

***Ab initio* modeling of quantum dot qubits: Coupling, gate dynamics, and robustness versus charge noise**

Hamza Jnane^{1,2,*} and Simon C. Benjamin^{1,2}

¹*Quantum Motion, 9 Sterling Way, London, N7 9HJ, United Kingdom*

²*Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, United Kingdom*



(Received 10 March 2024; revised 29 June 2025; accepted 12 September 2025; published 15 October 2025)

Electron spins in semiconductor devices are highly promising building blocks for quantum processors (QPs). Commercial semiconductor foundries can create QPs using the same processes used for conventional chips, once the QP design is suitably specified. There is a vast accessible design space; to identify the most promising options for fabrication, one requires predictive modeling of interacting electrons in real geometries and complex nonideal environments. In this work we explore a modeling method based on real-space grids, an *ab initio* approach without assumptions relating to device topology and therefore with wide applicability. Given an electrode geometry, we determine the exchange coupling between quantum dot qubits, and model the full evolution of a $\sqrt{\text{SWAP}}$ gate to predict qubit loss and infidelity rates for various voltage profiles. We determine full, three-dimensional solutions and introduce a method that can obtain near-identical predictions using far more efficient two-dimensional computations. Moreover we explore the impact of unwanted charge defects (static and dynamic) in the environment, and test robust pulse sequences. As an example we exhibit a sequence correcting both systematic errors and (unknown) charge defects, observing an order of magnitude boost in fidelity. The technique can thus identify the most promising device designs for fabrication, as well as bespoke control sequences for each such device.

DOI: [10.1103/rm43-nh9b](https://doi.org/10.1103/rm43-nh9b)

I. INTRODUCTION

Electron spins in gate-defined semiconductor quantum dots [1] are a strong candidate for qubit implementation [2–4]. Because of their small size, fast operations, and compatibility with current industry standards [5–8], silicon spin qubits hold great promise for the development of full-scale, mature-era quantum computers.

The vast design space provided by semiconductor foundries is highly enabling, while also presenting a challenge to identify the most promising device architecture. The iterative nature of chip development, coupled with the time and cost of a chip design cycle, makes it highly desirable to have accurate predictive modeling tools to speed up the discovery of scalable designs. Given a candidate chip layout defined with the use of standard commercial software (as employed for traditional chips), such tools would extract key metrics and enable one to optimize the design before committing to fabrication.

The electron spin qubits are confined by potentials generated by the device's electrodes, and the design space for electrode layout (and corresponding voltage ranges) is wide. Of particular interest are double quantum dot (DQD) potentials where two electrons can be isolated and experience exchange coupling: the spin-spin interaction resulting from underlying charge state symmetries. The strength J and its controllability ultimately limit the speed and quality of any native two-qubit gate [9–11]. Naturally, there is a long-standing effort to predict the exchange coupling for a given double quantum dot potential (and hence for a given electrode layout) by either analytic or numerical methods [12–15]. The task is complex, and typically simplifications to the device layout and the environment are adopted to make the task possible.

A key consideration in optimizing the fidelity of two-qubit gates is the sensitivity of the exchange coupling to charge noise [16–18]. Accounting for the qubits' environment is thus necessary for a predictive tool to be practically useful. Recently, several studies have addressed this challenge [19–21] and computed the exchange coupling for realistic scenarios. The authors have adopted techniques to make the otherwise-costly numerical simulations more tractable; for example, by tailoring the basis so as to enable a compact form for the Coulomb interaction, by coarse-graining the model in some direction(s), or by reexpressing

*Contact author: hjnane.science@gmail.com

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

the problem through a path integral formulation. Buongiorno *et al.* [20] limited the inclusion of charge noise to optimizing devices geometries to reduce the sensitivity of J to electrical fluctuations, while Cifuentes *et al.* [19] and Shehata *et al.* [21] explicitly added charge noise using a two-level fluctuator model. Recent experiments [22] confirmed the validity of this choice.

The approach taken in the present paper is *ab initio* in the sense that it makes very few assumptions regarding the anticipated physics but sees the key properties emerge once suitable parameters are found. We use a uniform real-space grid method that describes the relevant two-electron states for *any* reasonably smooth potential landscape without requiring that it be approximately locally harmonic, or that eigenstates be close to any given analytic form, etc. Since we do not use the low-lying eigenstates of the particle(s) as our means of representation, we are not constrained to low-energy dynamics. The representation fails only for states more highly curved than the resolution of the grid basis—more than 10^9 elements in some cases. Correspondingly, the numerical modeling is fairly demanding, but can tackle quite general scenarios. For the present study we focus on a flat-bottomed double-well potential derived, via a Poisson solver, from a realistic device's electrode geometry. We begin by identifying different J -coupling scenarios, including a suitable “off” configuration, where the notion of “left” and “right” qubits emerges as an excellent approximation to the true state.

We directly model the dynamics of a $\sqrt{\text{SWAP}}$ gate as the confining potential continuously deforms, propagating the full two-electron state forward with a split-operator (SO) method. At gate completion we reassess the validity of the qubit representation, i.e., whether there is increase in

the $(2, 0)$ and $(0, 2)$ configurations that correspond to qubit loss, and we report this separately from the fidelity of the gate operation within the $(1, 1)$ subspace. We observe the effect of a nonadiabatic voltage ramp on this loss probability, and verify that a suitable ramp introduces negligible loss. We then proceed to assess the impact of unwanted trapped charges in the environment, either as static entities or as fluctuators that switch charge position during the gate operation. By extracting the behavior of our full model into a reduced basis, we rapidly explore options for robust pulse sequences—i.e., a multistage gate that corrects for intrinsic axis error as well as charges in the environment. Adapting methods from the NMR literature [23–26] we exhibit a nine-pulse sequence with remarkable robustness regarding both effects, albeit at the cost of speed.

The tool we describe is capable of characterizing the impact of arbitrary charge defects, within arbitrarily changing electrode potentials and in a framework that fully describes qubit leakage. Moreover, this is possible both for two-dimensional (2D) and true three-dimensional (3D) particle pairs. As far we are aware, there is no prior-reported tool with these capabilities, although aspects have been previously explored; for example, charge noise modeled as two-level fluctuators [19,21] and first-principles methods to find exchange coupling [19–21]. A key motivation is to facilitate improved design cycle times for the fabrication of semiconductor quantum devices, since electrode configurations and potential ramping can be tested against various charge noise scenarios before commitment to a design (see Fig. 1).

This paper is organized as follows. In Sec. II we briefly explain how our double quantum dot and electron wave functions are modeled using real-space grids. In Sec. III we

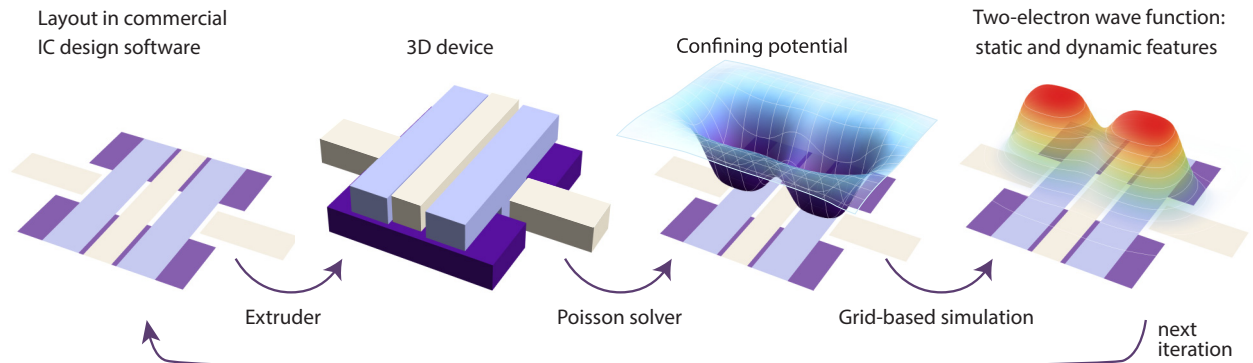


FIG. 1. Iterative design process for a quantum dot device. Starting from an idea of an integrated circuit (IC) layout, we would like to know the performance of the chip without sending it through the lengthy fabrication process. Using an extruder, we generate a 3D version of the chip for which we specified the different materials. This in turn allows us to extract realistic quantum dot potentials. The grid-based modeling tool presented in this paper then gives us access to the device’s key performance metrics. For instance, we could discard designs that show a small exchange coupling between neighboring quantum dots. On top of the static properties, we can also study the qubits’ dynamics and, for example, compute two-qubit gate fidelities, how they are impacted by the presence of charge noise, and how we can mitigate this effect. Finally, this process will inform new layouts and through similar iterations will lead to more promising devices that can be sent for fabrication.

study how our tool can be used to compute the exchange coupling in an idealized environment. In Sec. IV, we explore the dynamics of the exchange gate, and in Sec. V we study how it is impacted by the presence of charge noise. In Sec. VI we assess the mitigation power of different pulse sequences, and we conclude the paper in Sec. VII.

II. MODEL

A. Hamiltonian

We focus on the study of two electrons trapped in a DQD potential (see Fig. 2). Under the effective mass approximation, the Hamiltonian of the system is given by

$$H = \frac{\hbar^2}{2m^*} \mathbf{p}_1^2 + \frac{\hbar^2}{2m^*} \mathbf{p}_2^2 + V(\mathbf{r}_1) + V(\mathbf{r}_2) + \frac{e^2}{4\pi\epsilon_0\epsilon_r|\mathbf{r}_1 - \mathbf{r}_2|} + g(\mathbf{r}_1)\mu_B \mathbf{B} \cdot \mathbf{S}_1 + g(\mathbf{r}_2)\mu_B \mathbf{B} \cdot \mathbf{S}_2, \quad (1)$$

with $m^* = 0.19m_e$ the effective mass of an electron in silicon, $\epsilon_r = 11.68$ silicon's relative permittivity, and $g(\mathbf{r}_i)$ the position-dependent electron g -factor. The potential V is generated with the use of a Poisson solver on realistic devices. In this first study we ignore certain additional effects, while noting that their inclusion would be entirely possible within the approach and is an attractive direction for further work. Specifically, we ignore the impact of the magnetic field on the orbital motion of the electrons (through its associated vector potential) as we are concerned with flat or nearly flat 2D quantum dots subject to an in-plane field. Moreover, we ignore the valley degree of freedom as the valley splitting is usually large in silicon metal-oxide-semiconductor devices. Finally, we also ignore spin-orbit coupling, noting that it is small in silicon. Presently we remark on the ways our tool could be extended to encompass some of these additional features.

B. Grid-based simulation

1. Introduction to grid-based and split-operator methods

One of the canonical approaches to modeling either single or multiple quantum particles is to represent their state by storing a complex amplitude for each point in a regular grid—such a grid may be in real space, k space, or alternately in each representation. The approach is broadly a discrete variable representation [27], and the approach to driving dynamics used in this paper is a split-operator Fourier transform method, which dates back at least as far as the work of Feit and Fleck [28] in 1976. Widely used in a variety of contexts, the method involves repeatedly Fourier transforming between the real-space and the dual k -space representations of the state, described below.

It is worth noting that the method has recently received attention from researchers seeking efficient algorithms for modeling many-body systems on future quantum computing systems. The use of the Fourier transform is a particularly natural fit since this transformation is well-understood and efficient on a quantum machine. Indeed, the specific variant of the SO method that we use here is one that has been well-explored in that context (see, e.g., Refs. [29,30]).

2. State representation

It is convenient to begin in the k -space picture, and to start by describing a single particle in one dimension. The state of this system is represented as

$$\Psi_{\text{KS}}(x) = L^{-1/2} \sum_{k=-m}^{m-1} c_k \exp\left(\frac{2i\pi kx}{L}\right),$$

where we write the subscript KS for “ k space.” In the expressions in this paper we typically set the “box size” L equal to unity for simplicity (obviously, we can rescale it as appropriate in our calculations). Then

$$\Psi_{\text{KS}}(x) = \sum_{k=-m}^{m-1} c_k \psi_k(x), \quad \text{with } \psi_k(x) = \exp(2i\pi kx). \quad (2)$$

Since we used regularly spaced k , it follows that the state is periodic: it simply repeats outside the central box region $-\frac{1}{2} < x < \frac{1}{2}$, but of course we are interested only in this central region, and the confining potential means that the wave-function amplitudes of the states of interest will vanish well before reaching the border. We choose a scale such that the wave functions have very little amplitude outside the middle part of this box ($|x|, |y|$ less than $1/4$), and this is important because of the form of the Coulomb interaction, as explained in Appendix F.

We use various basis sizes: for each particle and each dimension, our index runs from $-m$ to $m-1$ for a total number of basis states of $M = 2m = 2^q$ for some integer q . This choice is made in some prior papers (e.g., Ref. [30]), while in others (e.g., Ref. [29]) an odd total number of k states is used, which slightly alters the form of the real-space states. Such states are found by the Fourier transform of the k -space representation. One finds

$$\Psi_{\text{RS}}(x) = \sum_{n=-m}^{m-1} b_n \phi_n(x),$$

where

$$\phi_n(x) = \frac{e^{i\pi(x-p_n)}}{\sqrt{M}} D_m(2\pi(x-p_n)) \quad \text{and} \quad p_n = \frac{n}{M}. \quad (3)$$

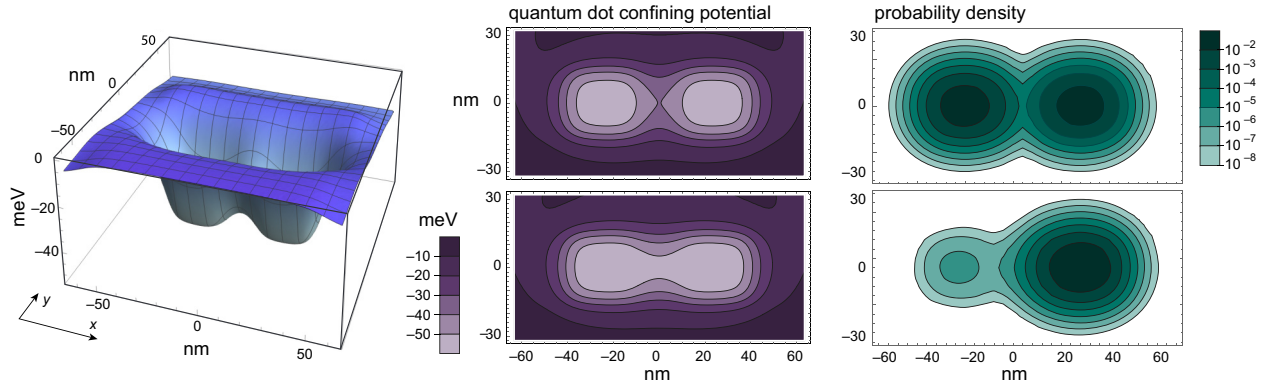


FIG. 2. Potential well constituting the double quantum dot (left and center) and states of the confined electrons (right). The 3D visualization and the upper contour plot show the “barrier up” case, while the lower contour plot shows the “barrier down” potential. The potential is expressed in mili-electron volt (meV) as a function of the position in nanometer (nm). The rightmost plots show probability densities on a logarithmic scale. The upper-right plot shows the ground state probability density for the “barrier up” scenario (due to symmetry the distribution is identical for either particle). We then explore the subspace corresponding to “a given electron is definitely on the left of the structure” and plot the probability distribution for *the other electron*; this reveals a small but nonzero probability that the second particle is also on the left, i.e., a (2,0) charge state that would not constitute a legitimate qubit configuration. The total probability of (2,0) and (0,2) is 0.04%.

Here D_m is expressed as

$$D_m(u) \equiv \frac{\sin(mu)}{\sin(\frac{u}{2})}. \quad (4)$$

One observes that D_m is a variant of the canonical Dirichlet kernel, obtained with the substitution $\sin(m) \rightarrow \sin(m + \frac{1}{2})$. As such, our function is a precursor to the Dirac delta function (or more precisely the Dirac comb [31], since D_m is periodic with period 2π). Each $\phi_n(x)$ is peaked at p_n , and these locations are simply our real-space grid points. With our simulation box running from $x = -\frac{1}{2}$ to $x = +\frac{1}{2}$, n runs from $-m$ to $m-1$, i.e., p_n runs from $-\frac{1}{2}$ through zero to $\frac{1}{2} - \frac{1}{M}$. Because of the periodicity, the points $\frac{1}{2}$ and $-\frac{1}{2}$ are identical [32]. Our basis [Eq. (3)] is variously referred to as the “dual basis,” or the “real-space basis,” or the “Dirichlet basis.”

Given that we are initially representing our state in the k -space form, Eq. (2), by storing the amplitudes c_k in our simulation software, the transformation to the real-space picture simply requires us to compute the b_n according to

$$b_n = \frac{1}{\sqrt{M}} \sum_{k=-m}^{m-1} \exp\left(\frac{2i\pi nk}{M}\right) c_k.$$

It is notable that $\phi_n(p_m) = 0$ for all $m \neq n$, i.e., where a given basis function is peaked, all other basis functions are zero. Consequently it is obvious how to encode any given target wave function $f(x)$ into this form; we need to evaluate the target function only at the grid points, simply writing

$$f(x) \approx \Psi_{\text{RS}}(x) = \sum_{n=-m}^{m-1} f(p_n) \phi_n(x). \quad (5)$$

We can naturally extend Eq. (5) to two or three dimensions with the obvious generalizations

$$\Psi_{\text{RS}}(\mathbf{r}) = \sum_{n_x, n_y} f(p_{n_x}, p_{n_y}) \phi_{n_x}(x) \phi_{n_y}(y), \quad (6)$$

with $\mathbf{r} = (x, y)$ for 2D quantum dots, and

$$\Psi_{\text{RS}}(\mathbf{r}) = \sum_{n_x, n_y, n_z} f(p_{n_x}, p_{n_y}, p_{n_z}) \phi_{n_x}(x) \phi_{n_y}(y) \phi_{n_z}(z), \quad (7)$$

with $\mathbf{r} = (x, y, z)$ for full 3D analysis. Note that we need not have the same basis size M for the various dimensions. Indeed it can be appropriate to have a larger basis along the x axis, which is the axis of the double quantum dot and therefore has more structure than the y direction.

Finally, we note that the spin degree of freedom is easily included by having one entire charge state of the form of Eq. (6) for *each* spin basis state. Moreover, for multiple particles, one needs only to take the tensor product of the respective one-particle states.

Although we do not address the valley degree of freedom, it could be incorporated similarly to the spin degree of freedom, provided that the effects of valley-orbit coupling are treated carefully. However, for such a model to be meaningful the x - y resolution would also need to be high enough to capture realistic interface roughness since the valley dynamics profoundly depends on such irregularity [33]. The computing resources to explore this are

beyond those of the present project, but appear tractable in principle.

Presently we model a strictly 2D quantum dot using the representation in Eq. (6), and we independently compute the full 3D solutions using Eq. (7). The time and memory requirements for numerical computations are, of course, far greater for the 3D case; for z -direction basis size M_z there is a multiplicative cost of order M_z^2 . Therefore, it is interesting to explore the extent to which 2D models can predict the results of a full 3D analysis. We explore a pseudo-3D approach that requires only the 2D representation. It exploits the fact that we are interested in quantum dots whose z dimension confinement is tight and relatively uniform, so that we can opt to “freeze out” this axis by assigning only a single basis state. Effectively we assume that the gap to the first excited z state is too large to be relevant to our calculations [1,34]. Details of the generalization are given in Appendix F. By comparison with the fully fledged 3D solution, we can evaluate the validity of this “shortcut.”

Readers may be interested to note that the formalism used here largely follows that in Ref. [30], with some revisions and changes of notation. That paper, however, focuses on the optimal way to use grid-based techniques with future quantum computers; while such machines should avoid the exponential random access memory (RAM) costs, there are downsides, including the restriction to unitary evolution that we need not be concerned with. This paper also includes a more comprehensive survey of the history of grid-based methods that may be of interest to some researchers.

3. Dynamics

To propagate a state in time we use the SO method. This scheme first splits the total evolution time t in N shorter time intervals $\delta t = t/N$ such that

$$e^{-iHt} = \underbrace{e^{-iH\delta t} \dots e^{-iH\delta t}}_{N \text{ times}}. \quad (8)$$

Then, as the Hamiltonian in Eq. (1) can be separated into a kinetic part and a potential part, each short-time propagator $e^{-iH\delta t}$ can be approximated with the use of Trotterization:

$$\begin{aligned} e^{-iH\delta t} &= e^{-i(H_{\text{kin}} + H_{\text{pot}})\delta t} \\ &= e^{-iH_{\text{pot}}\delta t/2} e^{-iH_{\text{kin}}\delta t} e^{-iH_{\text{pot}}\delta t/2} + O(\delta t^3). \end{aligned} \quad (9)$$

We find that second-order Trotter decomposition is sufficient for our purposes.

To obtain the time-evolved state $|\psi(t)\rangle$, we need to apply the operator $U_{\text{SO}}(\delta t) := e^{-iH\delta t}$ to the initial state $|\psi(0)\rangle$ N times. In the grid-based formalism this can be done efficiently by switching between the *real-space* and *k-space* representations. Indeed, because of our choice of

encoding, H_{kin} is diagonal in k space, while H_{pot} can be approximated as diagonal in real space (see Appendix F).

III. EXCHANGE COUPLING

In this section we consider the practical task of estimating the exchange coupling J of a DQD structure. As J is directly related to the speed of two-qubit gates, any device that cannot generate a substantial exchange coupling is unsuitable as a qubit-qubit gating system.

The J coupling causes the spin singlet state to acquire phase with respect to all triplet states, and thus induces a continuous SWAP operation for our two qubits. The effect is not due to any direct (e.g., dipolar) interaction between spins, but rather it is a consequence of fermionic particle exchange antisymmetry: the spin singlet state must be associated with a symmetric charge state, and conversely spin triplet states must be associated with antisymmetric charge states. These charge states are appreciably distinct in energy, and the energy gap is highly sensitive to the size and shape of the confining double quantum dot potential.

To be specific, for two electrons trapped in a DQD the exchange coupling is defined as the difference in energies between the first two eigenstates of the spinless two-electron system (which indeed have opposite exchange symmetry). These eigenstates can be obtained by diagonalization of the Hamiltonian within our real-space basis. However, in the case of two electrons in two dimensions with M grid points per particle per direction (a total of M^4 basis states), the diagonalization becomes rapidly intractable. Nevertheless, by exploiting the distinct symmetries of the eigenstates with respect to electron swapping and using a state-preparation technique known as “imaginary-time evolution” (see, e.g., Ref. [35]), the grid-based method provides an efficient way of preparing them.

A. State preparation

Intuitively, for two electrons in a double quantum dot, the ground state and the first excited state should be close to symmetric and antisymmetric combinations of finding one electron on the left and the other on the right, respectively.

Our approach to initializing the system into its ground state and first excited state (the lowest-lying symmetric and antisymmetric charge states, respectively) is simply an imaginary-time evolution. This is convenient as it exploits the same machinery that we use for modeling the dynamics of the system; we need only adjust a line in our code to change from it to t in the Schrödinger equation, together with a convergence test and an adaptive δt .

Starting from a guess initial state that has some overlap with the true ground state—such as a symmetric combination of two Gaussians centered in each dot—propagation of the state with the use of an imaginary time guarantees

convergence to the true ground state $|s\rangle$ [35]. The ground state and the first excited state have distinct symmetries, and imaginary-time evolution preserves the symmetry of the starting state. Hence, starting with an antisymmetric combination of Gaussians, we will achieve convergence to the antisymmetric state with the lowest energy—namely, the first excited state $|a\rangle$. We can then estimate the $|s\rangle$ and $|a\rangle$ respective energies by computing their expectation value with respect to the Hamiltonian and then determine the exchange coupling by computing their difference. This method is completely general and can be applied to any DQD structure.

For realistic potentials, we will find that the states $|s\rangle$ and $|a\rangle$ include a finite probability of finding both electrons in the same quantum dot. However, when the barrier is large, we expect to be able to approximate them by

$$\begin{aligned} |s\rangle &\approx \frac{1}{\sqrt{2}} (|LR\rangle + |RL\rangle), \\ |a\rangle &\approx \frac{1}{\sqrt{2}} (|LR\rangle - |RL\rangle), \end{aligned} \quad (10)$$

with the probability of finding the electrons in the states $|LL\rangle$ and $|RR\rangle$ decreasing exponentially with the barrier height. Although this probability should become small, it is important to characterize it since it represents states for which qubits are not defined—finding the system in such a state would correspond to irreversible qubit loss.

Throughout this paper we use $|L\rangle$ ($|R\rangle$) to denote the state of an electron that is definitely on the left (right) quantum dot. This notation will be especially useful when we are defining our qubit states in Eq. (11). However, it is important to note that when approximating the symmetric and antisymmetric state as in Eq. (10), we are referring to specific charge wave functions (the eigenstates) localized on each quantum dot.

B. Numerical results

We computed J using the *ab initio* method described in the previous section, for different basis sizes, choices of quantum dot dimensionality, and representations of the Coulomb interaction. For each such choice, we swept through a range of potentials from “barrier up” to “barrier down” (see Fig. 2); the potentials were obtained from a commercial Poisson-solver tool provided with a certain device layout involving a central electrode (see Fig. 1 and Appendix A). Throughout our numerical study, where we use a 3D potential this is created by introducing a z -direction ramp [see Fig. 4(a)] to the corresponding 2D potential. This choice was made in order that the behavior of the 2D and 3D models can be compared directly without factors arising from, for example, small variations in the z -direction field across the x - y plane that would occur

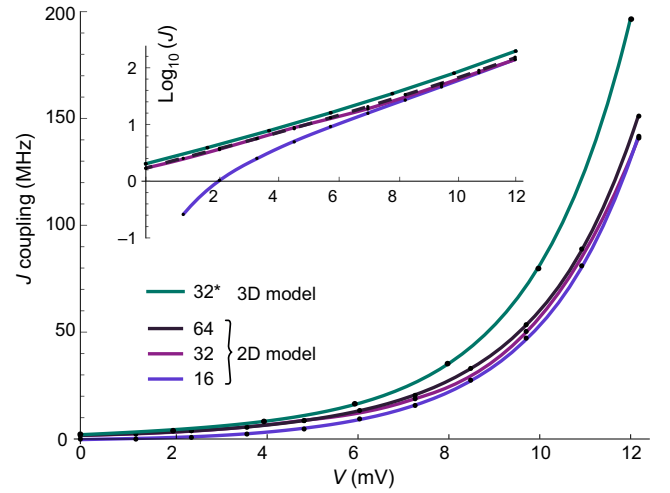


FIG. 3. Observed variation of the exchange coupling J with the barrier gate voltage V_g . The blue and purple lines correspond to a strictly 2D quantum dot modeled with 16, 32, and 64 basis states per particle, per dimension. One notes from the inset that the curves for 32 and 64 basis states are nearly identical (the 64 basis state line is shown dashed for visibility), while the lower basis size of 16 deviates in the low- J limit. The green curve corresponds to the far more computationally demanding 3D model; the basis size is 32 in the x direction (the axis along which the two quantum dots lie) and 16 in the orthogonal directions. One sees that the 2D model underestimates the J coupling strength appreciably.

in reality. The 3D numerical method does not depend on this simple structure, so its run-time and accuracy should be similar for any smoothly varying 3D potential.

Our first set of results are shown in Fig. 3, where several 2D quantum dot calculations (with various basis sizes) are compared with the far more computationally demanding 3D calculation. In all cases we retrieve the general exponential dependence of the exchange coupling with the barrier gate voltage, as expected from analytic treatments (see, e.g., Ref. [1]). The purple lines depict cases for a strictly 2D quantum dot; while noting broadly similar behavior for all resolutions, we observe that for the 16^4 case, there is a deviation from the expected behavior at low V_g (the “barrier up” scenario). The use of 32^4 is adequate to recover the expected exponential variation over the full range of V_g considered (see Appendix E for a more detailed convergence study). Further calculations (not shown) verified that a resolution of $(32 \times 16)^2$ suffices to obtain good low- J estimates, provided that the larger basis runs along the x axis (see Fig. 2, leftmost panel).

The green line represents the data from the computationally expensive full 3D quantum dot simulation. The potential differs from that in the 2D case by the addition of a z -direction component that ramps linearly up with depth, and an abrupt interface “wall” [see Fig. 4(a)]. The grid-based model used a total basis size of $(32 \times 16 \times 16)^2 \approx$

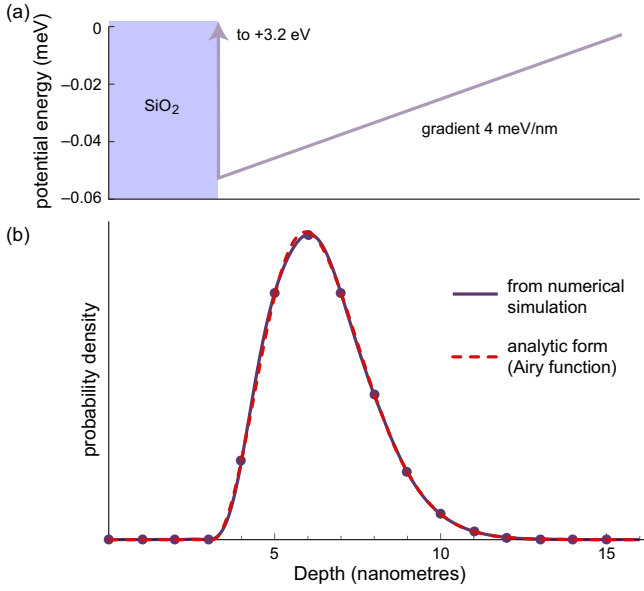


FIG. 4. (a) Variation in potential within the 3D double quantum dot in the z direction (the x,y location corresponds to a quantum dot minimum). The potential is linear, ramping at 4 meV/nm. (b) Probability density for an analytic Airy function solution to a one-dimensional problem with the potential from (a), but taking the step to be infinite. One sees that this analytic form is a near-perfect match to the probability density that is obtained from our *ab initio* calculation for the full 3D quantum dot potential.

67×10^6 , where the larger basis size 32 runs long the x axis (the axis along which the two minima of the double quantum dot lie). By repeating the 3D calculation for somewhat higher resolutions, we confirmed that there was negligible variation in the predicted J .

Intuitively, it is not unexpected that the introduction of finite width is significant. Recall that the Coulomb interaction actually *reduces* the exchange coupling, by forcing electrons further apart and reducing their amplitude in the crucial central region, where the state's symmetry is most significant. By allowing the electrons to move in a third dimension, we reduce the impact of the Coulomb interaction and thus increase the exchange coupling [1].

We investigated the extent to which a modified 2D model could replicate the J strength predictions of the full 3D model. We began by inspecting the probability density in the z direction, according to the full wave function solution. Specifically, we compared the numerically obtained probability density with the analytic solution to a one-dimensional model in which the interface step is infinite (noting that the finite step used in the 3D model, 3.2 eV, is extremely severe). The numerically obtained solution is remarkably close to the analytic form; see Fig. 4(b). We therefore proceeded to adjust the

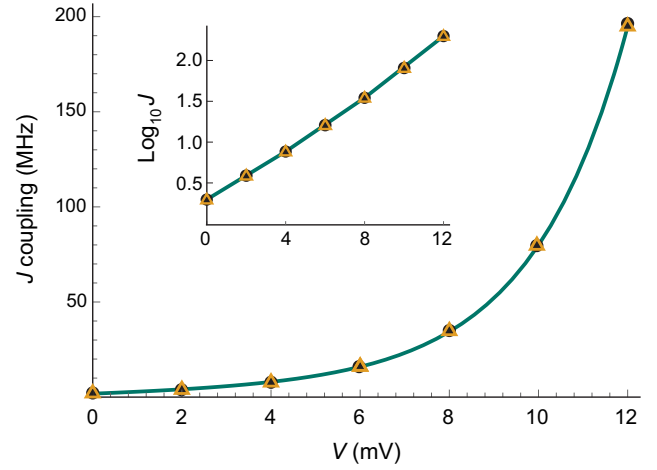


FIG. 5. Performance of our resource-efficient quasi-3D model, which uses a 2D space and an adjusted Coulomb interaction. The black dots correspond to the true 3D model, and are the same data as in the green line in Fig. 3. The triangles denote the predictions made from the quasi-3D model. One sees that the match is near perfect; in fact, the quasi-3D model slightly underestimates J by deviation of between 0.6% and 0.8%.

2D Coulomb interaction using the analytic Airy function solution, noting that the process does not use any information gained from the full 3D model. The method we used is explained in Appendix F. In essence, we derive a whole set of 2D Coulomb interaction matrices, each of which has a fixed Δz offset between the two particles. Then we find the average of these matrices, weighted by the Airy-function probability distribution. This has the effect of softening the Coulomb interaction at short range.

The J versus V_g curves for 2D quantum dots versus 3D quantum dots are compared in Fig. 5. One observes that the match is excellent, indicating that for quantum dots of this kind—i.e., with negligible irregularity in the z confinement over the lateral extent of the quantum dot—this of quasi-3D approach can offer an excellent trade-off of accuracy versus numerical efficiency [36].

Because the assignment of a mean z depth of the electrons is a choice that makes our models specific to only quantum dots of that geometry, in the rest of this paper we use the pure 2D Coulomb interaction. While noting, of course, that this is in some sense the least “realistic” option, we emphasize that the phenomena that we presently identify are qualitatively robust regarding the introduction of a small finite z depth: There is no qualitative impact on the physics observed during the dynamics. The only meaningful change will be the speed of the gates. Moreover, it is straightforward to recalculate any given set of results for a specific $\langle z \rangle$.

IV. EXCHANGE GATE DYNAMICS

We now focus on the dynamics of our two-electron system. Specifically, we are interested in extracting two-qubit gate fidelities and loss probabilities for different voltage profiles. But first, we need to define our qubits' states.

A. Qubit states

For two electrons in a DQD in the $(1, 1)$ charge configuration, the qubit states are defined as follows:

$$\begin{aligned} |00\rangle &:= \frac{1}{\sqrt{2}} (|LR\rangle - |RL\rangle) |\downarrow\downarrow\rangle, \\ |01\rangle &:= \frac{1}{\sqrt{2}} (|LR\rangle |\downarrow\uparrow\rangle - |RL\rangle |\uparrow\downarrow\rangle), \\ |10\rangle &:= \frac{1}{\sqrt{2}} (|LR\rangle |\uparrow\downarrow\rangle - |RL\rangle |\downarrow\uparrow\rangle), \\ |11\rangle &:= \frac{1}{\sqrt{2}} (|LR\rangle - |RL\rangle) |\uparrow\uparrow\rangle, \end{aligned} \quad (11)$$

where the arrows represent the spin states of the electrons. The state of a qubit is given by the spin of an electron found in a specific quantum dot. For instance, $|01\rangle$ represents the state in which we have an electron with spin down on the left quantum dot and an electron with spin up on the right quantum dot. This state is naturally given by the antisymmetrization of the distinguishable-electrons' state $|LR\rangle |\downarrow\uparrow\rangle$, in which we find the first electron on the left quantum dot with spin down and the second electron on the right quantum dot with spin up. Note that the singlet $S(1, 1)$ and triplet $T_0(1, 1)$ states can be retrieved as follows:

$$\begin{aligned} S(1, 1) &= \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle), \\ T_0(1, 1) &= \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle). \end{aligned} \quad (12)$$

To study two-qubit gates within our model, we need to be able to initialize our electrons in the qubit states defined in Eq. (11). However, it is important to appreciate that the valid qubit states defined in Eq. (11) will not suffice to completely describe the state of a real double quantum dot structure. This is because the true eigenstates of the system, $|s\rangle$ and $|a\rangle$, are only imperfectly described with the use of the $|LR\rangle$, $|RL\rangle$ states [with the imperfect association as given in Eq. (10)]. In reality there is always some finite probability associated with $(2, 0)$ and $(0, 2)$ charge configurations, i.e., $|LL\rangle$ and $|RR\rangle$, which lie outside the qubit subspace and thus constitute qubit loss outcomes. With that

said, the approximate association is given by

$$\begin{aligned} |00\rangle &\approx |a\rangle |\downarrow\downarrow\rangle, \\ |01\rangle &\approx \frac{1}{2} ((|s\rangle + |a\rangle) |\downarrow\uparrow\rangle - (|s\rangle - |a\rangle) |\uparrow\downarrow\rangle), \\ |10\rangle &\approx \frac{1}{2} ((|s\rangle + |a\rangle) |\uparrow\downarrow\rangle - (|s\rangle - |a\rangle) |\downarrow\uparrow\rangle), \\ |11\rangle &\approx |a\rangle |\uparrow\uparrow\rangle, \end{aligned} \quad (13)$$

with the approximation becoming better as the barrier gets larger. This encoding naturally enforces a coherent oscillation (with frequency J) between the states $|01\rangle$ and $|10\rangle$.

As noted earlier, adding the spin degree of freedom is done by taking the tensor product of the charge states defined in Eq. (6) with an array of length 2 encoding the spin state. The generalization to two particles is straightforward. It is worth realizing that as we are using a first-quantized representation, the antisymmetry of the wave function is enforced in the states and is conserved through the evolution in time. Finally, note that our solver cannot be directly applied to hole spin qubits in its current form. The construction of the qubit states would need to be modified, since holes exhibit stronger spin-orbit coupling.

B. Numerical results

While multiple two-qubit gates are made possible from the exchange interaction [11], in this work we focus on the entangling $\sqrt{\text{SWAP}}$ gate, which naturally appears when a homogeneous magnetic field is considered. Initially we thus suppose that the g -factor in each quantum dot is the same. In that case, the gate is realized by pulsing the barrier gate voltage such that $\int_0^T \sqrt{\text{SWAP}} J(t) dt = \pi/2$. In Sec. VI we study the impact of having different g -factors. For simplicity, we focus on simple pulse sequences in which we smoothly ramp the potential from one with a large barrier (exchange off) to one with a small barrier (exchange on). It is worth noting that our tool can handle any evolution of the potential with time.

Starting from the state $|01\rangle$ defined as in Eq. (13), we perform a $\sqrt{\text{SWAP}}$ operation by dynamically changing the barrier gate voltage according to the schedule given Fig. 6. The rising and falling times were chosen to prevent nonadiabatic effects (as discussed later), while minimizing gate time—ramping over the course of approximately 1 ns is consistent with current technological capabilities.

After the dynamics are simulated, we must measure the performance of the gate. Finding that the state at the end of the gate satisfies $P(|01\rangle) = P(|10\rangle) \approx \frac{1}{2}$ is of course insufficient to conclude that we indeed perform a $\sqrt{\text{SWAP}}$ gate. To characterize the quality of the gate, we need to introduce more nuanced measures. Suppose we are given a general quantum state $|\psi\rangle$ encoded in real space as

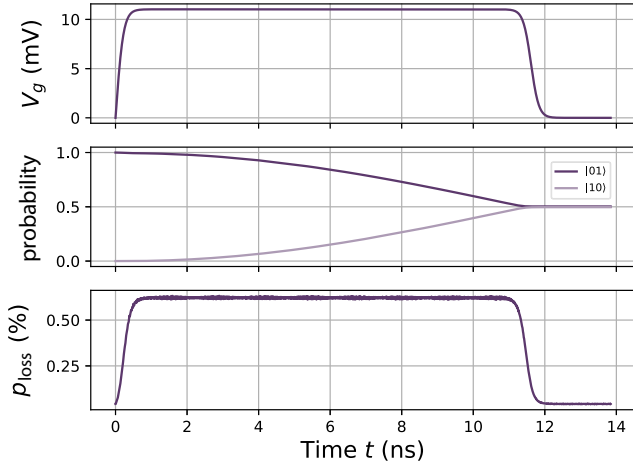


FIG. 6. Smooth $\sqrt{\text{SWAP}}$ pulse. Top: Barrier gate voltage profile, with V_g being the difference in potential between the bottom of the wells and the barrier at the midpoint ($x = y = 0$). We smoothly switch on the exchange interaction to minimize loss. Middle: Probability of finding the electrons in the $|01\rangle$ (dark) and $|10\rangle$ (light) states. We observe a near-perfect transfer to the desired superposition at the end of the process with infidelity $1 - F = 1.32 \times 10^{-5}$. Bottom: Probability p_{loss} of finding the electrons in the charge $(2, 0)$ or $(0, 2)$ configuration and hence outside the qubit subspace. It is worth noting that for our initial state we have a small probability $p_{\text{loss}} = 0.04\%$ of the electrons being in the $(2, 0)$ or $(0, 2)$ configuration. At the end of the process, we recover a practically identical value for p_{loss} and conclude that our adiabatic pulse does not increase the loss (even though if one were to perform a measurement of the charge distribution *midway* through the gate it *would* cause appreciable loss probability).

follows:

$$|\psi\rangle = \sum_i |\Omega_i\rangle (a_i^{\downarrow\downarrow} |\downarrow\downarrow\rangle + a_i^{\downarrow\uparrow} |\downarrow\uparrow\rangle + a_i^{\uparrow\downarrow} |\uparrow\downarrow\rangle + a_i^{\uparrow\uparrow} |\uparrow\uparrow\rangle),$$

where the constants can have any values provided that overall antisymmetry is respected. Here the set of states $\{|\Omega_i\rangle\}$ is some relevant basis of two-particle charge states—for example, the grid-based Dirichlet basis used in our model.

We wish to measure how close this state is to a given qubit state $|Q\rangle$ that would typically be written in the form

$$\begin{aligned} |Q\rangle &= a_{00} |00\rangle + a_{01} |01\rangle + a_{10} |10\rangle + a_{11} |11\rangle \\ &= \frac{1}{\sqrt{2}} (|LR\rangle (a_{00} |\downarrow\downarrow\rangle + a_{01} |\downarrow\uparrow\rangle + a_{10} |\uparrow\downarrow\rangle \\ &\quad + a_{11} |\uparrow\uparrow\rangle) - |RL\rangle (a_{00} |\downarrow\downarrow\rangle + a_{01} |\uparrow\downarrow\rangle \\ &\quad + a_{10} |\downarrow\uparrow\rangle + a_{11} |\uparrow\uparrow\rangle)). \end{aligned} \quad (14)$$

(Notice the different kets associated with a_{01} in each line, and similarly for a_{10}). In our target state we have used the

conventional $|LR\rangle$ notation to indicate that electron 1 is definitely in the left side of the structure, and electron 2 is definitely on the right (and conversely for $|RL\rangle$). States such as $|LL\rangle$ or $|RR\rangle$, with both electrons on the same side, are not legitimate qubit states. Therefore, in measuring the match between $|\psi\rangle$ and $|\phi\rangle$, we can start by projecting out any $|\Omega_i\rangle$ that correspond to the $(2, 0)$ and $(0, 2)$ configurations, recording the probability of being in this nonmeaningful subspace as p_{loss} .

The fidelity *within* the qubit subspace is then to be determined. Importantly, we are not concerned with the detailed shape of the charge distribution; thus, for example, if the a_i coefficients in Eq. (14) are correct, then the fidelity is unity regardless of the specifics of the charge state $|LR\rangle$ (and its label-exchanged converse $|RL\rangle$). Therefore, we write

$$F(|Q\rangle, |\psi\rangle) := \sum_{\text{all } |LR\rangle} |\langle Q|\psi\rangle|^2,$$

where we are summing over all variants of the target $|Q\rangle$ defined by Eq. (14) using a complete basis of states $|LR\rangle$ (i.e., all the states with a $(1, 1)$ charge distribution). Fortunately the calculation of this fidelity in the grid-based representation is straightforward.

This expression gives us the fidelity of a given state. The fidelity of the gate itself follows relatively straightforwardly simply by inspection of the state fidelity (versus the ideal) of two cases: that of an input state $|Q_{\text{in}}\rangle$ that is symmetric under qubit exchange, and that of an input state $|Q_{\text{in}}\rangle$ that is antisymmetric. This suffices to infer the state fidelity of any output, and hence the gate fidelity under any chosen definition. We chose the definition of gate fidelity as being the worst-case fidelity, i.e., the state fidelity for input $|Q_{\text{in}}\rangle$ that minimizes $F(|Q_{\text{out}}\rangle, |\psi\rangle)$ where $|Q_{\text{out}}\rangle$ is the ideal output. This will be any equal superposition of a symmetric and an antisymmetric qubit state, and thus the state $|01\rangle$ itself is suitable; see Eq. (13).

In this case, our pulse should ideally achieve the target state $|Q\rangle = (|01\rangle - i|10\rangle)/\sqrt{2}$. As noted earlier, if we begin from a state in the lowest two eigenstates, then there is a small initial amplitude associated with the states having a $(2, 0)$ or a $(0, 2)$ charge distribution. For the optimized gate, the eventual p_{loss} corresponds only to this initial imperfection. The increase of p_{loss} during the gate is because in this exchange coupling regime, the overlap with states outside the computational subspace is bigger (which is inevitable to obtain large J). The action of the gate itself introduces *zero loss probability* (to within the numerical noise in the model of approximately 10^{-7}). Moreover, the infidelity within the qubit subspace process is very small, $1 - F = 1.32 \times 10^{-5}$. We thus verify that with the chosen voltage profile, one achieves a near-perfect $\sqrt{\text{SWAP}}$ gate when starting from $|01\rangle$ (and by symmetry, also when starting from $|10\rangle$). As a comparison, if we

abruptly switch the barrier (see Appendix B), p_{loss} is dramatically increased and can exceed 1%, and even once this component is removed, we obtain only the limited fidelity $F = 97.9\%$. This underscores the importance of a proper voltage switching profile, i.e., achieving near-adiabatic dynamics.

Whereas the ideal system can be adjusted to very high (near-perfect) gate operation, this does not account for imperfect environments. We now discuss the impact of charge irregularities.

V. IMPACT OF CHARGE NOISE ON EXCHANGE GATE

To adequately model the noise hindering the performance of silicon spin qubits, we first need to understand its nature. Multiple experimental groups have performed noise spectroscopy and they found that noise follows a $1/f$ -like behavior [37–40]. Such noise is commonly associated with charge noise, and it is believed that it can be well-modeled with the use of a large number of two-level fluctuators [22]. Several studies have considered baths of fluctuators [22,41,42] to model this regime. Recent studies [43] have shown that, for some devices, only a few two-level fluctuators are present, breaking the $1/f$ -like model. We complement prior modeling work by exploring the interesting case of a single fluctuator strongly coupled to the DQD [19,21]. We leave more diverse two-level fluctuators (e.g., dipoles) for future work.

As shown in Ref. [21], considering the time it takes to perform a single $\sqrt{\text{SWAP}}$ gate, one expects that there will be more static charge defects than fluctuating charges within the period of a single gate operation. Hence, we first limit ourselves to static charges, before looking at the rarer, albeit more interesting, case of fluctuating charges.

A. Static charge

The trapped charge is modeled classically by adding an extra Coulomb interaction to Eq. (1) with respect to each electron in the DQD:

$$H_{\text{SC},i}(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0\epsilon_r|\mathbf{r} - \mathbf{r}_i|^2}, \quad (15)$$

with $\mathbf{r} = (x, y, z)$ and $\mathbf{r}_i$ the position of the charge and the position of the i th electron, respectively. The charge is randomly placed at the silicon oxide interface $z \approx 2$ nm above the DQD and on the symmetry axis of the double quantum dot (the x axis, i.e., $y = 0$). By placing the charge along this axis, we are exploring situations in which the charge has the most impact. In Appendix C, we explore the more general setting of off-axis charge defects.

When a single charge is located near a DQD, it displaces the trapped electrons, altering the overlap between their

TABLE I. Exchange coupling, loss probability, and state-to-state fidelity as a function of the position of the charge. The charge position (in the quantum dot line) is given as a distance from the center of the DQD, which is positioned at $(0, 0, 0)$. As the exchange coupling is a static property, it has been computed with the 32^4 resolution. However, as the loss and fidelities are obtained after simulation of the dynamics, we only used a 16^4 resolution, which we do not expect to change much (see Fig. 3).

	Charge position (nm)				
	50	75	100	150	200
J (MHz)	507	202	168	155	153
p_{loss} (%)	0.14	0.06	0.05	0.05	0.04
F (%)	22.41	92.11	99.10	99.95	99.99

wave functions and hence modifying the exchange coupling. This increases as the charge gets closer to the DQD (see Table I). However, the trend breaks down when the charge is between the two electrons. We assume that the gate has been calibrated in the absence of a charge defect, i.e., as operators we are unaware of it and thus we use the same pulse as in the noiseless case to perform our gate. As the exchange coupling is modified by the presence of the charge, the pulse no longer yields a high-quality gate.

In Fig. 7, we report the evolution of the qubits' state and p_{loss} for a charge positioned at $x = 50$ nm (purple) and $x = 100$ nm (green) with respect to the center of the double quantum dot structure ($x = y = 0$). Assuming that the system has previously relaxed into the eigenstates of the modified potentials, our initial state $|01\rangle$ differs from that computed earlier and now has a larger initial value of p_{loss} . We note that the control pulse still gives us an adiabatic evolution. Nevertheless, we find that the fidelity decreases drastically with charge proximity because of the timing error. In Table I, we report the evolution of F and p_{loss} for various charge positions.

B. Fluctuating charge

Although most charge defects may be static on the timescale of a $\sqrt{\text{SWAP}}$ operation, it is important to study the impact of a charge that moves during a gate operation. While there are a vast range of interesting scenarios that can be studied by the methods we use here (e.g., a charge moving randomly in three dimensions), we focus on a charge fluctuating instantaneously between two trap locations.

We take two approaches to exploring the effect. In the first, we specify that the charge oscillates between $\mathbf{r}_{\text{init}} = (100, 0, 2)$ nm (its initial position) and $\mathbf{r} = (x, 0, 2)$ nm for various values of x . We expect that the impact will be greater as the two positions are far from one another. We also suppose that the experiment has been calibrated such that one has modified the barrier gate voltage profile such that we obtain an optimal $\sqrt{\text{SWAP}}$ gate in the presence of a

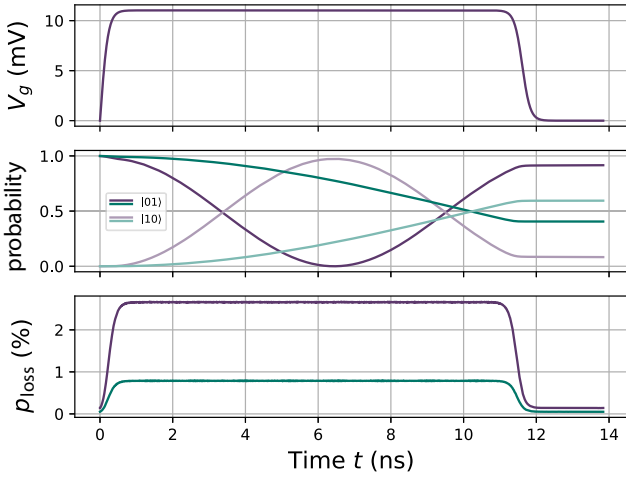


FIG. 7. Smooth $\sqrt{\text{SWAP}}$ pulse in the presence of charge noise. Top: As we assume the operator does not know that the defect charge is present, we use the evolution of the barrier gate that works optimally in the defect-free case (i.e., upper the panel is the same as in Fig. 6). Middle: Probability of finding the electrons in the $|01\rangle$ (dark) and $|10\rangle$ (light) states for a charge positioned at $x = 50$ nm (purple) and $x = 100$ nm (green), respectively. The presence of charge noise generates an error in the $\sqrt{\text{SWAP}}$ gate as it modifies J . There is also an increased value for p_{loss} during the gate operation, as compared to the noiseless gate (Fig. 6), but at the end of the gate it returns to the initial value and thus the operation does not *increase* the loss—it is still effectively adiabatic.

charge at $\mathbf{r}_{\text{init}}$. In the second approach, described presently in the context of robust pulses, we consider fluctuators with a fixed 10 nm separation but various mean locations. A charge could tunnel between nearby defects on the scale of a few nanometers. Here we consider a slightly worse case to show the power of our robust pulse sequence.

The nature of the two-level fluctuators that will be most problematic for quantum processes is an active topic in the literature, and the mismatch between whole-charge fluctuations and experimental power spectral densities have been documented in Ref. [21]. Here our aim is to demonstrate the flexibility of our numerical tool by investigating one potentially damaging form of a two-level fluctuator.

In Fig. 8, we study the impact on the gate of a charge oscillating between $\mathbf{r}_{\text{init}}$ and $\mathbf{r} = (75, 0, 2)$ nm. We randomly chose the times (dashed green lines) at which the charge moves and we limited the number of fluctuations to at most three (see Appendix D for other examples). We limit ourselves to three fluctuations as these scenarios become less and less probable as the number of fluctuations increases.

It is interesting to note that instantaneously changing the position of the charge during the gate has a similar effect as when we too-abruptly switch the barrier voltage (see Appendix B). The sudden (nonadiabatic) nature of the change is damaging. However, as the charge does not

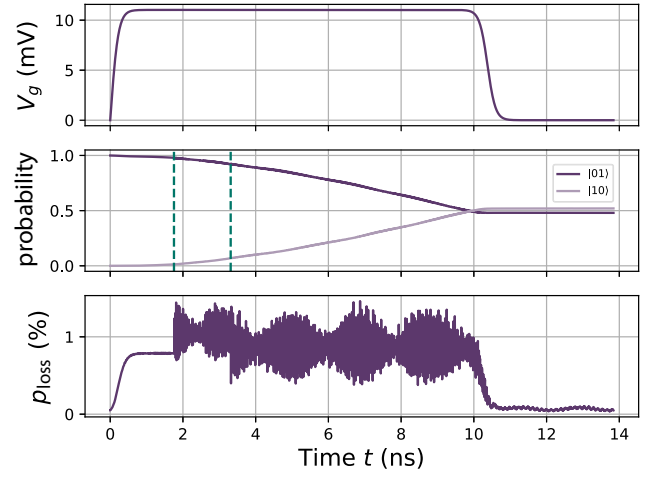


FIG. 8. Smooth $\sqrt{\text{SWAP}}$ pulse in the presence of a fluctuating charge. The charge oscillates between its initial position $\mathbf{r}_{\text{init}} = (100, 0, 2)$ nm and $\mathbf{r} = (75, 0, 2)$ nm at each green dashed line.

move too closely to the DQD in this example, the change in potential is small here, and hence the impact of the fluctuation is relatively minor (see the last row of Fig. 13 for more drastic effects). Regarding p_{loss} , we note that even after the end of the gate, we still have some oscillations. We take the average over the time remaining after the gate and find that $p_{\text{loss}} = 0.07\%$ and $F = 99.71\%$. Contrary to the previous cases, we now for the first time see an increase in p_{loss} , which is the worst type of error as it cannot be corrected. A fluctuating charge is thus more damaging than a static one when it comes to gate quality.

Now that we have identified how charge noise modifies the quality of the gate, we access the vast literature on robust pulse sequences to begin to explore methods to mitigate these errors.

VI. ROBUST PULSE SEQUENCES

A. Types of error

When a gate is being performed, three types of imperfection can arise. We already saw two of them in the previous section: First, the loss coming from driving the electrons into the $(0, 2)$ and $(2, 0)$ configurations (and thus outside the qubit subspace) when the potential is being modified. Second, the error generated by charge noise that modifies the exchange coupling J between electrons and that ultimately leads to uncertainty in the gate time, lowering the fidelity of the operation. Finally, a nonideality that we have ignored until now arises from magnetic detuning between quantum dots. If the g -factors between the quantum dots are different, the qubits within the double quantum dot will not experience a pure SWAP-type operation: Consider a Bloch sphere for the qubit subspace $|01\rangle, |10\rangle$ [as defined in Eq. (11)]. Then rather than an on-axis rotation, in the presence of a g -factor discrepancy the qubit state will

rotate around a tilted axis. We now consider this effect, i.e., we assume each quantum dot's g -factor is indeed different. For simplicity we assume that the g -factor is uniform across each half of the double quantum dot structure, changing abruptly at the center (i.e., at $y = 0$). This is obviously oversimplified, but allows us to make contact with prior treatments—note, however, that the numerical methods described here can tackle any spatially varying g factor.

While in the case of a well-characterized environment the first type of error (qubit loss) can be reduced by the use of an adiabatic pulse, we observed that in the presence of unknown charge fluctuations, it cannot be corrected. However, as we explore below, the other types of error can be mitigated even in the presence of unknown charge environments.

It is also worth observing that a two-qubit gate that is off-axis in the sense described above is nevertheless adequate as a computationally universal gate, given suitable single-qubit rotations. Therefore, one could argue that the natural rotation is acceptable (once characterized) and does not require correction at the pulse level. However, in a device with thousands or millions of such structures, the ability to homogenize their action is likely to be valuable.

B. Robust pulse sequence

Robust pulse sequences or composite pulse sequences have been devised and implemented over several decades by the NMR community to mitigate the effect of experimental imperfections [23]. They can also be used in the context of quantum computation to reduce the last two types of error mentioned above (see, e.g., Refs. [24,25]).

There are two different classes of composite pulses: those that are efficient for a subset of initial states and those that are error-tolerant for any initial state (also known as “fully compensating pulses”). In this work we focus on a fully compensating pulse that generates a $\sqrt{\text{SWAP}}$ gate.

This type of pulse (or pulse sequence) will generally take longer to apply than the naive one. Hence, grid-based methods may become impractical for the search for robust pulse sequences: the large number of time steps we need to propagate the full wave function is compounded by the need to assess each candidate sequence against a variety of charge defect scenarios. Fortunately, we can restrict the use of the full grid-based model to characterizing p_{loss} and providing certain key parameters that we can then use to construct a simpler model with a far smaller subspace. In our case, the subspace of interest is spanned by the states $|01\rangle$ and $|10\rangle$. In this subspace, the time-dependent Hamiltonian is given by

$$H(t) = J(V_g(t))\sigma_x + \Delta E_z\sigma_z, \quad (16)$$

with the dependence of J on V_g having been extracted from the grid-based method. Here ΔE_z is the difference in Zeeman energy between the two quantum dots due to their difference in g -factor and σ_z, σ_x are the standard Pauli Z and Pauli X operators, respectively. We set $\Delta E_z = J_{\text{on}}/20$ (with J_{on} the maximal exchange value obtained when the interaction is switched on), which is a typical value for the magnetic detuning [44]. Since ΔE_z is assumed to be fixed and nonzero, we cannot directly perform a pure x rotation for any value of our controllable parameter J . However, different values of J will result in rotations around different axes within the relevant quadrant of the x - z plane

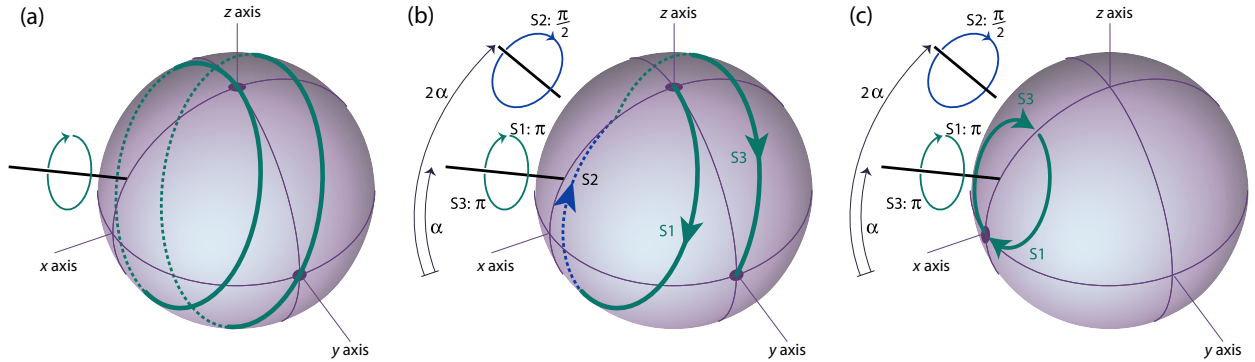


FIG. 9. (a) Off-axis nature of the “natural” gate when the two quantum dots have distinct g -factors: one cannot achieve a pure x rotation (thus the two states marked with purple dots do not evolve into one another). (b),(c) The basic “ABA” pulse sequence that corrects the off-axis rotation error. The first and last of the three steps (marked green) correspond to the same rotation, by π about an axis making an angle α with respect to the x axis. The middle step (marked blue) is a $\pi/2$ rotation about an axis that makes an angle 2α with respect to the x axis. In (b) one sees that the state $|01\rangle$ at the north pole undergoes a net rotation to $(|01\rangle + i|10\rangle)/\sqrt{2}$ as desired (the two filled purple dots mark these states). In (c) we see that the same sequence maps the state marked with the purple dot onto itself, acquiring only phase, since the first pulse leaves it as an eigenstate of the second pulse (i.e., on that pulse’s axis). Together, (b),(c) imply that we have synthesized the desired ideal rotation about the x axis. Note that the angle α is exaggerated for this schematic, as compared with the value in the pulse sequence ($\alpha \approx 7.8^\circ$).

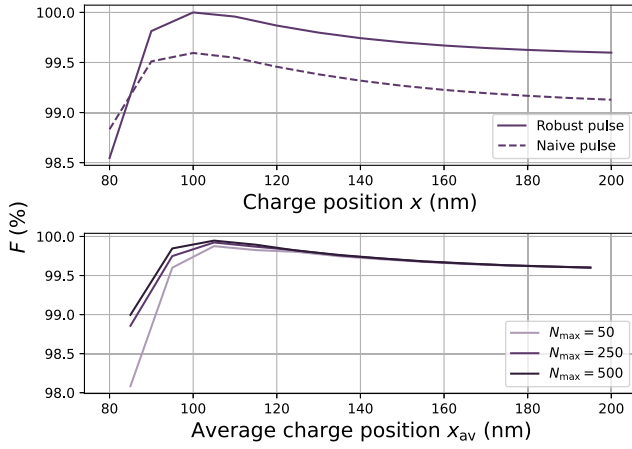


FIG. 10. Evolution of the fidelity when the robust pulse sequence is used for a static charge (top) and a fluctuating charge (bottom). For the fluctuating case, the charge oscillates between two traps located at a fixed 10 nm distance; the horizontal axis in the graph is the mean charge position. The number of fluctuations during the pulse is drawn uniformly at random between $N = 1$ and $N = N_{max}$. Additionally, the switching times are randomly chosen between $t = 0$ and $t = T_{\sqrt{\text{SWAP}}}$. Each curve is obtained by averaging 10^4 instances of such a random environment. For the naive case, we used a maximal J coupling equal to the strongest one appearing in the robust pulse sequence.

(see Fig. 9). This freedom allows us to construct interesting sequences.

The ideal composite pulse would implement a high-fidelity on-axis rotation (around the x axis), despite both the off-axis nature of the primitive evolution and the problem of charges in the environment. One should aim for a fully compensating sequence that does so for *any* input state, i.e., a good match to the ideal unitary.

We explored several potential sequences, and we report the performance of one successful option in Fig. 10. This is a relatively complex sequence with nine steps. In creating this sequence, our approach was to begin with a simpler sequence of the form ABA , which is well-known [26] to correct off-axis errors, confirming that this does so in the absence of charge noise (see Fig. 9). Then we divided this sequence into two equal parts as $(A(B/2))(B/2)A$, and looked for additional pulses that could be inserted into the middle in order to compensate for the charge noise effects. We adapted another solution used in the NMR literature [26] whereby we rotate the state by π about an axis approximately perpendicular to the x - z plane (requiring two pulses in our case) and then perform a full 2π rotation about an axis in the x - z plane, before reversing the earlier π rotation. The net effect is to accumulate charge-induced rotation of sign opposite the sign that occurs in the unembellished ABA sequence—thus the charge-induced errors that occur “naturally” are largely negated by those that we “deliberately” accumulate.

This specific fixed sequence is effective in a range of charge scenarios. With a numerical search, it can be further tuned (without presuming foreknowledge of the charge environment) to make it maximally effective against charge impurities at a given distance, at the cost that the sequence will no longer implement a perfect gate in the case of a pristine zero-charge environment. This is the approach taken for the sequence whose performance is shown in Fig. 10.

While the sequence we have explored here does indeed boost gate fidelity, this comes at the cost of greatly increasing the total gate time. Compared with the naive pulse that allowed us to perform a $\sqrt{\text{SWAP}}$ gate in $T_{\sqrt{\text{SWAP}}} \approx 12$ ns in Fig. 6, the robust pulse sequence leads to $T_{\sqrt{\text{SWAP}}} \approx 1.9$ μ s. We emphasize that we did not perform a systematic search for more compact sequences, and this is an interesting challenge for future work.

C. Numerical results

As we are interested in fully compensating pulses, our measure of fidelity should now focus on comparing the implemented unitary to the target one, rather than comparing specific states. In this section we define the fidelity F as [45]

$$F(U, U_{\text{target}}) := \frac{d + \text{Tr}(U^\dagger U_{\text{target}})^2}{d(d+1)}, \quad (17)$$

with $U_{\text{target}} = U_{\sqrt{\text{SWAP}}}$ restricted to the subspace spanned by the states $\{|01\rangle, |10\rangle\}$ and $d = 2$.

At the top of Fig. 10, we plot the evolution of F for different positions of a static charge impurity when using the naive and robust pulses. In this section we use a maximal J coupling equal to the strongest one appearing in the robust pulse sequence for the naive pulse. By tuning the robust pulse sequence such that the maximal fidelity is obtained when $x = 100$ nm, we obtain an increased fidelity over a large range of positions. As a consequence, the pulse cannot generate a perfect $\sqrt{\text{SWAP}}$ gate in the limit of an infinitely remote impurity (or no impurity). As the charge becomes very close to the DQD, we see that inevitably the fidelity starts to drop drastically. Broadly one would expect that the (unexpected, uncalibrated for) presence of a defect charge directly above the double quantum dot would be catastrophic for gate fidelity regardless of mitigation efforts—effectively that quantum dot structure would be, at least temporarily, nonfunctional as a computing component. If we wished to study these scenarios more comprehensively, a finer model of the impurity would be necessary to reach meaningful results (likely promoting the impurity to being modeled as a full quantum entity).

As the pulse sequence is 2 orders of magnitude longer than the naive one, we might expect to have a significant number of fluctuations during the process. It is important to note that by switching from the grid-based method to this

lower-dimension model, we lost the ability to track the loss probability. However, for the positions of the charge considered here, p_{loss} is small and is not drastically modified by the charge fluctuations as reported in Fig. 13.

At the bottom of Fig. 10, we plot the evolution of F for different average positions of the charge x_{av} in the quantum dot line (which is the worst case). Having an average position x_{av} represents the situation of a charge oscillating between two traps positioned at a fixed distance of 10 nm around x_{av} . For instance, for $x_{\text{av}} = 95$ nm, the charge oscillates between $x = 90$ nm and $x = 100$ nm. Given that the number of fluctuations N and their timings $\{t_i\}_{1 \leq i \leq n}$ are unknown, both are randomly generated such that N is uniformly selected between $N = 1$ and $N = N_{\text{max}}$, while the t_i are drawn randomly between $t = 0$ and $t = T_{\sqrt{\text{SWAP}}}$. Each curve is the result of averaging over 10^4 instances of such a random environment.

In this plot, we can distinguish two different regimes. On the one hand, when the average position of the charge is far from the DQD, the number of fluctuations has negligible impact. This aligns with the trend observed in Table I—the farther the charge is from the quantum dot, the smaller the change in the exchange coupling. Hence, fluctuation between two positions around x_{av} that yield a similar J leads to a fidelity similar to that of a fixed charge at x_{av} , irrespective of the number of fluctuations. This also explains why we retrieve a similar evolution as in the static case (solid purple line at the top of Fig. 10). On the other hand, when the charge oscillations occur closer to the quantum dot, the difference in the impact on J between the two traps is larger, resulting in a smaller fidelity. However, with an increasing number of fluctuations, the fidelity increases and tends to converge toward that of the static case.

In both the static charge scenario and the fluctuating charge scenario, our pulse sequence shows improvements on the fidelity over a large range of positions, thus accommodating various charge environments. We believe this demonstrates the modeling approach taken here can readily be used to seek and validate robust pulses, potentially allowing the discovery of various sequences that yield high-fidelity gates.

VII. FUTURE DIRECTIONS AND CONCLUSION

In this work we present a versatile modeling approach able to simulate electrons and their spins in double quantum dots. Using realistic potentials, the tools we use are able to identify promising devices by computing the exchange coupling, an important metric in the realization of two-qubit gates. Moreover, the tools can fully simulate the qubits' dynamics and allow one to study various voltage control pulses in order to increase gate fidelities as well as reduce the (highly damaging) risk of losing qubits.

Using a two-level fluctuator model, we explored different scenarios in which a single charge trapped near the DQD impacts the quality of the gate. For a static charge, we found that the fidelity can be quite heavily impacted, whereas the loss stays constant (provided a suitable adiabatic control pulse is used). However, for a randomly oscillating charge, there is an impact on both the fidelity and the loss. While the impact on the fidelity can be mitigated with the use of robust pulse sequences, as shown for a reduced model, the effect on the loss cannot be removed for unknown environments.

The versatility of the grid-based methods opens many other future directions. Our study demonstrated that a quasi-2D method can near-perfectly replicate the results of a far more numerical costly 3D solution. It would be interesting to explore this for cases where the z confinement is irregular, making the mapping to two dimensions more challenging. The complexity of the Hamiltonian could also be increased to incorporate more physical phenomena; expansion of our model by the addition of spin-orbit interaction terms will be interesting to study. The same is true for adding the valley degree of freedom and valley-orbit coupling terms. With the valley degree of freedom incorporated, increasing the model's resolution to capture interface roughness (at the interface where the electrons are confined) would be very interesting. Finally, the introduction of interactions between two-level fluctuators and the modification of the model to treat them as distinct quantum particles are other potential areas for investigation.

To conclude, our approach and the tools we have developed set the stage for a software pipeline that takes as input a chip layout defined in software used to design traditional chips, and returns two-qubit gate performances for realistic noise environments. It is worth noting that we have not investigated single-qubit gates or other types of two-qubit gate in this work, but it would be a natural extension of the methods here to do so.

ACKNOWLEDGMENTS

The authors are very grateful to James Williams for help throughout this research and in particular for generating the electrical potentials, derived from electrode structures, which we use in this work. We also thank Hans Hon Sang Chan, Andrew Fisher, Guido Burkard, Tyson Jones, and Richard Meister for helpful discussions. The numerical modeling involved in this study used the Quantum Exact Simulation Toolkit [46], and the recent development pyQuEST [47], which permits the user to use PYTHON as the interface front end. We are grateful to those who have contributed to all of these valuable tools. The authors acknowledge the use of the University of Oxford Advanced Research Computing facility [48] in carrying out this work and specifically the facilities made available

by the EPSRC Quantum Technology Hub in Computing and Simulation (Grant Agreement No. EP/T001062/1). The authors also acknowledge support from the EPSRC's Robust and Reliable Quantum Computing project (Grant No. EP/W032635/1) and the SeeQA project (Grant No. EP/Y004655/1).

H.J. developed the modeling tool, performed the numerical simulations, and wrote the manuscript. S.C.B. contributed to developing the method and to writing the manuscript, and wrote code to independently validate the results.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available because they contain commercially sensitive information. The data are available from the authors upon reasonable request.

APPENDIX A: DEVICE SPECIFICATIONS

For the device we consider (see Fig. 1), we used gates and oxide dimensions consistent with designs and expected fabricated dimensions from the IMEC silicon metal-oxide-semiconductor process. The silicon substrate is separated from the three gate layers by 8-nm-thick silicon dioxide. Each gate layer is modeled as 30-nm-thick Schottky contacts with a work function of 4.1 eV consistent with n^{++} -doped polysilicon with 5 nm silicon dioxide separating each layer. The first layer (the closest to the silicon surface) is used to define the channel through confinement gates with a separation of 64 nm. The second layer is used for plunger gates to form our potential wells; they are separated by 30 nm and have a length of 54 nm (due to the oxide layer between gate layers) and a width of 40 nm, making an area of 2160 nm². The third layer incorporates source and drain gates, which yields lateral confinement to our channel, and a barrier gate that sits between both plunger gates, with length 44 nm and width 20 nm. The plunger gates were set to 0.3 V and the barrier was swept from -0.1 to 0.4 V; all other gates were set to 0 V. The potential is generated with the use of nextnano's Poisson solver [49], and the potential landscape 2D slice was taken 2 nm below the Si/SiO₂ interface.

APPENDIX B: ABRUPT TRANSITION

The grid-based method allows us to study any type of evolution of the potential in time. In the main text we focus on the more realistic case in which we smoothly lower and raise the barrier to perform a $\sqrt{\text{SWAP}}$ gate, the intuition behind this choice being that by adiabatically modifying the potential, we will implement a better performing two-qubit gate. To validate this choice, we compare it with the extreme case in which we abruptly switch the coupling on. In Fig. 11, we see that by doing so, we largely

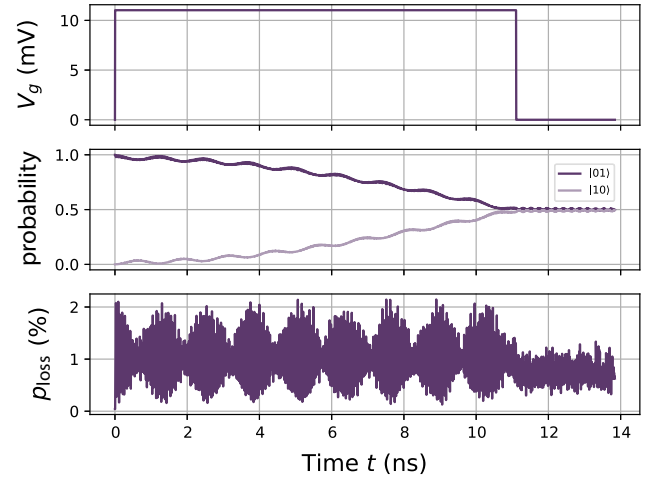


FIG. 11. Abrupt $\sqrt{\text{SWAP}}$ pulse. We abruptly switch the exchange interaction on and off and observe beatings due to the excitation of higher-energy charge states. As expected, the loss probability is highly increased with this method and can be as large as 1%.

increase p_{loss} (up to 1%). More precisely, by taking the average over the time remaining after the gate, we find that $p_{\text{loss}} = 0.73\%$ and $F = 97.06\%$. This result emphasizes the need for careful considerations of the control pulse.

APPENDIX C: CHARGE TRAPPED OUTSIDE THE QUANTUM DOT LINE

As said in the main text, we are not limited to the study of charges in the quantum dot line: we can position them anywhere we want. In this appendix, we look at the performance of the $\sqrt{\text{SWAP}}$ gate for three different positions of a single charge. To make a fair comparison, we position it at a fixed distance of 100 nm from the DQD but at different angles—namely, 0° (in the quantum dot line), 45° , and 90° .

In Fig. 12, we plot the evolution of the qubits' probability as well as p_{loss} for a given voltage profile (optimized for the noiseless case), and we report the final fidelities and loss probabilities in Table II. The results correspond to our intuition as the lowest fidelity is attained for a charge in the quantum dot line. It is worth noting that when the charge is placed perpendicularly to the quantum dot line (black), the probabilities of finding the electrons in the $|01\rangle$ and $|10\rangle$ states do not cross for this voltage profile, in contrast to the previous charge environments studied in this paper. This is because by placing the charge as such, we are pushing the trapped electrons apart from one another rather than bringing them closer and hence reduce the exchange coupling.

APPENDIX D: FLUCTUATING CHARGES

In this appendix we explore various scenarios involving multiple charge fluctuations between different positions,

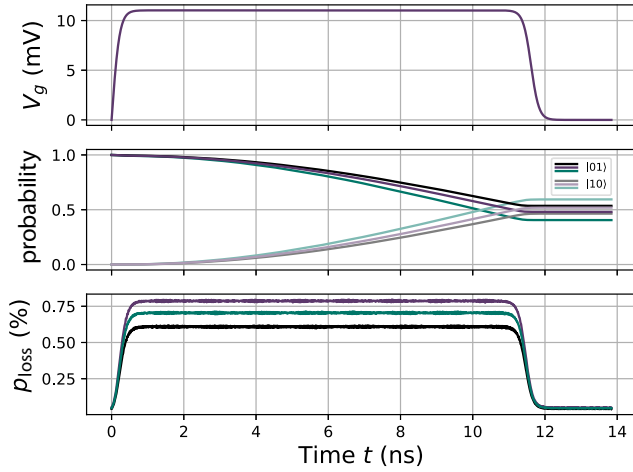


FIG. 12. Smooth $\sqrt{\text{SWAP}}$ gate for charges positioned at $(100, 0, 2)$ nm (green), $(0, 100, 2)$ nm (black), and $(50\sqrt{2}, 50\sqrt{2}, 2)$ nm (purple), respectively.

quantifying their impact on fidelity and loss probability, as illustrated in Fig. 13. Using a voltage control profile similar to that used for Fig. 8, we start with a charge placed at 100 nm from the DQD in the quantum dot line, leading to an initial $p_{\text{loss}} = 0.05\%$. We then perform a $\sqrt{\text{SWAP}}$ pulse and let the charge oscillate between this initial position and an additional charge trap located at 90, 75, and 50 nm (see the top, middle, and bottom of Fig. 13, respectively).

We find that the impact on fidelity is similar to that in the static case, with reductions attributed to timing errors, and the magnitude of the impact increasing as the charge approaches the DQD. Notably, a significant departure from the static scenario lies in the loss of adiabaticity during the gate operation due to the dynamic potential changes. This is evident in the evolution of p_{loss} , exhibiting pronounced shifts whenever a fluctuation occurs. Consequently, there is a significant increase in p_{loss} at the end of the gate, constituting the most detrimental type of error as it cannot be corrected. Similarly as for the fidelity, the closer the charge is to the DQD the more damaged the gate's performance. For oscillations between 100 and 50 nm, loss probabilities reach the order of 1 percent, rendering the gate impractical for use.

TABLE II. Loss probability and fidelity for different charge positions. Each charge is placed at a fixed distance of 100 nm from the center of the DQD. Their position can thus be characterized by their angle with respect to the quantum dot line (0° corresponds to having a charge in the quantum dot line).

	Charge position (deg)		
	0	45	90
p_{loss} (%)	0.05	0.05	0.04
F (%)	99.10	99.96	99.87

APPENDIX E: CONVERGENCE VERSUS BASIS SIZE

Figure 3(a) shows how the $J(V_g)$ curve can vary with the number of basis states in the model. While the general exponential dependence on V_g is observed when we use 16 basis states (per particle, per dimension, total 4096), the specific values can deviate from those obtained with higher resolutions. In contrast, there is very little difference between the basis sizes of 32 (total 1×10^6) and 64 (total 16×10^6). Given the computational resource costs, it is obviously interesting not only to confirm convergence but also to identify the basis size that is adequate. Therefore, we coded an implementation of our model with a variable basis size, and tested a series of choices—the results are shown in Fig. 14. One sees that above a basis size of around 22, the predicted J values converge steadily to about 140 MHz. Below this size, the prediction is unstable, while remaining within about 20% of the converged value.

APPENDIX F: COULOMB INTERACTION IN REAL SPACE

As explained in the main text, the SO modeling method that we use involves two representations for the system's state: The plane-wave (or “ k -space”) representation, where each stored amplitude corresponds to a component of the form $\exp(i2\pi\mathbf{k}_i \cdot \mathbf{r})$, and a second dual basis that results from a Fourier transform.

The confining potential $H_{\text{conf}} = V(\mathbf{r}_1) + V(\mathbf{r}_2)$, including any effects of unwanted charges in the local environment of the qubit, depends only on the real-space coordinates, and so we apply the corresponding unitary while we are in the real-space basis. Because the basis functions are not perfectly local (i.e., they are not Dirac delta functions for finite m), it follows that strictly speaking, the matrix representing $\exp(iH_{\text{conf}}\delta t)$ in the Dirichlet basis is not perfectly diagonal. However, the potential creating the quantum dot confinement, due to electrode voltages, material properties, and unwanted charges outside the primary quantum dot region, is smoothly varying and does not change dramatically over the length scale of the grid point separations. In the present study we ignore these off-diagonal components and take the on-diagonal components as simply

$$\langle n_{1,x}n_{1,y}n_{2,x}n_{2,y} | H_{\text{conf}} | n_{1,x}n_{1,y}n_{2,x}n_{2,y} \rangle = V(\mathbf{r}_1) + V(\mathbf{r}_2),$$

where $V(\mathbf{r})$ is as defined in Eq. (1) and

$$\mathbf{r}_1 = S(p_{n_{x,1}}\mathbf{i} + p_{n_{y,1}}\mathbf{j}), \quad \mathbf{r}_2 = S(p_{n_{x,2}}\mathbf{i} + p_{n_{y,2}}\mathbf{j}).$$

Presently we discuss the inclusion of a finite z depth; this is also ignored in the treatment of H_{conf} since the potentials vary little over the modest (order 5 nm) depth.

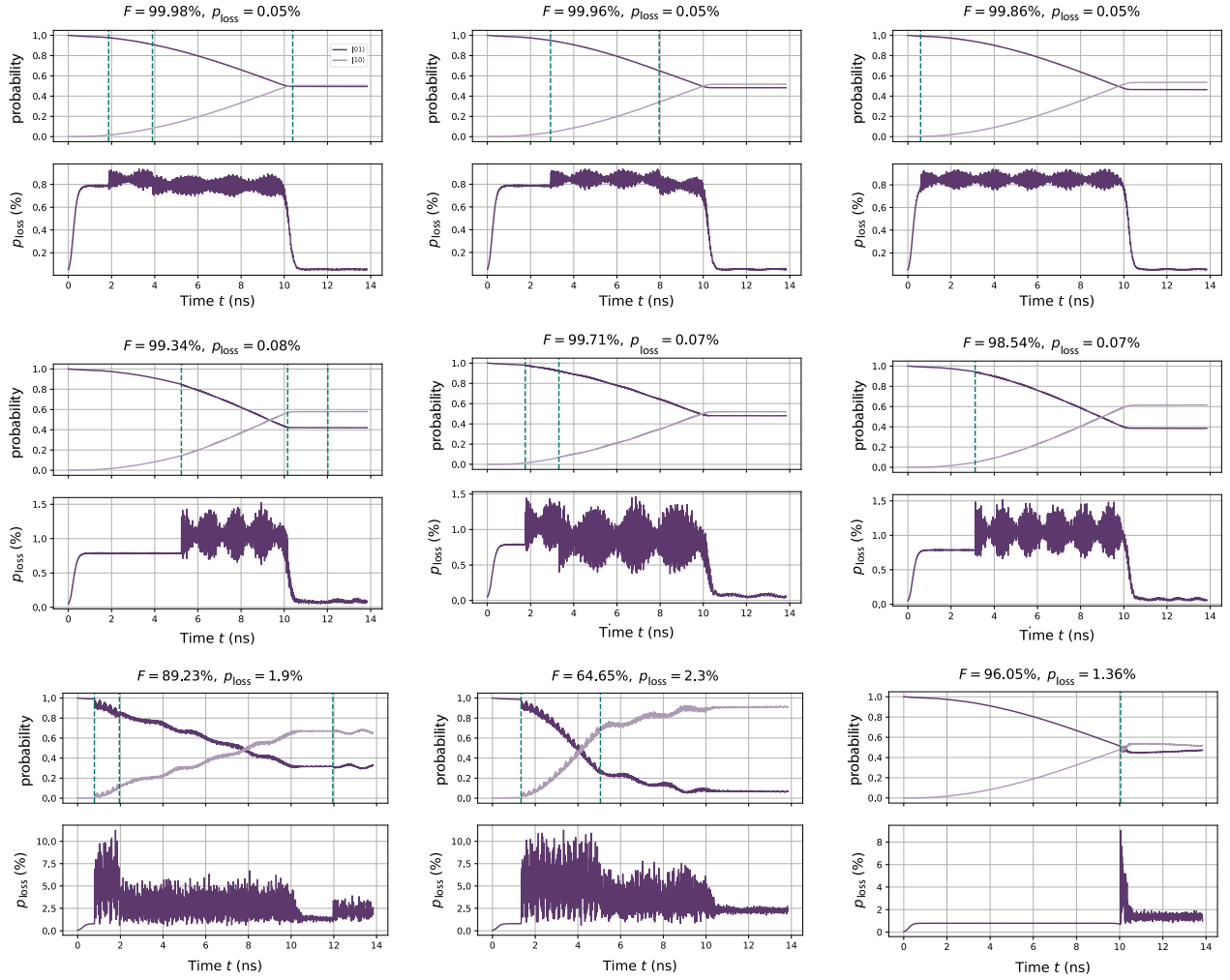


FIG. 13. Evolution of the probability of finding the qubits in the states $|01\rangle$ and $|10\rangle$ and the loss probability for different fluctuation scenarios. Initially the charge is located at $(100, 0, 2)$ nm and switches to another position at each green dashed lines. The voltage profile has been optimized for the $(100, 0, 2)$ nm case to yield a perfect $\sqrt{\text{SWAP}}$ gate. Oscillation between $(100, 0, 2)$ nm and $(90, 0, 2)$ nm at the top, $(100, 0, 2)$ nm and $(75, 0, 2)$ nm in the middle, and $(100, 0, 2)$ nm and $(50, 0, 2)$ nm at the bottom. The fidelity and loss probability are obtained by averaging over the time following the end of the gate.

The Coulomb interaction between the two electrons (the two qubits) in our model should be considered in more detail: it is singular and this is one of the challenges of modeling multielectron systems. Indeed the implications of the singularity are so strong that in one dimension the model has pathologies such as a singular ground state [50]. Fortunately in two-and-higher dimensions these states are well-behaved. In the remainder of this appendix we (1) derive the expression for the matrix elements of H_{Coul} in the real-space Dirichlet basis, for strictly 2D and for “pizza-box”-type 3D potentials; determine the numerical values of the on-diagonal elements for relevant cases; and (3) discuss the strength of the off-diagonal terms and how future work can include them in the simulation as a correction.

To keep the expressions in this appendix as clean as possible, we specify that the spatial “box” within which our

electrons are represented runs from $-\frac{1}{2}$ to $+\frac{1}{2}$ on both the x axis and the y axis, and therefore has unit area. Obviously, the expressions we obtain can be scaled to arbitrary sizes; moreover, the generalization to, for example, elongated boxes is straightforward.

1. 2D quantum dots

Because our basis is periodic (i.e., the wave functions simply repeat in the x and y directions with a period of unity), we should adopt a periodic function in place of the canonical nonperiodic Coulomb interaction. If we write the vector between the two particles as $\Delta \equiv \mathbf{r}_1 - \mathbf{r}_2$, when $|\mathbf{i} \cdot \Delta \mathbf{r}| = \frac{1}{2}$, then particle 1 is equidistant from its real partner particle 2 and an image of that particle—our choice should acknowledge that symmetry (and similarly in the y

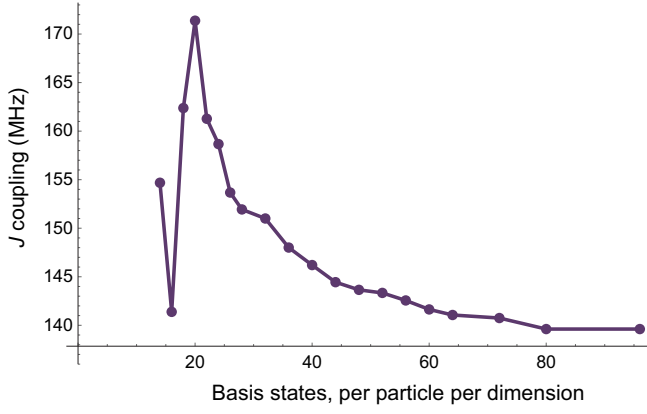


FIG. 14. J coupling strength obtained from a series of simulations with various basis set sizes, ranging from 14 to 96. Here we chose $V_g = 12$ mV. One observes that the series converges to 140 MHz. The model used here is the variant with strictly two dimensions and the standard Coulomb matrix, i.e., the purple lines in Fig. 3.

direction). A convenient choice is simply to use the canonical Coulomb interaction in the region near the origin and then repeat its use outside that region:

$$C(\Delta) = \frac{1}{|\Delta|} \quad \text{when } |\mathbf{i} \cdot \Delta| \leq \frac{1}{2}, |\mathbf{j} \cdot \Delta| \leq \frac{1}{2}, \quad (\text{F1})$$

$$C(\Delta + a\mathbf{i} + b\mathbf{j}) = C(\Delta) \quad \text{for all } a, b \in \mathbb{Z}.$$

This choice is appropriate for our scenario where the image charges are an artifact of the simulation and do not reflect any element of physical reality (i.e., the electrons in the quantum dot structure do not actually experience image charge effects). We must ensure the simulation box is large enough that the double quantum dot confinement region is only in the central part of the simulation box, so that there is negligible amplitude associated with states for which $|\mathbf{i} \cdot \Delta| > \frac{1}{2}$ or $|\mathbf{j} \cdot \Delta| > \frac{1}{2}$ (as such states experience the “wrong” Coulomb interaction). In the main text we report that we verify this both by tracking the total probability outside the central region and by doubling the simulation box size to ensure that properties of interest do not change (convergence with respect to box size).

We can then write the general matrix element as

$$\begin{aligned} & \langle n'_{1,x} n'_{1,y} n'_{2,x} n'_{2,y} | H_{\text{Coul}} | n_{1,x} n_{1,y} n_{2,x} n_{2,y} \rangle \\ &= K \int_{\text{box}} d\mathbf{r}_1 \int_{\text{box}} d\mathbf{r}_2 C(|\mathbf{r}_1 - \mathbf{r}_2|) \phi_{n'_{1,x} n'_{1,y}}^*(\mathbf{r}_1) \phi_{n'_{2,x} n'_{2,y}}^*(\mathbf{r}_1) \\ & \quad \times (\mathbf{r}_2) \phi_{n_{1,x} n_{1,y}}(\mathbf{r}_1) \phi_{n_{2,x} n_{2,y}}(\mathbf{r}_2), \end{aligned} \quad (\text{F2})$$

where K is the appropriate constant incorporating $e^2/4\pi\epsilon_0\epsilon_r$ and a factor accounting for the physical width

of our simulation box. From Eq. (3) we know

$$\begin{aligned} \phi_{ab}(\mathbf{r}) &= \frac{1}{M} \exp \left(i\pi \left(x - \frac{a}{M} + y - \frac{b}{M} \right) \right) \\ & \quad \times D_m \left(2\pi \left(x - \frac{a}{M} \right) \right) D_m \left(2\pi \left(y - \frac{b}{M} \right) \right), \end{aligned} \quad (\text{F3})$$

recalling that $M = 2^q$ is the total number of basis states associated with each dimension for each particle, and $m = M/2$.

Before proceeding, we note that because of the translational symmetry in the Eq. (F2) the value of the matrix element will be unchanged if we subtract any integer from all the x quantum numbers, and/or subtract any integer from all the y quantum numbers (wrapping around the cycle $-m$ to $m-1$ as needed). Therefore, we need only solve for the cases where $n_{1,x} = n_{1,y} = 0$ since the elements for nonzero $n_{1,x}, n_{1,y}$ can always be found by suitable shifts.

We now make the change of variables

$$\mathbf{S} = \mathbf{r}_1 + \mathbf{r}_2, \quad \Delta = \mathbf{r}_1 - \mathbf{r}_2.$$

Noting from the Jacobian that $d\mathbf{r}_1 d\mathbf{r}_2 = \frac{1}{4} d\mathbf{S} d\Delta$, we find the integral in Eq. (F2) will directly translate to

$$\int_{\text{box}} d\mathbf{r}_1 \int_{\text{box}} d\mathbf{r}_2 \rightarrow \frac{1}{4} \int_{\text{BOX}} d\Delta \int_{\text{rect}(\Delta)} d\mathbf{S},$$

where the Δ integral is over a region denoted “BOX” in capitals as it is centered at the origin but is twice the linear size (4 times the area) of the “box” regions, i.e., the regions $|\mathbf{i} \cdot \Delta| \leq 1$ and $|\mathbf{j} \cdot \Delta| \leq 1$. Meanwhile, the $\mathbf{S}$ integral is over a region denoted $\text{rect}(\Delta)$, which depends on Δ :

$$|\mathbf{i} \cdot \mathbf{S}| \leq 1 - |\mathbf{i} \cdot \Delta|, \quad |\mathbf{j} \cdot \mathbf{S}| \leq 1 - |\mathbf{j} \cdot \Delta|.$$

This constraint ensures that every $\mathbf{r}_1, \mathbf{r}_2$ point in the original integral is included, but points outside that space are not.

One could continue with the following steps using the Δ -dependent integration region [51]. However, it is convenient to observe that, because of the periodicity of the integrand,

$$\int_{\text{BOX}} d\Delta \int_{\text{rect}(\Delta)} d\mathbf{S} \rightarrow \int_{\text{box}} d\Delta \int_{\text{BOX}} d\mathbf{S},$$

where the region of the Δ integral becomes the unit-area box centered at the origin, i.e., $|\mathbf{i} \cdot \mathbf{S}| \leq \frac{1}{2}$ and $|\mathbf{j} \cdot \mathbf{S}| \leq \frac{1}{2}$, and the region of the $\mathbf{S}$ integral becomes the larger BOX referred to above. See Fig. 15 for an illustration of the equivalence.

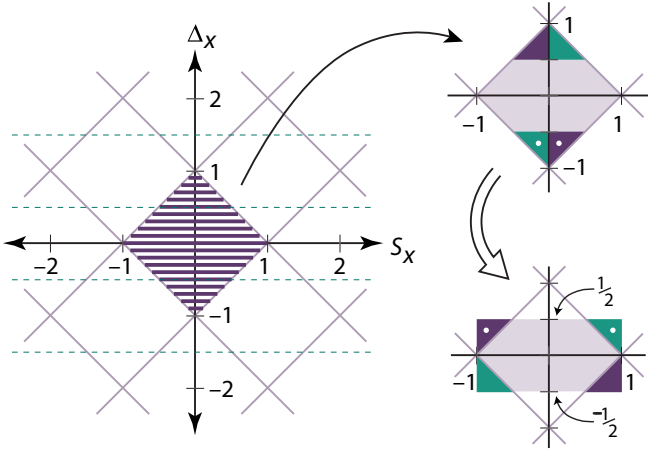


FIG. 15. Equivalent options for integration; the x coordinates are shown and an identical argument applies, independently, to the y coordinates. Left: The wave functions in Eq. (F2) are periodic, and one cell (i.e., the “box”) corresponds to sweeping $r_{1,x}$ and $r_{2,x}$ over the range $-\frac{1}{2}$ to $\frac{1}{2}$. Correspondingly, the Δ_x and S_x variables sweep the region shaded in dark blue, and the periodicity of the wave functions in these variables is indicated by the cyan diagonals. The dashed red lines indicate the periodicity of the other factor in the integrand, $C(|\Delta|)$. Right: Because of the indicated periodicities, we know that each triangle of a given color in the upper figure is equivalent to the same triangle in the lower figure. Consequently we can simplify the limits of the integral as in the main text.

With these observations we are left wishing to evaluate

$$\begin{aligned} & \langle n'_{1,x} n'_{1,y} n'_{2,x} n'_{2,y} | H_{\text{Coul}} | 0 0 n_{2,x} n_{2,y} \rangle \\ &= \frac{1}{4} \int_{\text{box}} d\Delta C(|\Delta|) f(\Delta), \end{aligned} \quad (\text{F4})$$

where

$$\begin{aligned} f(\Delta) &= \int_{\text{BOX}} d\mathbf{S} \phi_{n'_{1,x} n'_{1,y}}^* \left(\frac{\mathbf{S} + \Delta}{2} \right) \phi_{n'_{2,x} n'_{2,y}}^* \left(\frac{\mathbf{S} - \Delta}{2} \right) \\ &\times \phi_{00} \left(\frac{\mathbf{S} + \Delta}{2} \right) \phi_{n_{2,x} n_{2,y}} \left(\frac{\mathbf{S} - \Delta}{2} \right). \end{aligned} \quad (\text{F5})$$

$f(\Delta)$ can be simplified, first by recalling from Eq. (F3) that our basis states factor into x - and y -dependent functions, so that

$$f(\Delta) = f(\Delta_x, \Delta_y) = \frac{e^{i\Theta}}{M^4} g_x(\Delta_x) g_y(\Delta_y), \quad (\text{F6})$$

where $\Theta = n'_{1,x} + n'_{1,y} + n'_{2,x} + n'_{2,y} - n_{2,x} - n_{2,y}$,

and

$$\begin{aligned} g_x(\Delta) &= \int_{-1}^{+1} dS D_m \left(2\pi \left(\frac{S + \Delta}{2} - \frac{n'_{1,x}}{M} \right) \right) \\ &\times D_m \left(2\pi \left(\frac{S - \Delta}{2} - \frac{n'_{2,x}}{M} \right) \right) \\ &\times D_m \left(2\pi \left(\frac{S + \Delta}{2} \right) \right) \\ &\times D_m \left(2\pi \left(\frac{S - \Delta}{2} - \frac{n_{2,x}}{M} \right) \right), \end{aligned} \quad (\text{F7})$$

and similarly for $g_y(\Delta)$.

Finally, we note that we can subsume the quantum number $n_{2,x}$ into a new integer $n''_{2,x} = n'_{2,x} - n_{2,x}$, reducing the number of parameters, as follows. We examine $g_x(\Delta - n_{2,x}/M)$ and shift the integration variable $S \rightarrow S - n_{2,x}/M$, (which does not require an adjustment to the integration range, since that range corresponds to one period of the periodic integrand). Then we find

$$g_x \left(\Delta - \frac{n_{2,x}}{M} \right) = h_{n'_{1,x} n''_{2,x}}(\Delta),$$

where

$$\begin{aligned} h_{ab}(\Delta) &= \int_{-1}^{+1} dS D_m \left(2\pi \left(\frac{S + \Delta}{2} - \frac{a}{M} \right) \right) \\ &\times D_m \left(2\pi \left(\frac{S - \Delta}{2} - \frac{b}{M} \right) \right) \\ &\times D_m \left(2\pi \left(\frac{S + \Delta}{2} \right) \right) D_m \left(2\pi \left(\frac{S - \Delta}{2} \right) \right). \end{aligned} \quad (\text{F8})$$

Then we can write

$$\begin{aligned} f(\Delta_x \mathbf{i} + \Delta_y \mathbf{j}) &= \frac{e^{i\Theta}}{M^4} h_{n'_{1,x} n''_{2,x}} \left(\Delta_x + \frac{n_{2,x}}{M} \right) h_{n'_{1,y} n''_{2,y}} \left(\Delta_y + \frac{n_{2,y}}{M} \right). \end{aligned} \quad (\text{F9})$$

This is a useful form since it depends only on $h_{ab}(\Delta)$, which can be precomputed as a high-granularity lookup table for each required a, b . For the on-diagonal matrix elements, $a = b = 0$, so we need only precompute $h()$ once for a given choice of basis size M in order to obtain the diagonal approximation.

Given a precomputed $h()$ function, we still need to compute the outer $d\Delta$ integral from Eq. (F4). This is

conveniently performed in polar variables:

$$\begin{aligned}
& \frac{1}{4} \int_{\text{BOX}} d\Delta C(|\Delta|) f(\Delta) \\
&= \frac{1}{4} \int_0^{2\pi} d\theta \int_0^{\Delta_{\max}(\theta)} \Delta d\Delta C(\Delta) f(\mathbf{i}\Delta \cos \theta + \mathbf{j}\Delta \sin \theta) \\
&= \frac{e^{i\Theta}}{2M^4} \int_0^{2\pi} d\theta \int_0^{\Delta_{\max}(\theta)} d\Delta h_{n'_{1,x} n''_{2,x}} \left(\Delta \cos \theta + \frac{n_{2,x}}{M} \right) \\
&\quad \times h_{n'_{1,y} n''_{2,y}} \left(\Delta \sin \theta + \frac{n_{2,y}}{M} \right). \quad (\text{F10})
\end{aligned}$$

In the second line we were able to remove the singularity by canceling the Δ introduced from the area element, with $C(\Delta) = 1/\Delta$. The limit $\Delta_{\max}$ of the radial integral ensures that we sweep over our square, unit-area “box” area:

$$\begin{aligned}
\Delta_{\max}(\theta) &= \frac{1}{2} |\text{cosec}(\theta)| \text{ if } \frac{\pi}{4} < \theta < \frac{3\pi}{4} \text{ or } \frac{5\pi}{4} < \theta < \frac{7\pi}{4} \\
&= \frac{1}{2} |\sec(\theta)| \text{ otherwise.} \quad (\text{F11})
\end{aligned}$$

To summarize the analysis for the 2D problem, we find that the matrix elements of the Coulomb interaction $1/|\mathbf{r}_1 - \mathbf{r}_2|$ can be computed with the use of

$$\begin{aligned}
& \langle n'_{1,x} n'_{1,y} n'_{2,x} n'_{2,y} | H_{\text{Coul}} | 0 0 n_{2,x} n_{2,y} \rangle \\
&= K \frac{e^{i\Theta}}{4M^4} \int_0^{2\pi} d\theta \int_0^{\Delta_{\max}(\theta)} d\Delta h_{n'_{1,x} n''_{2,x}} \left(\Delta \cos \theta + \frac{n_{2,x}}{M} \right) \\
&\quad \times h_{n'_{1,y} n''_{2,y}} \left(\Delta \sin \theta + \frac{n_{2,y}}{M} \right), \quad (\text{F12})
\end{aligned}$$

where the function $h()$ is defined in Eq. (F8) and the relative quantum numbers $n''_{2,x} = n'_{2,x} - n_{2,x}$ and $n''_{2,y} = n'_{2,y} - n_{2,y}$. The phase Θ is as defined in Eq. (F6). We noted that elements for which the $n_{1,x}$ and $n_{1,y}$ quantum numbers are not zero can be found simply by shifting.

With these expressions we can calculate any matrix element; of particular interest is the element $\langle 0, 0, 0, 0 | H_{\text{Coul}} | 0, 0, 0, 0 \rangle$, which is the interaction for two electrons sharing the same basis state, i.e., the “shared grid point” case. This will be the matrix element with the greatest magnitude; the state’s amplitude for such an element will be zero

for antisymmetric charge states, but can be nonzero for symmetric charge states. The calculated values for three basis sizes are shown in the $z_{\Delta} = 0$ column of Table III.

2. 3D quantum dots

We consider a straightforward generalization to describe “pancake” three-dimensional quantum dots where the vertical confinement is far more severe than the x - y potential. We then make the simple assumption that the electron’s wave functions have a separable z component, and that they are “frozen” in the lowest possible z eigenstate. In effect, we have only a single basis state for the z direction of the model. This is an acceptable approximation unless the depth of the real quantum dot structure, more specifically the mean z separation, is significantly larger than the grid point spacing in the x - y plane; in that case, the 3D pixels would become “cigar-shaped” with the long axis vertical, yet the model could not properly account for vertical electron-electron repulsion *within* each such pixel.

Note that the grid-based method presented in this paper can naturally extend to fully model the third dimension with multiple basis states. In that case, the expressions in the previous section can be simply be adapted so that, for example, the polar integral (F10) is computed in cylindrical-polar coordinates. In terms of the resource costs of the numerical modeling of the two-electron system, introducing n basis states for the z direction would increase the RAM requirements of the simulation by n^2 . In the present paper we do not explore this, but it is an interesting theme for future work.

Here we assume

$$\Psi_{3D}(x_1, y_1, z_1; x_2, y_2, z_2) = Z(z_1)Z(z_2)\Psi_{2D}(x_1, y_1; x_2, y_2).$$

Here $\Psi_{2D}(\dots)$ is an instance of the 2D grid-based two-electron wave function that has been considered in the previous section.

We further assume that the function $Z(z)$ is part of an Airy function of the first kind, usually written $\text{Ai}(z)$ (see

TABLE III. Calculated strengths of the term $1/\sqrt{\Delta^2 + z_{\Delta}^2}$, where Δ is the separation of the electrons in the x - y plane, in the “shared grid point” case as defined in the main text. For 2D dots the relevant column is the $z_{\Delta} = 0$ column. Other columns correspond to an enforced z_{Δ} as discussed in Appendix F 2. See also Fig. 17.

Basis size	z_{Δ}							
	0	0.005	0.01	0.02	0.03	0.04	0.05	0.06
16	30.2	26.9	24.2	20.0	17.0	14.7	13.0	11.5
32	60.0	48.1	39.8	29.2	22.8	18.7	15.8	13.7
64	120.0	79.3	58.1	37.3	27.3	21.5	17.7	15.1

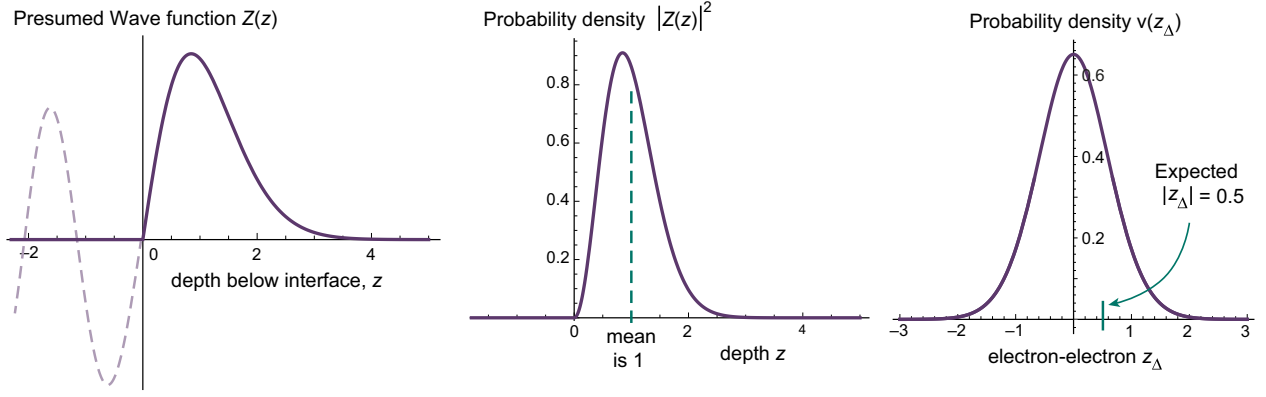


FIG. 16. Use if the Airy function in modeling a 3D structure. Left: A single electron's wave function has the z dependence shown by the purple line; it is zero for $z \leq 0$, and for positive z it is an Airy function of the first kind. The function is shifted so that its first root is at $z = 0$ and, as a useful reference, scaled so that the mean value of $\langle z \rangle = 1$ (as shown in the center panel). Right: Resulting probability distribution for the relative z coordinate between two such electrons; it is similar to a Gaussian, and the expected value of $|z_\Delta|$ is 0.5.

Fig. 16). Specifically,

$$Z(z) = N \text{Ai}\left(\frac{z - a_0}{L}\right) \quad \text{for } z > L a_0$$

$$= 0 \quad \text{otherwise.} \quad (\text{F13})$$

Here $a_0 \approx -2.3381$ is the first zero of the Airy function, $\text{Ai}(a_0) = 0$. The constant N is simply the normalization, and L is a constant determining how deep the z -axis distribution is. The treatment of this 3D scenario follows the 2D method closely, and Eq. (F1) for the periodic Coulomb interaction is still relevant; we do not need to introduce a periodicity in the z direction since the model has no such periodicity. It is convenient to still use $\mathbf{r}_1$ and $\mathbf{r}_2$, and their sum and difference $\mathbf{S}$ and $\mathbf{\Delta}$, where these vectors are understood to lie in the x - y plane. We additionally introduce z_1 and z_2 for the new dimension. Making the natural change of variables $z_S = z_1 + z_2$, $z_\Delta = z_1 - z_2$ and noting that the Coulomb interaction has no dependence on z_S , we find the relevant function is the probability density $v(z_\Delta)$, where

$$v(z_\Delta) = \frac{1}{2} \int_{-\infty}^{\infty} Z\left(\frac{z_S + z_\Delta}{2}\right)^2 Z\left(\frac{z_S - z_\Delta}{2}\right)^2 dz_S,$$

noting $\int_{-\infty}^{\infty} v(z_\Delta) dz_\Delta = 1$. Then in place of Eq. (F4), we now have

$$\langle n'_{1,x} n'_{1,y} n'_{2,x} n'_{2,y} | H_{\text{Coul}} | 0 0 n_{2,x} n_{2,y} \rangle$$

$$= \frac{1}{4} \int_{-\infty}^{\infty} dz_\Delta \int_{\text{BOX}} d\mathbf{\Delta} C(|z_\Delta \mathbf{k} + \mathbf{\Delta}|) f(\mathbf{\Delta}) v(z_\Delta). \quad (\text{F14})$$

This leads ultimately to a 3D generalization of the Eq. (F12) as follows:

$$\langle n'_{1,x} n'_{1,y} n'_{2,x} n'_{2,y} | H_{\text{Coul}} | 0 0 n_{2,x} n_{2,y} \rangle$$

$$= K \frac{e^{i\Theta}}{4M^4} \int_{-\infty}^{\infty} dz_\Delta v(z_\Delta) \int_0^{2\pi} d\theta \int_0^{\Delta_{\max}(\theta)} \frac{\Delta d\Delta}{\sqrt{z_\Delta^2 + \Delta^2}}$$

$$\times h_{n'_{1,x} n'_{2,x}}''(\Delta \cos \theta + \frac{n_{2,x}}{M}) h_{n'_{1,y} n'_{2,y}}''(\Delta \sin \theta + \frac{n_{2,y}}{M}). \quad (\text{F15})$$

Thus we introduce an offset z_Δ into the Coulomb interaction, and integrate over z_Δ with the probability density $v(z_\Delta)$. This can be performed numerically; while the need to integrate over z_Δ introduces a multiplicative time cost as compared with the 2D computation, the function $v(z_\Delta)$ is a simply Gaussian-like form and therefore requires only a relatively modest sampling resolution.

The result is to “soften” the Coulomb interaction in the sense that there will be appreciable reduction in the on-diagonal matrix elements for small $n_{2,x}$ and $n_{2,y}$, especially the $n_{2,x} = n_{2,y} = 0$ case, where the two electrons lie at the same grid point. This is intuitive since the additional dimension affords the electrons “more freedom to avoid one another,” so to speak.

As shown in the main text, the effect on the qubit-qubit interaction of adopting the 3D potential is to appreciably increase this coupling.

3. Off-diagonal terms

The expressions derived above allow us to evaluate both the on-diagonal and the off-diagonal matrix elements of H_{Coul} in the real-space Dirichlet basis. This matrix is not strictly diagonal except as the number of basis states $M \rightarrow \infty$ [52].

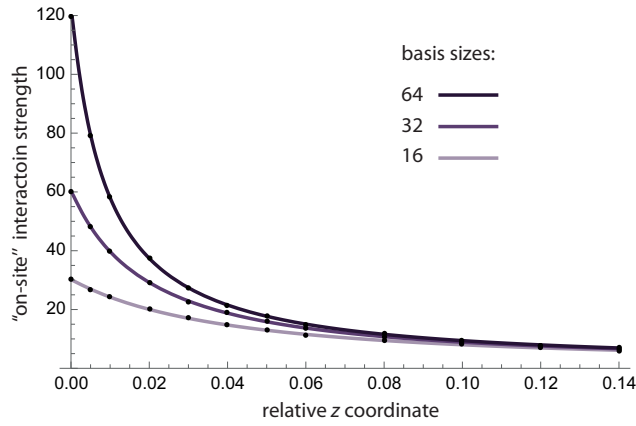


FIG. 17. Calculated strengths of the term $1/\sqrt{\Delta^2 + z_{\Delta}^2}$, where Δ is the separation of the electrons in the x - y plane, in the “shared grid point” case. Key values are also shown in Table III. Lines are fitted power series.

The computations in the main text simply ignore the off-diagonal terms. Computing their magnitude using the expressions above, one finds, for example, that in the 3D version and with $M = 64$ basis states, the off-diagonal elements with the greatest amplitude are weaker by more than an order of magnitude than the corresponding on-diagonal element. Moreover, the matrix elements are vanishingly small except near the diagonal [“near” meaning that in Eq. (F15), $n'_{1,x}$, $n'_{1,y}$, $n''_{2,x}$, and $n''_{2,y}$ are all small or zero].

In a future work it would be interesting to keep (at least) the most significant of the off-diagonal terms present in order to verify that the impact on the quantities of interest is negligible. One could, of course, modify the dynamical simulation code in various ways to do this, but it might be interesting to apply the method called “augmented split operator” described in Ref. [30]. This approach was actually suggested as an efficient method of including off-diagonal elements when the simulation itself is running on some future, fault-tolerant quantum computer; however, the method should translate well to the present classical code since it is ultimately just a protocol for efficiently manipulating a subset of the amplitudes.

[1] G. Burkard, T. D. Ladd, A. Pan, J. M. Nichol, and J. R. Petta, Semiconductor spin qubits, *Rev. Mod. Phys.* **95**, 025003 (2023).
[2] A. R. Mills, C. R. Guinn, M. J. Gullans, A. J. Sigillito, M. M. Feldman, E. Nielsen, and J. R. Petta, Two-qubit silicon quantum processor with operation fidelity exceeding 99%, *Sci. Adv.* **8**, eabn5130 (2022).
[3] X. Xue, M. Russ, N. Samkharadze, B. Undseth, A. Sammak, G. Scappucci, and L. M. K. Vandersypen, Quantum logic with spin qubits crossing the surface code threshold, *Nature* **601**, 343 (2022).

[4] A. Noiri, K. Takeda, T. Nakajima, T. Kobayashi, A. Sammak, G. Scappucci, and S. Tarucha, Fast universal quantum gate above the fault-tolerance threshold in silicon, *Nature* **601**, 338 (2022).
[5] M. D. Michielis, E. Ferraro, E. Prati, L. Hutin, B. Bertrand, E. Charbon, D. J. Ibberson, and M. F. Gonzalez-Zalba, Silicon spin qubits from laboratory to industry, *J. Phys. D: Appl. Phys.* **56**, 363001 (2023).
[6] A. M. J. Zwerver *et al.*, Qubits made by advanced semiconductor manufacturing, *Nat. Electron.* **5**, 184 (2022).
[7] M. Veldhorst, H. G. J. Eenink, C. H. Yang, and A. S. Dzurak, Silicon CMOS architecture for a spin-based quantum computer, *Nat. Commun.* **8**, 1766 (2017).
[8] R. Maurand, X. Jehl, D. Kotekar-Patil, A. Corna, H. Bohuslavskiy, R. Laviéville, L. Hutin, S. Barraud, M. Vinet, M. Sanquer, and S. De Franceschi, A CMOS silicon spin qubit, *Nat. Commun.* **7**, 13575 (2016).
[9] D. Loss and D. P. DiVincenzo, Quantum computation with quantum dots, *Phys. Rev. A* **57**, 120 (1998).
[10] D. P. DiVincenzo, D. Bacon, J. Kempe, G. Burkard, and K. B. Whaley, Universal quantum computation with the exchange interaction, *Nature* **408**, 339 (2000).
[11] T. Meunier, V. E. Calado, and L. M. K. Vandersypen, Efficient controlled-phase gate for single-spin qubits in quantum dots, *Phys. Rev. B* **83**, 121403(R) (2011).
[12] A. L. Saraiva, M. J. Calderón, and B. Koiller, Reliability of the Heitler-London approach for the exchange coupling between electrons in semiconductor nanostructures, *Phys. Rev. B* **76**, 233302 (2007).
[13] C. R. Anderson, M. F. Gyure, S. Quinn, A. Pan, R. S. Ross, and A. A. Kiselev, High-precision real-space simulation of electrostatically confined few-electron states, *AIP Adv.* **12**, 065123 (2022).
[14] H. E. Ercan, S. N. Coppersmith, and M. Friesen, Strong electron-electron interactions in Si/SiGe quantum dots, *Phys. Rev. B* **104**, 235302 (2021).
[15] M. J. Calderón, B. Koiller, and S. Das Sarma, Exchange coupling in semiconductor nanostructures: Validity and limitations of the Heitler-London approach, *Phys. Rev. B* **74**, 045310 (2006).
[16] M. D. Reed, B. M. Maune, R. W. Andrews, M. G. Borselli, K. Eng, M. P. Jura, A. A. Kiselev, T. D. Ladd, S. T. Merkel, I. Milosavljevic, E. J. Pritchett, M. T. Rakher, R. S. Ross, A. E. Schmitz, A. Smith, J. A. Wright, M. F. Gyure, and A. T. Hunter, Reduced sensitivity to charge noise in semiconductor spin qubits via symmetric operation, *Phys. Rev. Lett.* **116**, 110402 (2016).
[17] D. Culcer, X. Hu, and S. Das Sarma, Dephasing of Si spin qubits due to charge noise, *Appl. Phys. Lett.* **95**, 073102 (2009).
[18] E. Nielsen, R. W. Young, R. P. Muller, and M. S. Carroll, Implications of simultaneous requirements for low-noise exchange gates in double quantum dots, *Phys. Rev. B* **82**, 075319 (2010).
[19] J. D. Cifuentes, P. Y. Mai, F. Schlattner, H. E. Ercan, M. Feng, C. C. Escott, A. S. Dzurak, and A. Saraiva, Path-integral simulation of exchange interactions in CMOS spin qubits, *Phys. Rev. B* **108**, 155413 (2023).
[20] B. Buonacorsi, M. Korkusinski, B. Khromets, and J. Baugh, Optimizing lateral quantum dot geometries for reduced exchange noise, *arXiv:2012.10512* [cond-mat.mes-hall].

- [21] M. M. E. K. Shehata, G. Simion, R. Li, F. A. Mohiyaddin, D. Wan, M. Mongillo, B. Govoreanu, I. Radu, K. D. Greve, and P. V. Dorpe, Modelling semiconductor spin qubits and their charge noise environment for quantum gate fidelity estimation, *PhysRevB*. **108**, 045305 (2023).
- [22] A. Elsayed, M. Shehata, C. Godfrin, S. Kubicek, S. Massar, Y. Canvel, J. Jussot, G. Simion, M. Mongillo, D. Wan, B. Govoreanu, I. P. Radu, R. Li, P. V. Dorpe, and K. D. Greve, Low charge noise quantum dots with industrial CMOS manufacturing, *npj Quantum Inf.* **10**, 70 (2024).
- [23] M. H. Levitt, Composite pulses, *Prog. Nucl. Magn. Reson. Spectrosc.* **18**, 61 (1986).
- [24] K. R. Brown, A. W. Harrow, and I. L. Chuang, Arbitrarily accurate composite pulse sequences, *Phys. Rev. A* **70**, 052318 (2004).
- [25] J. A. Jones, Composite pulses in NMR quantum computation, *J. Ind. Inst. Sci.* **89**, 303 (2009).
- [26] J. Jones, Systematic errors and NMR composite pulses, <https://nmr.physics.ox.ac.uk/teaching/cp.pdf>.
- [27] J. C. Light and T. Carrington, Jr., Discrete-variable representations and their utilization, *Adv. Chem. Phys.* **114**, 263 (2000).
- [28] M. F. J. A. Fleck, Jr. and J. Morris, Time-dependent propagation of high energy laser beams through the atmosphere, *Appl. Phys.* **10**, 129 (1976).
- [29] R. Babbush, N. Wiebe, J. McClean, J. McClain, H. Neven, and G. Kin-Lic Chan, Low-depth quantum simulation of materials, *Phys. Rev. X* **8**, 011044 (2018).
- [30] H. H. S. Chan, R. Meister, T. Jones, D. P. Tew, and S. C. Benjamin, Grid-based methods for chemistry simulations on a quantum computer, *Sci. Adv.* **9**, eabo7484 (2023).
- [31] A good account of the Dirichlet kernel and its relation to the Dirac comb is provided at https://en.wikipedia.org/wiki/Dirichlet_kernel.
- [32] The equivalent to Eq. (3) for Ref. [29], with its odd number of basis states M , simply omits the phase prefactor, and has n running from $-m$ to m so that the grid points p_n run from $-(\frac{1}{2} - \frac{1}{2M})$ to $+(\frac{1}{2} - \frac{1}{2M})$.
- [33] J. D. Cifuentes *et al.*, Bounds to electron spin qubit variability for scalable CMOS architectures, *Nat. Commun.* **15**, 4299 (2024).
- [34] A. Saraiva, W. H. Lim, C. H. Yang, C. C. Escott, A. Laucht, and A. S. Dzurak, Materials for silicon quantum dots and their impact on electron spin qubits, *Adv. Funct. Mater.* **32**, 2105488 (2022).
- [35] L. Lehtovaara, J. Toivanen, and J. Eloranta, Solution of time-independent Schrödinger equation by the imaginary time propagation method, *J. Comput. Phys.* **221**, 148 (2007).
- [36] C. R. Anderson, Efficient solution of the Schroedinger–Poisson equations in layered semiconductor devices, *J. Comput. Phys.* **228**, 4745 (2009).
- [37] E. J. Connors, J. Nelson, L. F. Edge, and J. M. Nichol, Charge-noise spectroscopy of Si/SiGe quantum dots via dynamically-decoupled exchange oscillations, *Nat. Commun.* **13**, 940 (2022).
- [38] J. Yoneda, K. Takeda, T. Otsuka, T. Nakajima, M. R. Delbecq, G. Allison, T. Honda, T. Kodera, S. Oda, Y. Hoshi, N. Usami, K. M. Itoh, and S. Tarucha, A quantum-dot spin qubit with coherence limited by charge noise and fidelity higher than 99.9%, *Nat. Nanotechnol.* **13**, 102 (2018).
- [39] B. Paquelet Wuetz, D. Degli Esposti, A.-M. J. Zwerver, S. V. Amitonov, M. Botifoll, J. Arbiol, A. Sammak, L. M. K. Vandersypen, M. Russ, and G. Scappucci, Reducing charge noise in quantum dots by using thin silicon quantum wells, *Nat. Commun.* **14**, 1385 (2023).
- [40] J. S. Rojas-Arias, A. Noiri, P. Stano, T. Nakajima, J. Yoneda, K. Takeda, T. Kobayashi, A. Sammak, G. Scappucci, D. Loss, and S. Tarucha, Spatial noise correlations beyond nearest neighbors in $^{28}\text{Si}/\text{Si-Ge}$ spin qubits, *Phys. Rev. Appl.* **20**, 054024 (2023).
- [41] M. Kępa, N. Focke, Ł. Cywiński, and J. A. Krzywda, Simulation of $1/f$ charge noise affecting a quantum dot in a Si/SiGe structure, *Appl. Phys. Lett.* **123**, 034005 (2023).
- [42] D. L. Mickelsen, H. M. Carruzzo, and C. C. Yu, Interacting two-level systems as a source of $1/f$ charge noise in quantum dot qubits, *Phys. Rev. B* **108**, 195307 (2023).
- [43] J. S. Rojas-Arias, A. Noiri, J. Yoneda, P. Stano, T. Nakajima, K. Takeda, T. Kobayashi, G. Scappucci, S. Tarucha, and D. Loss, Inferring charge noise source locations from correlations in spin qubits, [arXiv:2505.05875](https://arxiv.org/abs/2505.05875) [cond-mat.mes-hall].
- [44] J. F. Chittock-Wood, R. C. C. Leon, M. A. Fogarty, T. Murphy, S. M. Patomäki, G. A. Oakes, J. Williams, F.-E. von Horstig, N. Johnson, J. Jussot, S. Kubicek, B. Govoreanu, D. F. Wise, M. F. Gonzalez-Zalba, and J. J. L. Morton, Radio-frequency cascade readout and coherent exchange control of spin qubits fabricated using a 300 mm wafer process, [arXiv:2408.01241](https://arxiv.org/abs/2408.01241) [cond-mat.mes-hall].
- [45] L. H. Pedersen, N. M. Møller, and K. Mølmer, Fidelity of quantum operations, *Phys. Lett. A* **367**, 47 (2007).
- [46] T. Jones, A. Brown, I. Bush, and S. C. Benjamin, QuEST and High Performance Simulation of Quantum Computers, *Sci. Rep.* **9**, 10736 (2019).
- [47] R. Meister, pyQuEST – A Python interface for the Quantum Exact Simulation Toolkit, 2022, <https://github.com/rmeister/pyQuEST>.
- [48] A. Richards, University of Oxford Advanced Research Computing, 2015.
- [49] S. Birner, T. Zibold, T. Andlauer, T. Kubis, M. Sabathil, A. Trellakis, and P. Vogl, nextnano: General purpose 3-D simulations, *IEEE Trans. Electron Devices* **54**, 2137 (2007).
- [50] R. Loudon, One-dimensional hydrogen atom, *Proc. R. Soc. A* **472**, 201505342 (2016).
- [51] As a check, this was done to ensure the numerical simulations come to the same value.
- [52] See however the approach in Ref. [29], where it is explained that indeed the Coulomb matrix is diagonal if one evaluates integrals only at the grid points, and this is a valid approach in that Coulomb matrix will converge successfully with increasing M .