Valley leakage and gate timing errors in SWAP operations of Si-based spin qubits

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We investigate the fidelity of a sequence of SWAP gates on a Si-based quantum dot (QD) spin qubit chain. We particularly examine how valley leakage and gate timing error affect the gate fidelity compared to charge noise, which is always present. In our Hamiltonian, each qubit is coupled via Heisenberg exchange to every other qubit in the chain, with the strength of the exchange interaction decreasing exponentially with qubit distance. Valley leakage is modeled through a dissipation term \( \gamma \) as appropriate for the experimentally observed intervalley tunneling effect. We show that randomness in the valley leakage parameter has little to no effect on the SWAP gate fidelity in the currently fabricated Si circuits. We introduce disorder in the forms of charge noise and gate timing error and average the fidelities of 10,000 calculations for each set of parameters. The fidelities are then plotted against \( J_{\text{SWAP}} \), the strength of the exchange coupling corresponding to the SWAP gate. We find that valley leakage decreases the fidelity of the SWAP operation—though the effect is small compared to that of the known charge noise—and that gate timing error creates an effective optimal value of \( J_{\text{SWAP}} \), beyond which infidelity begins to increase.

I. INTRODUCTION

Quantum dot semiconductor spin qubits are promising candidates to form the basis of a quantum computer. Such qubits benefit from long coherence times and relatively straightforward scalability. However, no one to date has demonstrated two-qubit gates on spin qubits with the fidelity required for the execution of quantum error-correcting codes, which are the basis of robust quantum computation. This level of fidelity is often referred to as the error-correction threshold, and is at least 99.9%. In order to achieve this error-correction threshold, recent experimental work \[1\] suggests that fast gate times are a key, so that the gate time is much shorter than any decoherence time. Gates based on the Heisenberg exchange underlying interqubit coupling in semiconductor spin qubits are very fast, since the exchange coupling can be controlled electrostatically. Such gates include the SWAP gate for single-spin qubits, while other multi-spin qubits have been designed so that all gates, single-qubit and two-qubit, are performed simply by tuning the Heisenberg exchange coupling \[2, 3\]. This paper addresses some of the key sources of infidelity of exchange-based SWAP gates on Si-based spin qubits. The issues we study here are not yet of immediate urgency to current experimental Si-based spin qubit circuits, where measurements have just started studying SWAP and multiqubit operations, simply because Si-based spin qubits are far behind in development compared with other competing quantum computing platforms such as superconducting circuits and ion traps. But the fundamental issues discussed theoretically in this work will be crucial in any future developments of Si-based spin quantum computing architectures.

In quantum computation, a SWAP gate is required to increase connectivity beyond nearest neighbors, i.e., to transport quantum information across the circuit. SWAP is performed for semiconductor spin qubits by lowering the barrier potential between two QDs, allowing for greater wavefunction overlap and subsequently greater exchange interaction \( J_{\text{SWAP}} \). This pulse of lowered potential lasts for time \( \tau = \frac{\pi}{J_{\text{SWAP}}} \) (\( h = 1 \)). One can also perform its root \( \sqrt{\text{SWAP}} \) by halving the gate time to entangle qubits. This makes SWAP, along with single-qubit gates, sufficient to achieve universal quantum computation \[4\]. SWAP is therefore an essential element of quantum computation, and obviously it must be error-free.

Silicon has been put forward as an ideal material for semiconductor QD qubits for several reasons. First, coherence times in Si are significantly longer than in GaAs systems, where nuclear-induced spin decoherence is a big problem. Silicon’s coherence times can be made even longer through a process known as isotopic purification, where \( ^{28}\text{Si} \), silicon’s only stable magnetic isotope, is removed in favor of the stable spin-0 isotopes \( ^{28}\text{Si} \) and \( ^{30}\text{Si} \), GaAs systems cannot be purified in such a manner because there are no stable spin-0 isotopes of gallium nor arsenic. Second, Si-based qubits can be more easily integrated into the existing semiconductor industry, which is already capable of creating complex silicon processors made up of a very large number of transistors, or classical bits, thus making scaling up an easier task in Si-based quantum circuits.

One disadvantage that Si-based qubits suffer from when compared to other semiconductor (e.g., GaAs) QD spin qubits is valley degeneracy. Bulk Si has six degenerate ellipsoidal valleys along the symmetry axes in the conduction band. This sixfold degeneracy becomes twofold in the size-confined Si [100] surface where the typical QDs hosting the spin qubit reside, with the other four valleys getting lifted in energy by virtue of the mass anisotropy. This twofold ground-state degeneracy is often found to be lifted by a relatively small valley splitting \( \Delta \), which depends on the interface sharpness and other factors that are often random and difficult to predict. For large \( \Delta \), the system behaves as a spin qubit since the valley degree of freedom is effectively frozen as long as the operational temperature is much smaller than the...
valley splitting. When $\Delta$ is small, however, it creates an avenue of decoherence during gate operation, known as valley leakage. This valley leakage problem, arising from any intervalley electron hopping, is independent of the problem associated with the higher valley thermal occupancy, and as such, may not necessarily be suppressed by making the temperature much lower than the valley splitting. Valley degeneracies also hinder the Pauli spin blockade, which is crucial to qubit initialization and readout [5]. Although much work has been done [6–9] to characterize valley leakage and develop methods to minimize information loss, some loss is inevitable, because of possible intervalley coupling.

Another well-known source of SWAP gate error is charge noise, which is ubiquitous and is thought to be the primary decohering problem in Si-based spin qubits since spin noise can be effectively suppressed in Si. For semiconductor spin qubits, charge noise comes from charged defects on the interface and from noise in the applied gate voltages, which are always present in the environment. This affects the exchange coupling directly, since the exchange coupling is fundamentally based on the interelectron Coulomb interaction between neighboring QDs [10]. Much work is being done to mitigate the effects of charge noise, including symmetric gate operation [11] and composite pulses [12].

As more experimental progress is made, we expect gate times to become shorter and for gate timing error to become increasingly relevant. Gate timing error refers to unintentional experimental errors in the gate duration $\tau$. This slight randomness in the SWAP time is inevitable, since the experimental controls cannot be absolutely precise.

We first introduce the model qubit Hamiltonian on which we base our work. We then analytically examine the effects of valley leakage and noise in the valley coupling. We then present our numerical results on SWAP fidelities in the presence of charge noise, valley leakage, and gate timing error. Finally, we present our conclusions.

**II. MODEL**

We use the following Hamiltonian,

$$H = \sum_{k=1}^{L-1} \sum_{n=1}^{L-k} J_{n}^{k} \sigma_{n} \cdot \sigma_{n+k} - i \gamma 1,$$

where $L$ is the length of the chain of spin qubits and $J_{n}^{k}$ refers to the exchange coupling strength between the $n$th and $(n+k)$th qubit. For example, $k = 1$ corresponds to nearest-neighbor coupling, $k = 2$ corresponds to next-nearest-neighbor coupling, and so on.

The non-Hermitian term $-i \gamma 1$ is a dissipative valley leakage term, making the time evolution operator nonunitary. This term represents the information loss from valley leakage arising from intervalley electron tunneling which effectively “removes” the electron from the qubit subspace, thus acting as a dissipation process. We use $\gamma$ as a phenomenological parameter to characterize the valley leakage—in reality, we expect $\gamma$ to be of the order of intervalley electron tunneling energy, which is typically 10–20% of the intravalley tunneling that contributes to the exchange energy in Eq. (1). Of course, $\gamma$ must be positive in order to properly simulate leakage, else the probability would increase exponentially with time. Based on recent experimental results [13], we estimate $\gamma$ to be no greater than one tenth the value of the nearest-neighbor coupling strength $J^2$, perhaps even much smaller.

Each spin in the chain in our model is coupled to every other spin in the chain. Previous work [14] simulated the effects of charge noise, but only including interactions between nearest and next-nearest neighbors. We extend the range of interactions to the whole length of the chain, including all qubits, with the interaction strength decreasing exponentially such that the $J_{n}^{k+1}/J_{n}^{k} \equiv \beta < 1$. For example, if $\beta = 0.2$, then $J_{n}^{3} = J_{n}^{1}/5 = J_{n}^{1}/25$. This is consistent with the energetics of interdot exchange couplings, which ultimately arise from the electron wavefunction overlaps between the QDs.

**III. CALCULATIONS**

We now turn our attention to calculating the fidelity of our sequence of SWAP gates. We define fidelity as

$$F = |\langle \psi | R^\dagger U | \psi \rangle|^2,$$

where $R$ is an operator which performs the SWAP gate sequence with perfect fidelity and $U$ represents the actual SWAP gate sequence with errors. In our case, the SWAP sequence is intended to transport a spin state from one side of the spin chain to the other, and then back again. Therefore, under ideal SWAP operations, we expect our sequence of gates to be equivalent to the identity, so that $R = 1$.

**A. Noise in the dissipative term**

Our simple dissipative model allows for the effects of $\gamma$ on fidelity to be calculated analytically. We find that

$$F = F_0 e^{-2\gamma t},$$

where $F_0$ is the fidelity without any valley leakage.

We now show that the additional effects of valley noise on the fidelity are negligible. Assuming that noise in $\gamma$ is independent from other sources of disorder, we can isolate it so that

$$\langle F \rangle = F_0 (e^{-2\gamma t}).$$

We then assume the quasistatic noise in the dissipation term $\gamma$, taken from a normal distribution with deviation
\(\sigma_\gamma,\) such that \(\gamma \sim \mathcal{N}(\gamma_0, \sigma_\gamma).\) The computation of \(\langle e^{-2\gamma t}\rangle\) is somewhat complicated by the fact that \(\gamma\) must be positive in order for our model in Eq. (1) to make any sense. This forces us to truncate our distribution at \(\gamma = 0\) and calculate the integral
\[
\langle e^{-2\gamma t}\rangle = \frac{1}{\alpha \sigma_\gamma} \sqrt{\frac{2}{\pi}} \int_0^\infty e^{-2\gamma t} e^{-(\gamma - \gamma_0)^2/2\sigma_\gamma^2} d\gamma
\]
where \(\text{erf}(x)\) is the Gaussian error function and
\[
\alpha = 1 + \text{erf}\left(\frac{\gamma_0}{\sigma_\gamma \sqrt{2}}\right).
\]

For reasonable values of our parameters, such that \(\sigma_\gamma/\gamma_0 < 0.1\) and \(t \ll 1,\) we see that
\[
\langle e^{-2\gamma t}\rangle \approx e^{-2\gamma_0 t},
\]
which is the same result as the noiseless case. We confirm the irrelevance of \(\sigma_\gamma\) numerically in Fig. [1].

We therefore ignore the effects of noise in \(\gamma\) completely in our simulations, and focus instead on the effects of charge noise, valley leakage, and experimental error in the gate timing.

### B. Numerical Calculations

Unlike the effects of valley leakage, we must treat the other sources of errors in our SWAP sequence, the charge noise and gate timing error, numerically. We examine two initial states, one being a spin eigenstate with the first spin up and the rest down, \(|\Psi_0\rangle = |\uparrow\downarrow\downarrow\downarrow\rangle\), and the other being an entangled state with the first two spins in a singlet state and the rest being spin down, \(|\Psi_0\rangle = |S\rangle \otimes |\downarrow\downarrow\downarrow\rangle\). In the eigenstate case, we transport the up spin from the first qubit to the sixth and then back again. The number of SWAP gates in this case is \(N = 2(L-1).\) In the singlet case, we transport the entanglement between the first and second qubit so that the first and sixth qubits are entangled and then back again. The number of SWAP gates in this case is \(N = 2(L-2).\)

For all calculations, we set \(\beta = 0.01\) and the length of the spin chain \(L = 6.\) We incorporate charge noise and gate timing error by choosing values from a normal distribution so that \(J^k \sim \mathcal{N}(J_0^k, \sigma_J)\) and \(\tau \sim \mathcal{N}(\tau_0, \sigma_\tau),\) where \(J_0^k\) and \(\tau_0\) are the base (noiseless) values. We assume that \(\sigma_J\) scales linearly with \(J\) and that \(\sigma_\tau\) is a constant value, arising from experimental clock errors in the gate timing. Because \(\tau_0 \propto J_{\text{SWAP}}^{-1},\) charge noise also causes errors in the gate duration. The gate timing error \(\sigma_\tau\) is an additional source of error in the duration \(\tau,\) separate from that caused by charge noise. For each value of \(\sigma_J\) and \(\sigma_\tau,\) we average the fidelity over 10,000 different realizations of disorder in order to obtain a benchmarked typical fidelity.

In Fig. [2] we plot the infidelity \(1 - F\) as a function of \(J_{\text{SWAP}}/J^1\) for several values of \(\sigma_J.\) The valley leakage and gate timing errors are also included. As charge noise \(\sigma_J\) increases, the fidelities decrease. With our model, we confirm the irrelevance of \(\sigma_\tau\) numerically.

We explicitly show the effects of gate timing error in Fig. [3]. Evidently, gate timing error only affects the fidelity for large values of \(J_{\text{SWAP}}.\) This makes sense from the point of view that \(J_{\text{SWAP}} \propto \tau^{-1},\) so that as \(J_{\text{SWAP}}\) increases, so does the ratio of \(\sigma_\tau/\tau.\) With the presence of any gate timing error, there is an optimal value of \(J_{\text{SWAP}}\) beyond which the fidelity will begin to decrease. This conclusion is especially relevant when considering the effect of valley leakage through the \(\gamma\) term.

The effects of valley leakage are seen in Fig. [4]. We see that as valley leakage becomes a more significant factor, SWAP fidelities decrease. With our model, we are able to analytically conclude that the effects of valley leakage are completely accounted for by an exponential factor of \(e^{-2\gamma_0 t},\) assuming that \(\sigma_\gamma\) is small. This implies that as one increases the SWAP coupling strength and decreases the gate duration \(\tau,\) the effects of valley leakage can be overcome. This is in fact what our calculations showed when excluding the effects of gate timing error—any effects of the valleys can be completely overcome by simply increasing \(J_{\text{SWAP}}.\) However, as \(\tau\)
FIG. 2. The infidelity $1 - F$ as a function of $J_{\text{SWAP}}/J^1$ for several values of $\sigma_J$ is shown. For both cases, the spin chain has a length of six. In decreasing order, the dotted lines correspond to the fidelity of the SWAP sequence assuming that the single gate fidelity matches the value achieved by Petta et al. [15], the value achieved by Nichol et al. [16], and the value necessary for quantum error-correcting codes. The plot on the left is for the initial state of $|\Psi_0\rangle = |↑↓↓↓↓⟩$ and the plot on the right is for the initial state of $|\Psi_0\rangle = |S\rangle \otimes |↓↓↓↓⟩$. For both plots, $\sigma_J/J^1 = 0.01$ and $\gamma_0/J^1 = 0.10$.

FIG. 3. The infidelity $1 - F$ as a function of $J_{\text{SWAP}}/J^1$ for several values of $\sigma_\tau$ is shown. For both cases, the spin chain has a length of six. In decreasing order, the dotted lines correspond to the fidelity of the SWAP sequence assuming that the single gate fidelity matches the value achieved by Petta et al. [15], the value achieved by Nichol et al. [16], and the value necessary for quantum error-correcting codes. The plot on the left is for the initial state of $|\Psi_0\rangle = |↑↓↓↓↓⟩$ and the plot on the right is for the initial state of $|\Psi_0\rangle = |S\rangle \otimes |↓↓↓↓⟩$. For both plots, $\sigma_J/J^1 = 0.01$ and $\gamma_0/J^1 = 0.10$.

gets shorter and shorter, the gate timing error dominates, and the infidelity reaches a minimum before increasing. This minimum infidelity is dependent on all three of our parameters—gate timing error, charge noise, and valley leakage.

We note that the fidelities that we obtain for the singlet state are better than for the eigenstate case. This is because our SWAP sequence simply requires $2(L - 1)$ SWAPs for the eigenstate case and $2(L - 2)$ SWAPs for the singlet case. Naturally, as the number of gate operations increases, the fidelity of the entire sequence decreases.

IV. SUMMARY AND CONCLUSION

We calculate the fidelity of a sequence of SWAP gates on a silicon quantum dot spin qubit chain. We include crosstalk between qubits as well as charge noise in the exchange couplings $J^k_n$. We extend previous work by im-
implementing exchange interactions among all spin qubits, rather than assuming only nearest-neighbor and next-nearest-neighbor interactions. We do this by assuming that the overlap of the two wavefunctions decreases exponentially with distance, such that $J^k = \beta^{k-1}J^1$. We also include new physics by implementing a dissipation term to simulate valley leakage associated with intervalley tunneling and by considering the effects of gate timing error associated with gate operations. The effects of valley leakage on the fidelity are completely accounted for in our model by a simple exponential factor of $e^{-2\gamma_0 t}$ for experimentally relevant values of $\sigma_\gamma$ (as high as 0.1 $J^1$). Therefore, we ignore the effects of valley noise in our simulation, and instead focus on how the magnitude of the valley parameter itself affects the fidelity.

We consider the effects of gate timing error $\sigma_\tau$ on SWAP fidelity by selecting $\tau$ from a normal distribution centered on $\tau_0 = \frac{\pi}{4J_{\text{SWAP}}}$ with deviation $\sigma_\tau$. $J_{\text{SWAP}}$ in this case refers to the expected value of $J_{\text{SWAP}}$ rather than the true value after accounting for $\sigma_J$. Gate timing error constitutes an additional error source on the gate duration $\tau$ beyond that caused by charge noise.

We numerically calculate the fidelity of a sequence of SWAP gates that transports a spin state from the left side of a six-qubit chain to the right side, and back again. We consider two cases for initial conditions. In the first case, where $|\Psi_0\rangle = |\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle$, we “transport” the first spin to the sixth and then back to the first. In the second case, where $|\Psi\rangle = |S\rangle \otimes |\downarrow\downarrow\downarrow\rangle$, we “transport” the entanglement from the second qubit to the sixth and then back to the second. We examine how the fidelity of the SWAP sequence is affected as we vary parameters corresponding to charge noise, valley leakage, and gate timing error.

We reach several conclusions from our results. First, we affirm that charge noise has an extremely detrimental effect on gate fidelities, and that in order for SWAP gates using Heisenberg exchange to be reliable enough to implement error-correcting codes, relative charge noise ($\sigma_J/J$) must be less than 0.01, which is a challenge for semiconductor spin qubits, but perhaps not impossible. Second, the presence of any gate timing error causes a minimum in the infidelity at some value of $J_{\text{SWAP}}/J^1$. This value is an optimal coupling strength, beyond which fidelity begins to increase. This optimal coupling strength changes with $\sigma_\gamma$ and $\gamma_0$, but it is always present. Therefore, any hope of completely overcoming valley leakage by simply making the exchange coupling stronger and the gate duration shorter should be considered with skepticism. Third, valley leakage affects the fidelity of the SWAP operations as expected, with fidelity decreasing as $\gamma_0$ increases. However, we do not expect $\gamma_0/J^1$ to be much greater than 0.1, and our results seem to imply that even with the leakage parameter saturated at this experimental maximum, the fidelity is not far off from the fidelity achieved with a much lower value of $\gamma_0$. We do not claim that valley leakage is a non-issue, simply that we do not see the same dramatic improvements in fidelity when turning down valley leakage as we do when turning down charge noise. Thus, an important conclusion is that at the current stage of Si qubit development, charge noise is a much more overwhelming problem than valley leakage, but in the future, when charge noise is under better control, it is possible for the valley leakage problem to detrimentally affect the SWAP gate fidelity.
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