By then constructing the \( G \) matrix, as in equation [3], we determine the corresponding virtual voltages \( \bar{U} \) in terms of gate voltages \( \bar{V}_g \). Fig. 6 shows the full virtual voltage space transformation corresponding to Fig. 1c; highlighting how it simplifies the analysis as there are no transitions from QDs 1 and 3. To prove this method enables controlling each QD independently from its neighbours, in Fig. 6b, we plot the charge stability diagram when sweeping simultaneously the virtual voltages \( U_{1,2} \) and \( U_{3,4} \) in the x and y axis respectively, after applying the virtual voltage extraction protocol.

FIG. 6. Virtual voltage space measured once the entire \( G \) matrix is extracted. a) Corresponding virtual voltage of Fig. 1c, with charge state denoted as reference. The reference charge \( * \) is identical to that used in Fig. 1c. b) To show independent control of all QDs, all four virtual voltages are swept, \( U_1 \) and \( U_2 \) simultaneously along the horizontal and \( U_3 \) and \( U_4 \) along the virtual axis.

VII. EXTENDING TO A 2\( \times \)N ARRAY OF QDs

To extract the virtual voltages in a 2\( \times \)N array of QDs, we envision a protocol in which 2\( \times \)2 subsets of QDs are defined at a time. High voltages are applied to the remaining gates to produce a strong inversion, resulting in the extension of the source and drain charge reservoirs close to the location of the square array (see Fig. 7 for a specific example of a 2\( \times \)5 array). We start by forming the four dots closest to the source reservoir (1-4) while we bias the remaining gates to extend the drain reservoir to the location of dots 3 and 4 (panel a). Then we extract the virtual voltages of the subset following the protocol described in section VI. After, we shift the 2\( \times \)2 array by one location in the horizontal direction to form QDs (3-6) and bias the remaining gates to extend the source and drain reservoirs accordingly (panel b). The process continues (panel c) until the 2\( \times \)2 subset closest to the drain reservoir is studied (panel d). Once all the required gradients have been extracted, we construct the transformation matrix \( G \) and obtain the virtual voltages.

The voltages applied on the gates to extend the reservoirs will be comparatively larger than the voltages required to tune the full 2\( \times \)N QD array to the few-electron
FIG. 7. Extending the 2×2 QD array protocol to a 2×N array. During the tuning process, only four QDs are formed at a time as shown for a 2×5 array in panels (a) to (d).

This difference in bias voltages could modify the shape of the 2×2 QD subset resulting in a different capacitive coupling to the environment. Particularly, for corner dots in silicon nanowire transistors, where the capacitive coupling to the source and drain electrodes is a small fraction of the overall QD capacitance. From Fig. 4, we determine a gradient change of ~2° every 0.25 V, from which we estimate a slope difference of ~4 to 8° between the multi and low electron regimes. From Eq. 3, we can predict which gradients in the low electron regime are going to be steeper or shallower than the ones measured with our protocol. Hence, we can subtract/add the average estimated deviation to the measured gradients to obtain an even better estimate of $G$ in the few electron regime. Finally, virtual voltage extraction methodology presented in this section could be particularly useful to study direct and cross coupling capacitance variability across QDs in large 2×N arrays.

VIII. OUTLOOK

In this paper, we have developed the relationship between gate voltage and virtual voltage space for a 2×N array of QDs in terms of the gradients of the DTR transitions obtained whilst probing two QDs at a time. We then propose a protocol of the different measurements required to construct our transformation matrix $G$ between gate and virtual voltage space. To automate the process, we have developed an algorithm to extract the appropriate gradients. This is done by utilising the Houff transform of a stability diagram when probing two gate voltages at a time. To manage the complexity of the Hough’s $\theta$ histogram obtained from experiment data, we train an ensemble of regression models to correctly predict the two most prevalent DTR gradients. We have then tested our protocol on experimental data of a 2×2 QD array. We outline how the protocol can be extended to a 2×N array of QDs.

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DATA AVAILABILITY

The data and code that support the findings of this study are openly available in the following GitHub repository [49].

Appendix A: Threshold experimental data

We have developed an automated thresholding protocol, which does not require any fitting parameters, but rather uses information theory to determine the threshold between noise and signal. Experimentally in an RF reflectometry setup, the reflected signal goes through an IQ mixer, allowing the measurement of both the in-phase (I) and quadrature (Q) components. From the measured I and Q, one can calculate the magnitude ($M = \sqrt{I^2 + Q^2}$) and phase ($\Phi = \tan^{-1}(Q/I)$), where changes in the phase are proportional to the changes in capacitance of the system ($\Delta C$) [50]. In particular, at regions of charge bistability an additional capacitance appears, resulting in a phase shift ($\Delta\Phi$) that can be approximated as:

$$\Delta\Phi \approx -\frac{2Q_L \Delta C}{C_p} \quad (A1)$$

where $Q_L$ is the loaded quality factor of the resonator and $C_p$ is the parasitic capacitance of the system. Besides this shift, in gate-defined QD, an additional capacitance associated to the two-dimensional charge inversion layer generated by the gate will also contribute to $\Delta\Phi$ [51]. This effect is visible in Fig. 8, as the background signal of the charge stability diagram increases as the resonator gate voltage, $V_g$, is increased. Over large voltage ranges, such a background is typically modelled as a sigmoid function, however, locally we can approximate it as...
a linear expression. Thus to flatten the data, we fit a linear plane, resulting in Fig. 8b.

The next step is to threshold the data. For most gate voltage combinations the QDs have a particular charge stable configuration which does not generate a signal. Only regions of charge bistability, the electrons tunnel cyclically driven by the effect of the RF voltage producing a phase response. This means that for most combinations we do not measure a signal, which only arises at a charge transition. Thus, we expect to have a large peak in the intensity distribution representing the background, that should be Gaussian in nature. To determine what values of I and Q to threshold from, we use the point that minimises the Kullback-Leibler divergence \( D_{KL} \) between the square root of the intensity distribution \( p(x) \) and that of a fitted Gaussian distribution \( q(x) \). By taking the square root of the intensities of the histogram data, it broadens the peak, allowing us to distinguish weak signals in the data. The Kullback-Leibler divergence \( D_{KL} \) calculates the information loss of approximating the distribution of our data \( p(x) \) by a Gaussian \( q(x) \):

\[
D_{KL}(p(x)|q(x)) = \sum_{x \in X} p(x) \ln \left( \frac{p(x)}{q(x)} \right) \tag{A2}
\]

By minimising \( D_{KL} \), we have found the data-points of \( p(x) \) that are best described by \( q(x) \) and thus represent our background, as shown in Fig. 9.

The data points below the threshold are then set to zero, in Fig. 8c however, we have plotted the points that are above the threshold for clarity. The reason to threshold I and Q separately is because certain transitions appear stronger in one domain than in the other. Therefore data points that appear as a signal in either I or Q are taken into account. The last step is to thin the data set, to remove any aliasing effects. This is done by using peak detection both along the x and y axis are taken into account, as shown in Fig. 10.

The thinned data that is then passed to the Hough transform is shown in Fig. 8d, in which we observe some random noise. This is not an issue for the Hough transform, as these data points are unlikely to generate a peak in the \( \theta \) histogram due to their random orientation.

**Appendix B: Ensemble regression models:**

The data-set that was used to train the model was created by generating 64,000 random stability diagrams of a 2×2 QD array. The data set contains examples of
single, double and quadruple dots. From the stability diagrams generated, the $\theta$ histograms were extracted. The histograms were standardised by being 500 data-points long, ranging from 0 to $\pi/2$. This ensures that only negative gradient lines are fitted to the data and thus excluding any ICT. The intensities of these histograms were normalised to have a maximum value of one. Since the capacitance used to generate these theoretical stability diagrams are known, the gradients of the two DTR transitions of interest can be calculated according to Eq. 3, which act as the labels for the data-set. To normalise the labels, the gradients were converted to their corresponding $\theta$ values and divided by $\pi/2$, such that the labels range between zero and one.

The aim of ensemble regression is to train multiple different regression models to carry out the same task. By then taking the average predictions, one obtains a more accurate and robust model than any of its constituents. The standard deviation between the different predictions of the ensemble models is utilised to determine how confident we are of the predicted value. The four regression models used consist of a neural network and three decision tree based algorithms, namely: random forest, bagging regression and extra trees regression. Out of the four models, the neural network is the one that can model more arbitrary functions, but requires more hyper-parameters to be tuned during training. For the neural network, as a non-linear transform a ReLu activation function is used between each layer. He initialisation is used to ensure that gradients of the activation function do not vanish to zero. Between each layer, a 0.05 probability dropout is used as regularisation to ensure the model doesn’t over-fit and the learning rate is set to $10^{-4}$. The learning cure was used during training to ensure that the model did not over fit the training data. The trained models were then evaluated on the test data as shown in Fig. [11], which shows that the model works very well, with an $R^2$ value of 0.978 and an average accuracy for $\theta_1$ of 97.36% and 99.29% for $\theta_2$. For $G$ however, we are interested in knowing $\phi$, which is the complementary angle to $\theta$, making the conversion of the two trivial.

**Appendix C: Parameters used in simulated data:**

The numerical values used for the capacitance and cross capacitance matrices for the simulations are summarised in Table [11].

For which the following $G$ matrix was used to measure in virtual voltage space in Fig. [6b]:

$$G = \begin{pmatrix} 1 & 0.2643 & 0.0991 & 0.0919 \\ 0.3390 & 0.9772 & 0.1278 & 0.2470 \\ 0.1211 & 1.077 & 0.9796 & 0.2402 \\ 0.1516 & 0.2182 & 0.3330 & 0.9521 \end{pmatrix} \quad (C1)$$

**Table II.** Capacitance $C$ and cross capacitance $Cc$ matrices used to generate Fig. [1] and Fig. [6] (rounded to four decimal places). The capacitances used have no physical units, as we are only interested in their relative ratios, as these will give rise to a particular stability diagram.

| $C$ matrix | $Cc$ matrix |
|------------|-------------|
| 1.6199 -0.4084 -0.0662 -0.0364 1.0225 0.0486 0.0272 0.0106 | 0.0408 1.8513 -0.0558 -0.3077 0.0587 0.9519 0.0119 0.0569 |
| -0.0662 -0.0558 1.6845 -0.3806 0.1481 0.0322 1.0549 0.0467 | -0.0364 -0.3077 -0.3806 1.8772 0.0483 0.0287 0.0973 0.9783 |

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FIG. 11. Predicted $\theta$ values by the model versus their true value on the 6,500 test data points. Error bars are also plotted, which correspond to the standard deviation between the predicted values of the four different models that make the ensemble. The better the trained model, the closer the data should resemble $y = x$.

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