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Impact of charge noise on electron exchange interactions in semiconductors

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The electron exchange interaction is a promising medium for the entanglement of single-spin qubits in semiconductors as it results in high-speed two-qubit gates. The quality of such entangling gates is reduced by the presence of noise caused by nearby defects acting as two-level fluctuators. To date, the effect of charge noise has been calculated assuming a Gaussian distribution of exchange interaction frequencies between the qubits equivalent to a linear coupling of charge noise with the exchange interaction. In reality the coupling can differ significantly from this linear-coupling approximation depending on the inter-qubit tunnel coupling, detuning of the qubit system, and the magnitude of charge noise. We derive analytical expressions for the frequency spectra of exchange oscillations that encompasses both linear and non-linear coupling to charge-noise. The resulting decoherence times and decay profiles of the exchange oscillations vary considerably. When compared with recent experiments our model shows that non-linear charge-noise coupling is significant and requires consideration to characterise and optimise exchange-based entangling gates.

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INTRODUCTION

To achieve universal quantum computation with error correction, all qubit operations including initialisation, single- and two-qubit gates, and measurement require errors to be less than 1%^{1,2}. Many promising single-spin semiconductor multi-qubit systems^{3–8} have performed gate operations between the qubits mediated by the exchange interaction. Electrical tuning of the strength of the exchange interaction J causes it to couple to charge noise thus becoming a significant source of errors. There has been great interest in understanding, characterising, and minimising charge noise in these qubit systems since it is known to limit qubit coherence times^{9–15}. Many theoretical studies of charge noise have directly attributed the exchange interaction frequency between qubits to have a Gaussian distribution, equivalent to a linear coupling between charge noise and J . An alternative approach is to consider the distribution of charge noise itself as a Gaussian distribution, as expected for an array of nearby electrical two-level fluctuators (TLFs)^{16,17} such as lattice or surface defects¹⁸. The resulting distribution of J can then be calculated exactly for a given dependence of the exchange interaction on the difference in electro-chemical potential, referred to as the detuning, between the electrons. Accounting for the noise distribution in terms of detuning fluctuations (rather than fluctuations in the exchange interaction frequency) allows for the inclusion of more physically-realistic, non-linear couplings of J to charge noise.

Here, we present how this non-linear coupling approach can give rise to non-Gaussian distributions of the qubit exchange interaction frequency, and hence qubit decoherence. The exact form of the coupling depends on the relation of the exchange strength to detuning and the operating regime. Several models that describe the exchange interaction as a function of detuning exist in the literature, but here we focus on the two most popular models. The Hubbard model^{7,19,20} is discussed in the main text whilst the empirical exponential model^{9,21} is discussed in Supplementary Information I. For each model, we derive how to

account for the non-linear charge-noise coupling analytically. In particular, we investigate its effect on the amplitude, coherence time, the time profile of decay of exchange oscillations, and ultimately gate fidelity as a function of the charge-noise magnitude and detuning. Importantly, we identify when these effects differ significantly from the linear coupling case. This identification allows us to consider how to account for coupling to charge noise in exchange-based qubits under different operating regimes which ultimately ensures that the appropriate model is used to characterise coherent exchange oscillations in multi-qubit systems.

Exchange-based two-qubit operations in semiconductor qubits are performed on single electron spins by sweeping the detuning potential ϵ of a double-dot system across a (1,1) to (2,0) equivalent charge transition. Here the left and right numbers correspond to the ground state electron numbers on the left and right dots respectively. This charge transition forms an anti-crossing between the $S(1,1)$ and $S(2,0)$ singlet spin states whose ground state energy levels are depicted in Fig. 1 along with the triplet T^0 state. The two-spin system near the anti-crossing is described in the two-spin product basis ($|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$) by the Hamiltonian H ,

$$H = \begin{bmatrix} E_Z + \Delta E_Z & 0 & 0 & 0 \\ 0 & -\frac{J}{2} + \frac{\Delta E_Z}{2} & \frac{J}{2} & 0 \\ 0 & \frac{J}{2} & -\frac{J}{2} - \frac{\Delta E_Z}{2} & 0 \\ 0 & 0 & 0 & -E_Z - \Delta E_Z \end{bmatrix},$$

where E_Z is the electron-spin Zeeman energy in a global magnetic field, and ΔE_Z is the difference in the Zeeman energy between the two qubits. The exchange strength J at a given point in detuning ϵ is derived using the Hubbard model to be,

$$J(\epsilon, t_c) = \frac{\epsilon}{2} + \sqrt{\frac{\epsilon^2}{4} + t_c^2}, \quad (1)$$

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Fig. 1 Pulse scheme to observe coherent exchange oscillations in exchange-coupled atom qubits in silicon. Singlet ($S(1,1)$) and triplet (T^0) state eigenspectrum as a function of detuning ϵ for a two electron-spin, double-dot system that forms an anti-crossing centred around $\epsilon = 0$. As the electrons (red dots) are pulsed from separate dots to the same dot, the exchange strength $J(\epsilon)$ increases. Using an appropriate gate pulse scheme (red line, upper left inset), coherent oscillations in the two-electron spin probabilities (e.g. $|\uparrow\downarrow\rangle$) can be measured (blue line in right inset) as a function of the wait time t_w at the detuning position $\epsilon = \mu_\epsilon$. Here the $|\uparrow\downarrow\rangle$ probability oscillates up and down while decaying over time characterised by the decoherence time T_2^{SWAP} . Charge noise shifts the position of the detuning pulse around the intended detuning μ_ϵ with a probability described by a Gaussian distribution of standard deviation σ_ϵ (upper inset). The resultant distribution in exchange interaction frequencies is the main factor that limits the decoherence time T_2^{SWAP} which characterises the decay envelope (red line, right inset).

where t_c is the inter-dot tunnel coupling of the anti-crossing. Multiple exchange-based qubit gates are possible based on this interaction including the CROT^{6,22}, CZ^{5,23}, and $\sqrt{\text{SWAP}}$ ^{3,7} gates. All these gates have the potential to be detrimentally affected by charge noise. For the purpose of this work, we focus on the $\sqrt{\text{SWAP}}$ gate to directly compare our model to experimental results using atom-bound electrons in silicon⁷. In the case of phosphorus donor atoms in silicon, t_c is controlled by the physical inter-dot separation²⁴ set by atomic precision lithography during fabrication and ΔE_Z is determined by the spin state of the donor-atom nuclei. Gate voltage pulses can then be used to control J over five orders of magnitude²⁵ to implement an exchange-based gate such as the $\sqrt{\text{SWAP}}$ gate.

In general, to perform a $\sqrt{\text{SWAP}}$ gate the double-dot system must first be initialised in a $(1,1)$ ground state far from the anti-crossing ($\epsilon \ll 0$) where the exchange interaction is effectively turned off and the computational basis is the eigen-basis of the two-qubit system. The detuning is quickly ramped closer to the centre of the anti-crossing ($\epsilon = \mu_\epsilon$) to increase J (such that $J \gg \Delta E_Z$) where the singlet and triplet T^0 states become the basis states. The system will oscillate between the $S(1,1)$ and T^0 states for a wait time t_w before being pulsed back into the $(1,1)$ region and measured as depicted by the red pulse scheme in the Fig. 1 upper-left inset. If J and the characteristic decay time of the exchange oscillations T_2^{SWAP} are sufficiently high, coherent oscillations in the two-spin probabilities (blue line in Fig. 1 right inset) can be measured as a function of t_w . Any charge noise, whose magnitude has a standard deviation of σ_ϵ when integrated over the experiment's duration, present in the system will shift the resulting detuning around the intended value μ_ϵ for a given pulse (inset in Fig. 1). Averaging over many of these pulses affected by this charge noise will create a distribution of interaction

frequencies that become the main limitation to T_2^{SWAP} , particularly for isotopically purified systems where the Overhauser field is weak²⁶. In this work we model the coherent time evolution of a pair of electron spins due to this distribution of exchange interaction strengths caused by the presence of charge noise with a Gaussian distribution. We focus on the decay envelope of these coherent oscillations which we model as having the form $A \exp(-(t_w/T_2^{\text{SWAP}})^a)$. We show how T_2^{SWAP} , the initial oscillation amplitude A , the decay profile (characterised by constant a), and maximum gate fidelity $F_{\text{max}}^{\sqrt{\text{SWAP}}}$ vary with noise σ_ϵ and detuning ϵ and note the significance of non-linear coupling to charge noise in different regimes.

RESULTS AND DISCUSSION

Derivation of non-linear coupling to charge noise

When considering the charge noise arising from a nearby ensemble of TLFs, one would expect the distribution of charge noise to be Gaussian^{16,17}. In the case of semiconductors, these TLFs typically take the form of crystal lattice defects, or surface defects^{10,27}. Previous studies that model the effects of charge noise directly attribute the noise as a Gaussian distribution of the exchange oscillation frequency $\Omega = \sqrt{J^2 + \Delta E_Z^2}$ ^{9,13} for simplicity. This frequency distribution approximates the dependence of J on ϵ to always be linear. In this work, we show that this approximation is not always appropriate particularly when J , ϵ , and σ_ϵ are of similar magnitude. We note that while the amplitude of the charge noise possesses a Gaussian distribution, the power spectral density (PSD) is not constant for all frequencies i.e. it is not a white Gaussian distribution. In semiconductor systems the PSD of charge noise has been found to have a $1/f$ frequency dependence^{10,15,18,28–30}. Regardless of the frequency dependence of the charge noise PSD, a particular experiment will be impacted by the total noise integrated over a particular bandwidth related to the time-scales of the experiment¹⁴. The magnitudes of this total charge noise resulting from a $1/f$ spectra follow a Gaussian distribution with respect to ϵ characterised by the standard deviation σ_ϵ which will form the basis of our charge-noise analysis.

By treating ϵ as directly having a Gaussian distribution we can more realistically model the charge noise and account for any non-linearity in $J(\epsilon)$ (and hence the overall oscillation frequency Ω). The likelihood of reaching each individual detuning value is described by the detuning's probability density function (PDF) $\mathcal{E}$ i.e.

$$\mathcal{E} = \frac{1}{\sqrt{2\pi}\sigma_\epsilon} \exp\left(-\frac{(\epsilon - \mu_\epsilon)^2}{2\sigma_\epsilon^2}\right), \quad (2)$$

around the targeted detuning position μ_ϵ . Note that here we are only defining the distribution of the charge noise magnitude in line with a quasi-static noise approach. To calculate the impact of this Gaussian detuning PDF we map the detuning PDF to a corresponding exchange oscillation frequency PDF $\mathcal{F}$ via the exchange strength PDF $\mathcal{J}$ which we will derive below. If the dependence of J on ϵ is approximately linear within the likely range of ϵ values due to charge noise, the Gaussian ϵ PDF leads to a Gaussian J PDF as pictured in Fig. 2a. It is also possible that the J dependence on ϵ is non-linear. The non-linear coupling case is more likely for larger magnitudes of charge noise (compared to the tunnel coupling t_c) as depicted in Fig. 2b. Here the deviation of $J(\epsilon)$ from the linear approximation causes the PDF of J to be biased towards certain values (lower values in the case depicted by Fig. 2b) and appear as a skewed Gaussian distribution. We note only a linear transformation would leave the distribution proportionately unchanged. This change in the J PDF will cause noticeable changes in the frequency and decoherence of coherent oscillations which we will now quantify.

Fig. 2 Impact of charge noise on exchange oscillations. The probability density functions (PDFs) of the exchange-interaction strength J as a result of coupling to **a** low-magnitude (blue) and **b** high-magnitude (red) charge noise that causes a Gaussian distribution in detuning values ϵ . For low charge-noise magnitudes **a** the variation in J is well explained by the gradient ($dJ/d\epsilon$, blue dotted line) causing a proportional Gaussian distribution in J . For high charge-noise magnitudes **b** the variation in J deviates from the linear approximation ($dJ/d\epsilon$, red dotted line). This deviation causes a skewed-Gaussian distribution in $J(\epsilon)$ as the $J(\epsilon)$ values of less than average ϵ values are brought closer to the mean while the $J(\epsilon)$ values of above average ϵ values are taken further away from the mean. **c** Normalised PDFs of the frequency components $\mathcal{F}$ (coloured lines) for various magnitudes of charge noise characterised by σ_ϵ relative to the tunnel coupling $t_c = 4.3$ GHz when $\Delta E_Z = 117.53$ MHz. The intended detuning is chosen to be $\mu_\epsilon = 0$ as an example. **d** Fourier transforms of the corresponding PDFs in **c** depicting the relevant exchange oscillations as a function of the wait time t_w for given charge-noise values. For these examples, the Hubbard model has been used for the exchange-strength dependence on detuning.

We ultimately require the frequency spectrum of the exchange oscillations described by the PDF $\mathcal{F}$ since we can retrieve the exchange oscillations as a function of detuning pulse wait time t_w by taking the Fourier transform of $\mathcal{F}$. Fitting the envelope of the derived exchange oscillations to a function of the form $\propto \exp(-(t_w/T_2^{\text{SWAP}})^\alpha)$ allows us to determine both the decoherence time T_2^{SWAP} and the decay profile characterised by the parameter α . For example, $\mathcal{F}$ is calculated (using a method that will be outlined below) and plotted in Fig. 2c for various values of σ_ϵ from $0.1t_c$ to $100t_c$ while choosing $\mu_\epsilon = 0$ for simplicity. These values of σ_ϵ are computed for a device with $t_c = 4.3$ GHz similar to recent experimental results⁷ assuming the bulk value of the phosphorus nuclear hyperfine constant $\Delta E_Z = 117.53$ MHz. The corresponding Fourier transforms of these same $\mathcal{F}$, representing the exchange oscillations in the up-down two-spin state probability ($\uparrow\downarrow$), are shown in Fig. 2d. Performing similar calculations for various PDFs permits a thorough study of the exact effects of charge noise on electron exchange interactions.

In the case of low charge noise ($\sigma_\epsilon = 0.1t_c$, blue line) the detuning does not deviate far from $\epsilon = 0$. The resulting exchange oscillation frequencies ω are therefore narrowly distributed around the inter-dot tunnel coupling t_c (value of $J(\epsilon = 0)$) and several, relatively-fast oscillations can be seen within the decoherence time (see Fig. 2d, blue line). As the charge-noise magnitude increases, however, i.e. $\sigma_\epsilon = 10t_c$ (red line), the distribution of ω broadens and skews to lower frequencies

resulting in slower oscillations. In extreme cases such as $\sigma_\epsilon = 100t_c$ (green) the distribution of ω narrows again and ω becomes dominated by the constant ΔE_Z since the noise dominates the detuning and shifts the entire system away from the anti-crossing. The resulting hyperfine dominated oscillations are slow (see Fig. 2d, green line) with longer decoherence times, although we will see later, these oscillations occur with amplitudes approaching zero which is not yet accounted for in Fig. 2d. The variation in resulting exchange distributions already displays that exchange strength distributions can be highly non-linear depending on their coupling to charge noise and independent of the nature of the noise itself.

To explicitly calculate the exchange PDF $\mathcal{J}$ as a function of a particular exchange strength j we use the PDF definition $\mathcal{J}(j) = \frac{\partial}{\partial j} P(J \leq j)$ where $P(J \leq j)$ is the probability that the exchange strength is less than or equal to the value j . This probability can be mapped to an equivalent probability in terms of the detuning by rearranging Eq. 1 and integrating $\mathcal{E}$ for all ϵ up to $j(\epsilon)$ to give,

$$P(J \leq j) = P\left(\epsilon \leq j - \frac{t_c^2}{j}\right), \quad (3)$$

$$= \frac{1}{\sqrt{2\pi}\sigma_\epsilon^2} \int_{-\infty}^{j - \frac{t_c^2}{j}} \exp\left(-\frac{(\epsilon - \mu_\epsilon)^2}{2\sigma_\epsilon^2}\right) d\epsilon. \quad (4)$$

The exchange PDF is then related to $P(J \leq j)$ ³¹ by,

$$\mathcal{J}(j) = \frac{\partial}{\partial j} P(J \leq j), \quad (5)$$

$$= \frac{\partial}{\partial j} \left(j - \frac{t_c^2}{j} \right) \frac{\partial}{\partial \left(j - \frac{t_c^2}{j} \right)} \left[\frac{1}{\sqrt{2\pi\sigma_e^2}} \int_{-\infty}^{j - \frac{t_c^2}{j}} \exp\left(-\frac{(\epsilon - \mu_e)^2}{2\sigma_e^2}\right) d\epsilon \right], \quad (6)$$

$$= \frac{1 + \left(\frac{t_c}{j}\right)^2}{\sqrt{2\pi\sigma_e^2}} \exp\left(-\frac{\left(j - \frac{t_c^2}{j} - \mu_e\right)^2}{2\sigma_e^2}\right). \quad (7)$$

In a similar fashion, we derive the frequency distribution $\mathcal{F}(\omega) = \frac{\partial}{\partial \omega} P(\Omega \leq \omega)$ for a particular frequency value ω using the relation $\Omega = \sqrt{J^2 + \Delta E_Z^2}$ which gives,

$$\mathcal{F}(\omega) = \left(1 + \frac{t_c^2}{\omega^2 - \Delta E_Z^2}\right) \frac{\omega}{\sqrt{2\pi\sigma_e^2(\omega^2 - \Delta E_Z^2)}} \exp\left(-\frac{\left(\sqrt{\omega^2 - \Delta E_Z^2} - \frac{t_c^2}{\sqrt{\omega^2 - \Delta E_Z^2}} - \mu_e\right)^2}{2\sigma_e^2}\right). \quad (8)$$

Coherent exchange oscillations are then obtained by taking the Fourier transform of the frequency distribution $\mathcal{F}(\omega)$ (as was discussed in the examples shown in Fig. 2 for various magnitudes of charge noise) by analytically accounting for both the PDF of the charge noise and its coupling to the exchange interaction. The above method is also generalisable to other formulations for the charge noise PDF and the exchange detuning dependence.

The above derivation does not include the impact of changes in the oscillation amplitude caused by tilting of the axis of rotation based on the relative magnitudes of J and ΔE_Z . J causes rotations of the two-qubit state between the $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ states whilst ΔE_Z causes rotations in terms of the phase difference. It is the projection of the combination of these rotations on to the measurement basis that determines the decreased value of the initial amplitude A . The initial amplitude of an oscillation is defined as $A(\epsilon) = J(\epsilon)^2 / (J(\epsilon)^2 + \Delta E_Z^2)$ for a particular detuning position. Note that this initial amplitude does not take qubit readout or initialisation errors to account, and hence does not necessarily correspond to the oscillation amplitudes directly measured in an experiment. Based on the dependence of A , similar to above, we derive its probability density $\mathcal{A}(a)$ as a function of a particular amplitude a ,

$$\mathcal{A}(a) = \frac{\Delta E_Z}{2(1-a)^2} \left(1 + \frac{t_c^2}{\Delta E_Z^2} \left(\frac{1-a}{a}\right)\right) \sqrt{\frac{1-a}{2\pi a \sigma_e^2}} \exp\left(-\frac{\left(\Delta E_Z \sqrt{\frac{1-a}{1-a}} - \frac{t_c^2}{\Delta E_Z} \sqrt{\frac{1-a}{a}} - \mu_e\right)^2}{2\sigma_e^2}\right). \quad (9)$$

The oscillations are ultimately dampened by the mean μ_A of this distribution calculated as,

$$\mu_A = \int_{-\infty}^{\infty} a \mathcal{A}(a) da. \quad (10)$$

The combination of $\mathcal{F}(\omega)$ and $\mathcal{A}(a)$ allows us to completely simulate the resultant exchange oscillations for a given detuning position and charge noise taking non-linear effects into account.

Quantifying effect of non-linear coupling to charge noise

We consider the Hubbard-model with an exchange dependence of $J(\epsilon, t_c) = \epsilon/2 + \sqrt{\epsilon^2/4 + t_c^2}$ where we use the above derivation to simulate exchange oscillations ($t_c = 4.3$ GHz) as a function of both the detuning position relative to the centre of the (1,1)–(0,2) charge anti-crossing ϵ , and the magnitude of the charge noise σ_e . In Supplementary Information II we present similar calculations for constant $\sigma_e = 1$ GHz, and varying t_c and ϵ . For each simulation we fit the function $\exp(-(t_w/T_2^{\text{SWAP}})^a)$ to the envelope of decaying

oscillations to extract T_2^{SWAP} and a as fitting parameters which have previously been used to identify charge-noise mechanisms⁹. The results are presented in Fig. 3a and b respectively. In Fig. 3a, we observe a region where T_2^{SWAP} is minimal, close to the separation of two distinct regions where a corresponds to either a Gaussian ($a = 2$) or an exponential ($a = 1$) decay as both effects are a result of non-linear coupling to charge noise. In Fig. 3a, for any given magnitude of charge noise, the decoherence time T_2^{SWAP} is highest for large negative ϵ values, far from the anti-crossing, where the electrons are effectively uncoupled. T_2^{SWAP} decreases inversely proportional to $\partial J / \partial \epsilon$ ^{32,33} (i.e. the smaller the change in J , the longer the coherence) which is lowest far from the anti-crossing (as is the case for a linear coupling to charge noise). Figure 3a shows that for most detuning positions T_2^{SWAP} decreases as σ_e increases (until $\sigma_e > 10$ GHz), as the larger magnitude charge noise decoheres the qubits faster.

The exception to this trend in T_2^{SWAP} is approximately in the region where both $-\epsilon < 10$ GHz and $\sigma_e \sim t_c$ in this case. For these detuning values, we see that T_2^{SWAP} has a minimum around $\sigma_e \sim t_c$. This minimum is because (i) for small values of charge noise there is little disturbance to the two qubit system so the change in J is also small as for the $\sigma_e = 0.1 t_c$ (blue) case in Fig. 2c, d, and (ii) for large values of charge-noise the system is ‘shaken’ so strongly that pulses often reach particularly large negative detunings where the exchange-oscillation frequency ω is approximately constant leading to a minimal variation in J (albeit far from the intended value) as for the $\sigma_e = 100 t_c$ (green) case in Fig. 2c, d. It is only for values that lie between these two cases (i and ii) where time is spent at intermediate detuning values that the charge noise leads to significant changes in J and hence relatively significant decoherence similar to the red and orange examples in Fig. 2c, d. Naively one might expect the best T_2^{SWAP} values to occur at low σ_e , far from the centre of the anti-crossing, but these values are of little practical use without also considering the exchange oscillation decay envelope, quality factor, and amplitude.

The shape of the decay characterised by the exponent a in the fit to $\exp(-(t_w/T_2^{\text{SWAP}})^a)$ would be expected to either be 1 (exponential decay) if caused by a few nearby TLFs³⁴, or 2 (Gaussian decay) if caused by a large ensemble of fluctuators³⁵. However, in Fig. 3b we observe two distinct regions where a varies from 1 to 2 using the same noise mechanism/distribution. The bright region at low σ_e is when the decay profile is approximately Gaussian as expected for a large ensemble of charge-noise fluctuators. Yet, for very high σ_e the decay is approximately exponential (dark red). The region of exponential decay corresponds directly to when $\mathcal{F}(\omega)$ has been skewed asymmetrically as shown by the large charge-noise magnitude examples in Fig. 2a. One trivial case of this is when the exchange strength is very weak when detuned far from the anti-crossing ($\Delta E_Z \gg J$) such that the overall oscillation frequency distribution asymptotically approaches ΔE_Z . As a consequence, the distribution is truncated at that frequency as in the $\sigma_e = 100 t_c$, green distribution in Fig. 2c. Realistically, there is also a distribution in the change in Zeeman energy (ΔE_Z) itself due to the presence of an Overhauser field but this is negligible compared to typical values for t_c and σ_e especially in ²⁸Si²⁶ hence it is not considered in this study. Overall, the results in Fig. 3b show that a qubit system can exhibit either exponential ($a \sim 1$) or Gaussian ($a \sim 2$) decay simply with varying magnitudes of either charge-noise, detuning, or tunnel coupling. This variation demonstrates that to draw conclusions on the underlying charge-noise mechanism present in devices from the oscillation decay profile (a value) one must first rule out the role of non-linear coupling to charge noise which is dependent on experimental parameters such as the noise magnitude and qubit detuning. A more detailed look at the transition between the exponential and Gaussian decay regimes will be discussed in the following section.

Fig. 3 Quantifying the impact of charge noise on exchange oscillations. Using the Hubbard model for the detuning dependence of J we extract the **a** decoherence time T_2^{SWAP} , **b** α from the decay profile of the oscillation envelope function $\exp(-(t_w/T_2^{\text{SWAP}})^\alpha)$, **c** quality factor Q , **d** initial amplitude A of exchange oscillations, and **e** maximum fidelity of a $\sqrt{\text{SWAP}}$ gate $F_{\text{max}}^{\sqrt{\text{SWAP}}}$ as a function of the charge noise standard deviation σ_ϵ and detuning position ϵ relative to the anti-crossing calculated using $t_c = 4.3$ GHz to match⁷. The error bars (A–D) in **b** represent the corresponding data points from experimental exchange oscillations⁷ whose oscillations and parameters are displayed in Fig. 4 and Table 1 respectively. The blue error bars (B) in each figure corresponds to experimental parameters used to achieve coherent exchange oscillations by⁷. The dotted white line in **b** depicts the contour where $\sigma_\epsilon = J$ (which causes α to transition from 1 to 2) forming a boundary between regions of exponential and Gaussian decay. The lower right values (white) in **b** are left out due to practical time resolution limitations of the calculations. The darker values inside the white dotted line in **c** achieved quality factors $Q < 1$, whilst the values to the left of the black dotted line in **d** achieved initial oscillation amplitudes $A > 0.5$. The brighter values in **e** below the black dotted line shows where σ_ϵ is low enough to achieve a maximal fidelity $F_{\text{max}}^{\sqrt{\text{SWAP}}} > 0.9$.

Of particular interest is the boundary between the exponential and Gaussian decay regimes which distinguishes between experiments with low noise (below the boundary) where a linear mapping of the charge noise is sufficient, and high noise (above the boundary) where non-linear effects should be considered. We can approximate the boundary's position between the two

regimes by determining the function of σ_ϵ with respect to ϵ that satisfies the following condition;

$$|J(\mu_\epsilon + \sigma_\epsilon) - J(\mu_\epsilon - \sigma_\epsilon)| \sim 2\sigma_\epsilon \left. \frac{\partial J}{\partial \epsilon} \right|_{\epsilon=\mu_\epsilon}, \quad (11)$$

which defines the point at which variation of J across a noisy detuning range is approximately equal to the expected linear variation. Based on approximations for $\epsilon \ll t_c$ and $\epsilon \gg t_c$ we find the boundary (dashed line in Fig. 3b to be $\sigma_e \propto \sqrt{\epsilon^2 + t_c^2}$ (see Supplementary Information III for more details). It is important to determine whether non-linear effects of charge noise are significant before characterisation or optimisation of qubit operation to avoid predicting/extracting incorrect decoherence times or charge-noise magnitudes.

To help determine the optimal operating conditions for a two qubit operation, we calculate both the quality factor Q (number of oscillations within T_2^{SWAP}) and the initial oscillation amplitude A which is presented in Fig. 3c and d respectively. Ideally we want both these values to be as high as possible ($Q \gg 1$, and $A \gg 0.5$) to ensure a high-fidelity 2-qubit gate. We see in Fig. 3c that Q follows a very similar trend to T_2^{SWAP} in Fig. 3a. However, the Q values do not experience the same increase in magnitude at high charge-noise magnitudes because the increasing decoherence times of the oscillations are more than compensated for by the decreasing exchange oscillation frequency that approaches ΔE_Z at these values. To achieve a $\sqrt{\text{SWAP}}$ gate with non-negligible fidelity, Q must be at least greater than one (lighter region below white dotted line in Fig. 3c) to reasonably complete two-qubit operations before significant levels of dephasing reduce the oscillation amplitude and hence gate fidelity. For the same reason, the initial amplitude A is ideally close to one such that it is not limiting the fidelity of the $\sqrt{\text{SWAP}}$ gate. The value of A is expected to be less than one if ΔE_Z is at any point comparable to the magnitude of J , since the axis of the exchange rotations will be tilted. We observe in Fig. 3d that A is closest to one (dark red) for low charge noise σ_e with detuning values close to the anti-crossing. When ϵ is negative and large, then ΔE_Z is significant relative to J regardless of the magnitude of charge noise and the resultant oscillation amplitude is small. When σ_e is large, the charge noise will lead to unintended pulse detuning values where ΔE_Z is also significant, again decreasing the amplitude. Even though T_2^{SWAP} and Q were found to be high in these regimes, we expect the low amplitude of exchange oscillations so significantly limit the $\sqrt{\text{SWAP}}$ gate fidelity. Realistically, noisy systems can compromise oscillation amplitude, quality factor, and/or speed to optimise the gate fidelity of a two-qubit quantum gate.

For all calculations, we have set ΔE_Z to 117.53 MHz, the bulk hyperfine value for single phosphorus donor atoms in silicon³⁶. While this hyperfine value can vary for different numbers of donor atoms in the quantum dots^{25,37,38}, we expect the same trends to apply for realistic values of ΔE_Z as they vary by less than an order of magnitude. Additionally, the hyperfine value is less than typical tunnel couplings (several GHz) and hence would only contribute to a small shift in the plots of T_2^{SWAP} , α , and Q . The value of ΔE_Z does however determine the crossover point ($A = 0.5$, dotted line in Fig. 3d) for the amplitude with respect to both ϵ and σ_e . This crossover point signifies where the exchange interaction starts to dominate the hyperfine interaction and therefore the onset of two-spin correlations would be observed³⁹. In order to estimate the crossover point, we define the ratio $\beta = t_c/\Delta E_Z$. The crossover point then occurs when $\epsilon = t_c(1 - \beta^2)/\beta$ which is approximately

$\epsilon \sim -\beta t_c = -t_c^2/\Delta E_Z$ when $\beta \gg 1$. Hence, the tunnel coupling has a particularly strong effect on the detuning position at which the oscillation amplitude drops off, which is directly related to the practicality of switching the exchange interaction on and off. For example, when $t_c = 4.3$ GHz and $\Delta E_Z = 117.53$ MHz as in Fig. 3d we find the detuning of the crossover point to be $\epsilon = -157$ GHz. To achieve an exchanged-based $\sqrt{\text{SWAP}}$ gate care should be taken to ensure noise is sufficiently low to reach the regime where both $Q > 1$ and $A > 0.5$ (ideally well above these thresholds) for a given tunnel coupling and practical detuning range.

A practical metric for quantifying how close a quantum gate is to the intended ideal case is the gate fidelity. While one could determine the gate fidelity by simulating the time evolution of the complete density matrix of the two qubit system using the values for ϵ , σ_e , α , and T_2^{SWAP} extracted here, we find this simulation to be outside the scope of this work. Instead, the upper bound of the $\sqrt{\text{SWAP}}$ gate fidelity $F_{\text{max}}^{\text{SWAP}}$ is defined as

$$F_{\text{max}}^{\text{SWAP}} = A \exp(-(4Q)^{-\alpha}), \quad (12)$$

reflect the total oscillation amplitude at the time corresponding to a quarter oscillation required for a $\sqrt{\text{SWAP}}$ gate. This definition of $F_{\text{max}}^{\text{SWAP}}$ includes the reduction in gate fidelity due to off-axis rotations caused by ΔE_Z and the qubit decoherence, but ignores the qubits' readout and initialisation and the qubits' phase information which the density matrix would be required for. The results for $F_{\text{max}}^{\text{SWAP}}$ as a function of ϵ and σ_e are shown in Fig. 3e where we intuitively see the highest fidelities occurring for low σ_e such that charge noise has minimal impact on the qubits, and low ϵ where exchange oscillations are fastest close to the anti-crossing. For large σ_e , the fidelity is limited by the incoherent exchange oscillation frequencies caused by charge noise, and for large ϵ the reduced amplitude becomes the main limitation to gate fidelity. In between these two regions is a small section in the upper-right corner of the bright area of Fig. 3e (corresponding to $F_{\text{max}}^{\text{SWAP}} > 0.9$) where high gate fidelity can still be achieved by compensating for the larger charge noise magnitude by operating further away from the anti-crossing in detuning where the coupling to the charge noise is weaker. Therefore, point A ($F_{\text{max}}^{\text{SWAP}} = 0.94$) is more promising than point B ($F_{\text{max}}^{\text{SWAP}} = 0.81$) as point A falls within this compensation region where the gate fidelity is theoretically expected to be higher.

We now compare the results for the simulated exchange oscillations to that experimentally realised by He et al.⁷ in their precisely placed phosphorus donor atoms in silicon double quantum dot device. The inherent tunnel coupling of their device was $t_c = 4.3$ GHz based on the physical separation of the donor qubits. Exchange oscillations were performed at four different detuning values (A–D) represented by the error bars in Fig. 3b. We note the blue error bars for B represent the detuning position used to perform a $\sqrt{\text{SWAP}}$ gate. The results of the fits to the experimental data are summarised in Table 1 and displayed in Fig. 4. As ϵ becomes more negative (and the overall oscillation frequency Ω decreases) we observe T_2^{SWAP} increase as the charge noise couples more weakly to the exchange oscillations when further from the centre of the anti-crossing. Here the electrons are

Table 1. Summary of experimental parameters extracted at various detuning positions from two-qubit experiments using donor atom qubits in silicon.

	ϵ (GHz)	σ_e (GHz)	Ω (MHz)	T_2^{SWAP} (ns)	Q	α	A	$F_{\text{max}}^{\text{SWAP}}$
A	-30 ± 2	3 ± 1	618 ± 38	4.7 ± 2.0	2.99 ± 1.42	1.88 ± 0.10	0.96 ± 0.01	0.94 ± 0.03
B	-63 ± 3	13 ± 2	329 ± 14	4.7 ± 0.9	1.57 ± 0.36	1.48 ± 0.12	0.87 ± 0.01	0.81 ± 0.04
C	-89 ± 20	49 ± 10	249 ± 43	5.7 ± 1.8	1.49 ± 0.68	0.96 ± 0.13	0.75 ± 0.07	0.61 ± 0.14
D	-148 ± 9	35 ± 8	172 ± 6	14.4 ± 3.8	2.50 ± 0.73	1.30 ± 0.16	0.54 ± 0.03	0.54 ± 0.03

Fig. 4 Impact on charge noise on the determination of optimal exchange-gate operating conditions. Normalised oscillations of the experimentally measured two-spin probability (open circles, offset for clarity) of the up-down state as a function of the detuning-pulse wait time t_w with a two-qubit donors-in-silicon system from He et al.⁷. The four sets of oscillations correspond to four different detuning positions (A-D) as outlined in Table 1. The decay of each oscillation was fitted proportionally to $\exp(-t_w/T_2^{\text{SWAP}})^\alpha$ (solid lines) which shows how α can vary from 1 to 2 with detuning position.

more bound to the individual dots and both the absolute value of J and its variation over a fixed detuning range decrease.

All resulting exchange oscillations presented in Fig. 4 were found to have sufficient amplitudes that the dual-spin probabilities ($P_{\uparrow\downarrow}$ and $P_{\downarrow\uparrow}$) cross over at some point in time, and most of the four points achieved quality factors greater than one ($Q > 1$)⁷ suitable to demonstrate a $\sqrt{\text{SWAP}}$ gate. Interestingly α transitions between Gaussian ($\alpha = 2$) and exponential ($\alpha = 1$) depending on the particular experimental measurement. The range of α values observed in the model displays how an experiment with the same source of charge noise can exhibit different exchange oscillation decay behaviours based on the presence of non-linear coupling to charge noise in differing regimes. The chosen detuning positions happen to cross the boundary between linear and non-linear charge-noise coupling regimes where the charge noise σ_c is of comparable energy to both t_c and ϵ . We find σ_c values in the range of 3–49 GHz for experiments A–D where the variation in noise is largely due to varying experimental pulse-cycle times, number of repeated measurements per data point, and wait-time resolution of the experiments which all affect the overall integrated noise of the individual measurements as highlighted and improved upon by Kranz et al.¹⁴ in a similar donor-based device. In particular, the faster oscillations closer to the anti-crossing require less total experiment time to measure. Additionally, the sub-nanosecond detuning pulses are likely distorted from the intended square pulse, especially for short time-scales. Thus, while the type of decay profile (Gaussian or exponential) is not necessarily an effective tool to identify noise mechanisms it can be useful to characterise the coupling of charge noise to the exchange interaction and identify useful regimes for a $\sqrt{\text{SWAP}}$ gate. For example, our analysis highlights how point A would have produced better results than the point B used in⁷ in terms of quality factor Q , measured oscillation amplitude, and hence $\sqrt{\text{SWAP}}$ gate fidelity. While T_2^{SWAP} stayed approximately equal, the oscillation frequency $\Omega = 580$ MHz increased to achieve a higher quality factor $Q = 3$. The increased Ω would also allow completing the same two-qubit gate experiment in a shorter period of time, introducing less integrated noise over the course of the measurement.

Here we have presented our analytical method for directly accounting for the impact of charge noise on electron exchange interaction. By attributing a PDF to the qubit detuning due to charge noise, and including the exact coupling to the exchange

interaction it is possible to precisely derive the resultant coherent oscillations. We present this method in the specific case of the Hubbard model detuning dependence of the exchange interaction strength whilst also demonstrating how it is generalisable to other detuning dependences. Overall, this method is perfectly suited to accounting for non-linear coupling effects arising from charge noise magnitudes comparable to qubit detunings or tunnel couplings, as opposed to simple linear approximations. For this reason, we also approximate the regime, defined by $\sigma_c \gtrsim \sqrt{\mu_c^2 + t_c^2}$, where the effects of non-linear coupling to charge noise are too large to successfully utilise the linear approximation method.

The transition from linear coupling to non-linear coupling also corresponds to a transition between Gaussian and exponential decay of the coherent oscillations respectively. This transition from Gaussian to exponential decay was also reflected in the fits to recent experimental coherent oscillations using the exchange interaction to achieve a $\sqrt{\text{SWAP}}$ gate⁷. All experiments in a similar parameter regime would require the analytical method presented here to be able to: characterise coherent oscillations and correctly extract dephasing times and charge noise magnitudes; and to optimise qubit detunings and inter-qubit couplings for exchange-based two-qubit gates. Note that it is the charge noise integrated over the duration of the experiment that is relevant for this analysis. Importantly, all variations in the coherent oscillations presented here were independent of the source or mechanism of the charge noise. Instead, the coupling to the charge noise, dictated by the detuning dependence of the exchange interaction strength and the experimental operating conditions (such as detuning, charge noise, and inter-qubit tunnel coupling) can visibly alter the characteristics of resultant coherent oscillations.

METHODS

Analytical coherent exchange oscillations

Most of the results in this work are determined via theoretical calculations. We derive the PDF of the frequency of exchange oscillations for a Gaussian PDF of the two-qubit detuning caused by charge noise, and a coupling of the qubits to the charge noise via the exchange interaction described by the Hubbard model. The exchange oscillations are then determined by taking the Fourier transform of the frequency PDF.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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REFERENCES

- Wang, D. S., Fowler, A. G. & Hollenberg, L. C. L. Surface code quantum computing with error rates over 1%. *Phys. Rev. A* **83**, 020302 (2011).
- Hill, C. D. et al. A surface code quantum computer in silicon. *Sci. Adv.* **1**, e1500707 (2015).
- Nowack, K. C. et al. Single-shot correlations and two-qubit gate of solid-state spins. *Science* **333**, 1269–1272 (2011).
- Veldhorst, M. et al. A two-qubit logic gate in silicon. *Nature* **526**, 410–414 (2015).
- Watson, T. F. et al. A programmable two-qubit quantum processor in silicon. *Nature* **555**, 633–637 (2018).
- Zajac, D. M. et al. Resonantly driven CNOT gate for electron spins. *Science* **359**, 439–442 (2018).
- He, Y. et al. A two-qubit gate between phosphorus donor electrons in silicon. *Nature* **571**, 371–375 (2019).
- Kandel, Y. P. et al. Coherent spin-state transfer via Heisenberg exchange. *Nature* **573**, 553–557 (2019).
- Dial, O. E. et al. Charge noise spectroscopy using coherent exchange oscillations in a singlet-triplet qubit. *Phys. Rev. Lett.* **110**, 146804 (2013).

10. Shamim, S., Weber, B., Thompson, D. W., Simmons, M. Y. & Ghosh, A. Ultralow-noise atomic-scale structures for quantum circuitry in silicon. *Nano Lett.* **16**, 5779–5784 (2016).
11. Das Sarma, S., Throckmorton, R. E. & Wu, Y.-L. Dynamics of two coupled semiconductor spin qubits in a noisy environment. *Phys. Rev. B* **94**, 045435 (2016).
12. Buterakos, D., Throckmorton, R. E. & Das Sarma, S. Crosstalk error correction through dynamical decoupling of single-qubit gates in capacitively coupled singlet-triplet semiconductor spin qubits. *Phys. Rev. B* **97**, 045431 (2018).
13. Throckmorton, R. E., Barnes, E. & Das Sarma, S. Environmental noise effects on entanglement fidelity of exchange-coupled semiconductor spin qubits. *Phys. Rev. B* **95**, 085405 (2017).
14. Kranz, L. et al. Exploiting a single-crystal environment to minimize the charge noise on qubits in silicon. *Adv. Mater.* **32**, 2003361 (2020).
15. Connors, E. J., Nelson, J. J. & Nichol, J. M. Charge-noise spectroscopy of Si/SiGe quantum dots via dynamically-decoupled exchange oscillations. Preprint at <https://arxiv.org/abs/2103.02448> (2021).
16. Shnirman, A., Makhlin, Y. & Schön, G. Noise and decoherence in quantum two-level systems. *Phys. Scr.* **102**, 147 (2002).
17. Nakamura, Y., Pashkin, Y. A., Yamamoto, T. & Tsai, J. S. Charge echo in a cooper-pair box. *Phys. Rev. Lett.* **88**, 047901 (2002).
18. Connors, E. J., Nelson, J. J., Qiao, H., Edge, L. F. & Nichol, J. M. Low-frequency charge noise in Si/SiGe quantum dots. *Phys. Rev. B* **100**, 1615305 (2019).
19. Shi, Z. et al. Coherent quantum oscillations and echo measurements of a Si charge qubit. *Phys. Rev. B* **88**, 075416 (2013).
20. Fogarty, M. A. et al. Integrated silicon qubit platform with single-spin addressability, exchange control, and single-shot singlet-triplet readout. *Nat. Commun.* **9**, 4370 (2018).
21. Shulman, M. D. et al. Demonstration of entanglement of electrostatically coupled singlet-triplet qubits. *Science* **336**, 202–205 (2012).
22. Petit, L. et al. High-fidelity two-qubit gates in silicon above one Kelvin. Preprint at <https://arxiv.org/abs/2007.09034> (2020).
23. Veldhorst, M. et al. An addressable quantum dot qubit with fault-tolerant control-fidelity. *Nat. Nanotechnol.* **9**, 981–985 (2014).
24. Broome, M. A. et al. High-fidelity single-shot singlet-triplet readout of precision-placed donors in silicon. *Phys. Rev. Lett.* **119**, 046802 (2017).
25. Wang, Y. et al. Highly tunable exchange in donor qubits in silicon. *npj Quantum Inf.* **2**, 16008 (2016).
26. Tyryshkin, A. M., Lyon, S. A., Astashkin, A. V. & Raitsimring, A. M. Electron spin relaxation times of phosphorus donors in silicon. *Phys. Rev. B* **68**, 193207 (2003).
27. Queisser, H. J. & Haller, E. E. Defects in semiconductors: Some fatal, some vital. *Science* **281**, 945–950 (1998).
28. Freeman, B. M., Schoenfeld, J. S. & Jiang, H. W. Comparison of low frequency charge noise in identically patterned Si/SiO₂ and Si/SiGe quantum dots. *Appl. Phys. Lett.* **108**, 253108 (2016).
29. Petit, L. et al. Spin lifetime and charge noise in hot silicon quantum dot qubits. *Phys. Rev. Lett.* **121**, 076801 (2018).
30. Struck, T. et al. Low-frequency spin qubit energy splitting noise in highly purified ²⁸Si/SiGe. *npj Quantum Inf.* **6**, 40 (2020).
31. Stephens, M. E., Goodwin, B. W. & Andres, T. H. Deriving parameter probability density functions. *Reliab. Eng. Syst. Saf.* **42**, 271–291 (1993).
32. Hu, X. & Das Sarma, S. Charge-fluctuation-induced dephasing of exchange-coupled spin qubits. *Phys. Rev. Lett.* **96**, 100501 (2006).
33. Thorgimsson, B. et al. Extending the coherence of a quantum dot hybrid qubit. *npj Quantum Inf.* **3**, 32 (2017).
34. Ithier, G. et al. Decoherence in a superconducting quantum bit circuit. *Phys. Rev. B* **72**, 134519 (2005).
35. Lyon, A. Why are normal distributions normal? *Br. J. Philos. Sci.* **65**, 621–649 (2014).
36. Feher, G. Electron spin resonance experiments on donors in silicon. I. Electronic structure of donors by the electron nuclear double resonance technique. *Phys. Rev.* **114**, 1219 (1959).
37. Büch, H., Mahapatra, S., Rahman, R., Morello, A. & Simmons, M. Y. Spin readout and addressability of phosphorus-donor clusters in silicon. *Nat. Commun.* **4**, 2017 (2013).
38. Hile, S. J. et al. Addressable electron spin resonance using donors and donor molecules in silicon. *Sci. Adv.* **4**, eaaq1459 (2018).
39. Broome, M. A. et al. Two-electron spin correlations in precision placed donors in silicon. *Nat. Commun.* **9**, 980 (2018).

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AUTHOR CONTRIBUTIONS

S.G. and Y.H. fabricated the device. D.K. derived the analytical expressions and performed the modelling with helpful discussion from S.G., Y.H., and L.K. The manuscript was written by D.K. and M.Y.S. with input from all other authors. M.Y.S. supervised the project.

COMPETING INTERESTS

M.Y.S. is a director of the company Silicon Quantum Computing Pty Ltd. D.K., S.K.G., Y.H., and L.K. declare no competing interests.

ADDITIONAL INFORMATION

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