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Thermodynamic effects of single-qubit operations in silicon-based quantum computing ☆

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ABSTRACT

Silicon-based quantum logic is a promising technology to implement universal quantum computing. It is widely believed that a millikelvin cryogenic environment will be necessary to accommodate silicon-based qubits. This prompts a question of the ultimate scalability of the technology due to finite cooling capacity of refrigeration systems. In this work, we answer this question by studying energy dissipation due to interactions between nuclear spin impurities and qubit control pulses. We demonstrate that this interaction constrains the sustainable number of single-qubit operations per second for a given cooling capacity.

1. Introduction

Environmentally-induced decoherence is typically considered the main obstacle for scalable quantum computing [1,2]. Known remedies include decreasing qubit coupling to the environment [3, 2] and quantum error correction (QEC) [4,5]. Then the challenge lies in trading between the overheads of QEC and decoupling techniques. What often goes overlooked in this analysis is the effect of qubit controls on the environment itself. While the direct effects of the control pulse coupling to the environment may in principle be minimized, e.g., by shielding, the indirect, or qubit-mediated, environmental coupling is a fundamental challenge. In turn, the latter may result in a net environmental energy increase, which inevitably must be removed. For some quantum algorithms, e.g., quantum linear systems [6], it is believed that logical circuit widths of hundreds of millions of qubits will be required to perform better than classical competitors. With QEC overheads pushing the qubit count higher, even small thermal effects, in aggregate, could constrain quantum computing's ultimate scalability.

In this letter, we report the first study of this problem for a phosphorus donor nuclear spin qubit in silicon [7]. We investigate the thermodynamic implications of qubit control pulses coupling with silicon substrate impurities. We choose this system for its attractive features: long qubit coherence times; potentially scalable manufacturing via CMOS techniques; and tremendous recent experimental advances in controlling a single donor atom [8–11] or, alternatively, small clusters of atoms [12]. The decoherence mechanism is mainly due to the interaction with unavoidable inclusions of ^{29}Si isotope (nuclear spin $\frac{1}{2}$) that may range in concentration from 4.7% in natural occurring silicon to below 100 PPM in highly purified samples [13]. The ^{31}P-donor nuclear and electron spin coherence times are well characterized both theoretically [14–16] and experimentally [8,17,10]. For example, at 100 mK, in isotopically purified ^{28}Si, donor nuclear and electron spin coherence times of up to 30 s [10] and 1 s [17], respectively, have been demonstrated, potentially supporting thousands of successive operations. Further, the use of topological QEC codes promise to bring fault tolerance within reach [18].

One's ability to coherently manipulate the nuclear spin of a ^{31}P donor is important not only for single qubit operations but also for two-qubit gates between neighboring donor electron spin qubits [19]. The coherent control of ^{31}P nuclear spins is achieved by using resonant RF pulses [9,11]. The direct effect of such drive pulses on the qubit's environment is negligible, thanks to the large difference in the gyromagnetic ratio between electron and nuclear

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spins ($\gamma_e \gg \gamma_{^{31}\mathrm{P}} > \gamma_{^{29}\mathrm{Si}}$). However, the nuclear spin of a ^{31}P donor indirectly couples to nuclear spins of neighboring ^{29}Si impurity atoms via the donor qubit's electron. The donor electron enables Fermi contact interaction between the electron spin, and the nuclear spins of the ^{31}P and ^{29}Si, resulting in effective nuclear spin–spin coupling. Therefore, coherent rotations of the donor's nuclear spin translate into a net change of the ^{29}Si nuclear spin bath's Zeeman energy. If the net change is positive, energy is added to the substrate raising its effective temperature. In turn, the thermalization process will increase phonon-mediated spin interactions that may result in decoherence. To avoid this, energy dissipated by qubit control operations must be removed by a refrigerator and may not exceed available cooling capacity. Dilution refrigerators appear to be the most likely solution, although their cooling capacity rapidly diminishes as the operating temperature decreases (e.g., see Fig. 3 in [20]) potentially limiting gate operation rates.

To evaluate the magnitude of the bath heating effect, we compute the net Zeeman energy change of ^{29}Si spins as a function of the number of single-qubit rotations, impurity concentration, and impurity spatial distribution. We find that a random single rotation about the X axis decreases the average ^{29}Si ensemble energy, i.e., the spin bath experiences a cooling effect. However, for a sequence of random single-qubit gates, the average energy change is positive, resulting in bath heating. Further, the amount of heating depends on the sequence of single-qubit gates. As an arbitrary qubit operation may be decomposed in many ways, our results suggest that future quantum compilers could optimize selected gate sequences to reduce thermal effects.

2. Materials and methods

We begin by introducing a model for the qubit and its environment. The qubit is defined by the nuclear spin $\hat{\mathbf{I}}_\mathrm{P}$ of a donor ^{31}P atom implanted into a silicon substrate. We set the physical qubit volume to 5 nm^3, defined by twice the typical estimate of the Bohr radius of a donor electron [21]. The qubit environment then includes nuclear spins of neighboring residual ^{29}Si atoms $\hat{\mathbf{I}}_\mathrm{n}$ (index n runs over all lattice sites occupied by ^{29}Si) and the spin of the donor electron $\hat{\mathbf{S}}_e$.

When placed in a uniform magnetic field B_0^z aligned along Z axis, the Hamiltonian of the qubit $\hat{H}_q = \omega_\mathrm{P}\hat{I}_\mathrm{P}^z$, where $\omega_\mathrm{P} = \gamma_\mathrm{P} B_0^z$ and γ_P is the gyromagnetic ratio for the ^{31}P nucleus. Similarly, we denote the free Hamiltonian for the donor electron spin, $\hat{H}_e = \Omega_e \hat{S}_e^z$ and the neighboring ^{29}Si nuclear spins, $\hat{H}_\mathrm{Si} = \sum_n \omega_n \hat{I}_{\mathrm{Si}_n}^z$, where $\Omega_e = \gamma_e B_0^z$, $\omega_n = \gamma_{\mathrm{Si}_n} B_0^z$ and $\gamma_e(\gamma_{\mathrm{Si}_n})$ are the electron (^{29}Si nucleus) gyromagnetic ratio.

Single-qubit gates are typically implemented as rotations along the X, Y, Z axes by exposing the qubit to time-varying magnetic fields aligned along the axis of rotation. Here, we concentrate on the impact of single-qubit rotations around the X axis. The Hamiltonian that describes such rotations is

$$\hat{H}_d = \cos(\omega_d t)[\Omega_e^x \hat{S}_e^x + \Omega_\mathrm{P}^x \hat{I}_\mathrm{P}^x + \Omega_\mathrm{Si}^x \sum_n \hat{I}_n^x], \tag{1}$$

where B_0^x and ω_d are the amplitude and the frequency of the AC magnetic field along the X axis, $\Omega_e^x = \gamma_e B_0^x$, $\Omega_\mathrm{P}^x = \gamma_\mathrm{P} B_0^x$, and $\Omega_\mathrm{Si}^x = \gamma_\mathrm{Si} B_0^x$. Note that Eq. (1) includes terms corresponding to the effects of the drive field on ^{29}Si nuclear spins as well as the donor electron spin. As we will show later, the standard "resonant" choice of the driving frequency, results in a negligable effect on the electron spin because $\Omega_e \gg \omega_\mathrm{P}$.

Next, we include the effects of the nuclear spin environment. The qubit and ^{29}Si nuclear spins are coupled to the donor electron spin $\hat{\mathbf{S}}_e$ via the Fermi contact interaction. This coupling, in particular, is the leading cause of donor electron spin decoherence [14–16,22]. In addition, as we will show, this interaction provides a mechanism for an indirect coupling of ^{29}Si nuclear spins with X-axis qubit rotation pulses. And while the effects of the environment on the qubit can be largely mitigated e.g., by using dynamic refocusing sequences and higher isotopic purity silicon, removing the effects of qubit control pulses on the spin bath entirely is complex as each qubit will couple to a different random local spin bath. The basic Hamiltonian describing the contact interaction between the donor electron spin and neighboring nuclear ^{31}P and ^{29}Si spins is

$$\hat{H}_{eN} = \sum_{n\in\mathrm{Si,P}} a_n \hat{\mathbf{S}}_e \cdot \hat{\mathbf{I}}_n = \sum_{n\in\mathrm{Si,P}} a_n (\hat{S}_e^x \hat{I}_n^x + \hat{S}_e^y \hat{I}_n^y + \hat{S}_e^z \hat{I}_n^z), \tag{2}$$

where hyperfine coupling constants a_n between the donor electron and the n-th nuclear spin are given by

$$a_n = \frac{2\hbar\mu_0}{3}\gamma_e\gamma_n|\Psi(\mathbf{R}_n)|^2. \tag{3}$$

Here μ_0 is the vacuum permeability and $\Psi(\mathbf{R}_n)$ is the donor electron wave function at the nucleus location $\mathbf{R}_n$. Several approaches to modeling the wavefunction $\Psi(\mathbf{R}_n)$ can be found in the literature [23–25]. For our numerical simulations below we adopt the approximation used to describe the original ENDOR experimental data [26] with the understanding that its validity is limited to about 20 nuclear shells around the donor [27].

In addition to the hyperfine coupling mediated interaction, nuclear spins couple via a direct dipole–dipole interaction. However, this interaction results in pairwise nuclear spin flipping that does not change the overall Zeeman energy of the nuclear spin bath. Also, the dipole–dipole interaction strength is typically weaker than the strength of the hyperfine interaction. Therefore, it is not included in our model.

Finally, besides the ^{29}Si nuclear spins, ^{31}P impurities can be introduced during the qubit implantation process. In turn, they can also be polarized by qubit control pulses, leading to additional thermodynamic effects. However, since even in isotopically purified silicon, the number of ^{29}Si impurities exceeds the number of undesired ^{31}P donors, we will exclusively focus on estimating the energy deposition to ^{29}Si environment.

Putting it all together, we arrive at the total Hamiltonian describing the dynamics of single qubit control pulses coupling to the ^{29}Si spin bath for a X-axis drive field,

$$\hat{H} = \hat{H}_e + \hat{H}_N + \hat{H}_d + \hat{H}_{eN}, \tag{4}$$

where $\hat{H}_N = \hat{H}_\mathrm{Si} + \hat{H}_q$.

In the total Hamiltonian, Eq. (4), three terms may, in principle, change the Zeeman energy of ^{29}Si nuclei which in turn, can result in an environmental temperature change. These are the driving term $\hat{H}_d$ and the two hyperfine coupling terms $\sum_n a_n \hat{S}_e^x \hat{I}_n^x$ and $\sum_n a_n \hat{S}_e^y \hat{I}_n^y$. However, because the Zeeman energy of the electron is much larger than the Zeeman energies of phosphorus and silicon nuclei, i.e., $2\hbar\Omega_e \gg \{2\hbar\omega_\mathrm{P}, 2\hbar\omega_n\}$, the latter terms can be treated as a small perturbation. It can be shown, by applying perturbation theory, that these terms indeed cancel out to the first and the second order, providing an effective spin–spin coupling that preserves Zeeman energies of the nuclei (a so-called secular term). To see this behavior we derive the effective Hamiltonian $\hat{H}'$ using the method of small rotations [28]. Accordingly,

$$\hat{H}' = U_r \hat{H} U_r^{-1} \tag{5}$$