Cavity-assisted quantum computing in a silicon nanostructure*

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We present a scheme of quantum computing with charge qubits corresponding to one excess electron shared between dangling-bond pairs of surface silicon atoms that couple to a microwave stripline resonator on a chip. By choosing a certain evolution time, we propose the realization of a set of universal single- and two-qubit logical gates. Due to its intrinsic stability and scalability, the silicon dangling-bond charge qubit can be regarded as one of the most promising candidates for quantum computation. Compared to the previous schemes on quantum computing with silicon bulk systems, our scheme shows such advantages as a long coherent time and direct control and readout.

Keywords: quantum computing, dangling-bond state

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1. Introduction

Quantum computing (QC)[1–10] offers methods for efficiently solving problems that are not solvable with a classical computer[11] in a reasonable time scale. Of the promising technologies, solid-state systems[12] are especially attractive because of their stability and expected scalability.[13] The key challenges are to control the coupling strength of qubits and to form stable architectures. Recently, the approaches to the quantum control of spin- and charge-based systems in bulk semiconductors have been studied in detail,[14–18] allowing one to consider further two-dimensional (2D) architectures based on charge qubits[19] associated with dangling-bond (DB) pairs of the surface silicon atoms, which couple to a microwave stripline resonator via electrical control.

In this paper, we propose a realizable architecture of cavity quantum electrodynamics (QED) via artificial atoms (DB pairs) on the 2D hydrogen-terminated silicon surface coupled to a one-dimensional (1D) stripline resonator within a simple circuit that can be fabricated on a low-dimensional microelectronic chip. The charge qubit[20–24] corresponds to one excess electron shared between two nearby DBs. We describe a technique for electrically coupling the DB pair state of the 2D silicon surface to the microwave stripline resonator on a chip.[25–27] The logical gate operations including single- and two-qubit gates $\sqrt{i\text{swap}}$ can be implemented by controlling the evolution time of the combined systems. Due to its intrinsic stability and scalability, the silicon dangling-bond charge qubit is one of the most promising candidates for quantum computation. Our scheme has advantages over the proposed bulk silicon quantum computing in long coherent time and direct control and readout.

The structure of this paper is organized as follows. In Section 2, we discuss the realization of cavity QED with the pairs of DBs with an excess electron coupling to a coplanar stripline resonator. In Section 3, we show the evolution of the combined system and implement a set of universal logical gates by choosing the proper evolution time. In Section 4, we analyze the main resource of decoherence and come to a compendious conclusion.

2. Low dimensional implementation of cavity QED

2.1. Two-level atomic system

Our scheme is to create, control, and read out the charge qubits on the hydrogen-terminated surface of a bulk silicon crystal[28–30] doped with phosphorus atoms. The goal is to devise a QC architecture with charge qubits which correspond to single excess electrons shared between DB pairs[31,32] of the surface silicon atoms.

The DBs of the surface silicon atoms can be essentially regarded as quantum dots.[33,34] Physically, a DB is formed by passivating the P-doping silicon crystal whose surface is covered by a monolayer of hydrogen atoms, with each hydrogen atom connected to one surface silicon atom, which breaks the electron structures of the surface silicon atoms and produces unpaired electrons. A scanning tunneling microscope (STM) tip removes a hydrogen atom at the selected site,[33] thereby constructing a DB. The DB can host a second oppositely-

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spinning electron, which would make it negatively charged (henceforth denoted as DB$^-$), and this excess electron is provided by the phosphorus donor near the DB site (see Fig. 1(a)).

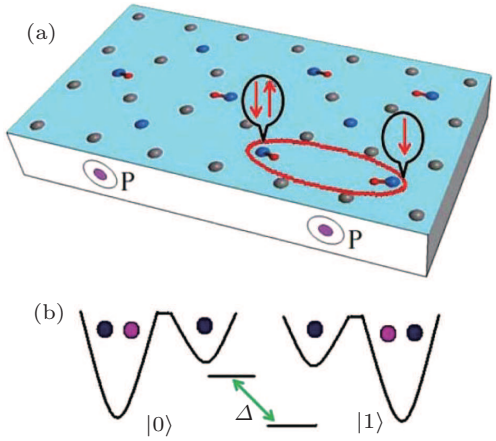


Fig. 1. (color online) (a) The structure of DB pairs on the hydrogen-terminated surface of bulk silicon doped with phosphorus atoms. H-terminated (red) Si (blue, without H-terminated Si atoms are presented in grey) with Si dimers on the surface and P (purple) dopants in the bulk. DBs exist for the surface Si atoms with a terminating H removed. (b) DB$^-$–DB and DB–DB$^-$ pairs modeled as double-well potentials.

A charge qubit is constructed by creating two nearby DBs sharing an excess unpaired electron from a phosphorus donor. The pair of DBs has a strict lower separation (5.43 Å) determined by the lattice constant of the atom on the surface of the silicon crystal. The DBs of a pair must be sufficiently close to each other (< 15 Å) so that the Coulomb repulsion between the DBs prevents the pair from having two excess electrons instead of just one excess electron remaining.[33] The pair of DBs can be modeled as a double-well potential, applying an external electric field to the DB pair; there would be an energy difference between the two potentials and the excess electron would tunnel between the DBs. When the unpaired electron appears in the left DB of the pair (i.e., DB$^-$–DB), the qubit corresponds to a logical zero state $|0\rangle$. In contrast, the qubit corresponds to logical state $|1\rangle$ if the right DB is negative (DB–DB$^-$). As we can see in Fig. 1(b), the energy difference between the states $|0\rangle$ and $|1\rangle$ is $\Delta = T$ ($\hbar = 1$) with T the tunneling rate of the excess electron between the DBs of the pair. Thus we can consider just whether there is an excess in the left potential. We fabricate our charge qubit on a chip and apply it in a circuit (see Fig. 2(a)). The Hamiltonian describing the circuit can be written as[27]

$$\hat{H}_{\rm Q} = \sum_{n=0,1} E_{\rm C}(n-n_{\rm g})^2 |n\rangle\langle n| - \Delta\left(|n+1\rangle\langle n| + {\rm h.c.}\right), \quad (1)$$

where $n_{\rm g} = C_{\rm g}V_{\rm g}$ is the total polarization charge due to the gate voltage, the charge energy is $E_{\rm C} = e^2/(2C_\Sigma)$, and the total capacitance is $C_\Sigma = C_{\rm g} + C_{\rm c}$, with $C_{\rm c}$ and $C_{\rm g}$ the equivalent chip and gate capacitances, respectively. Restricting $n_{\rm g} \in [0,1]$ by using gate voltage $V_{\rm g}$, Hamiltonian (1) can be rewritten as

$$\hat{H}'_{\rm Q} = \frac{1}{2}E_{\rm C}(1-2n_{\rm g})\hat{\sigma}_z - \Delta\hat{\sigma}_x, \quad (2)$$

where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the Pauli matrices with eigenbasis $\{|n=0\rangle, |n=1\rangle\}$.

Thus it can been seen that the DB pair of the surface silicon atoms is the same as a two-level atom with effective electric fields along the x and the z directions.

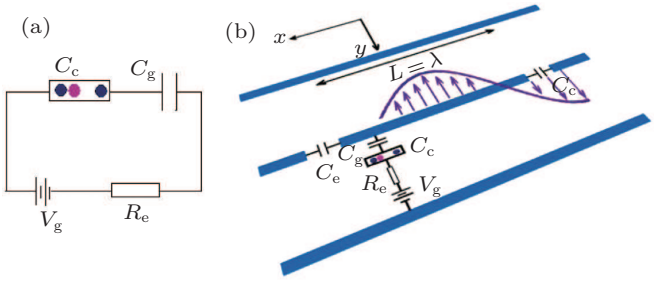


Fig. 2. (color online) (a) The circuit diagram of the charge qubit of a DB pair fabricated on a chip. The chip with equivalent capacitance $C_{\rm c}$ is coupled to the gate $V_{\rm g}$ through $C_{\rm g}$. Here $R_{\rm e}$ is the environment impedance. (b) Schematic diagram of charge qubits of DB pairs capacitively coupled to a coplanar stripline resonator. The coupling can be controlled by the electric field along the x axis.

2.2. Combined system: charge qubits of DB pairs coupled to a stripline resonator

The charge qubits of the DB pairs are located in the center of the coplanar stripline resonator (see Fig. 2(b)). Except for a DC part of the electric field $V_{\rm g}^{\rm DC}$, the quantum part $v = V_{\rm rms}^0(\hat{a}^\dagger + \hat{a})$ provided by the resonator should also be considered with the root-mean-square voltage $V_{\rm rms}^0$ in the center of the resonator. Thus Eq. (2) becomes

$$\begin{aligned}\hat{H}''_{\rm Q} &= \frac{1}{2}E_{\rm C}(1-2n_{\rm g}^{\rm DC})\hat{\sigma}_z - \Delta\hat{\sigma}_x \\ &\quad + \frac{eC_{\rm g}}{2C_\Sigma}V_{\rm rms}^0(\hat{a}^\dagger + \hat{a})\hat{\sigma}_z. \end{aligned} \quad (3)$$

Coupling the oscillator mode of the resonator to the charge qubit of the DB pair and at the same time using the coordinate system transformation $R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$, we have the Hamiltonian of the combined system in the form

$$\begin{aligned}\hat{H} &= \omega_{\rm r}\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + R\hat{H}''_{\rm Q} \\ &= \omega_{\rm r}\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \frac{\Omega}{2}\hat{\sigma}_z + g(\hat{a}^\dagger + \hat{a})\left(\cos\theta\hat{\sigma}_z + \sin\theta\hat{\sigma}_x\right), \end{aligned} \quad (4)$$

where $\omega_{\rm r}$ is the frequency of the resonator, the energy splitting of the charge qubit is $\Omega = \sqrt{E_{\rm C}^2(1-2n_{\rm g}^{\rm DC})^2 + 4\Delta^2}$, and $\theta = \arctan[2\Delta/E_{\rm C}(1-2n_{\rm g}^{\rm DC})]$ is the corresponding mixing angle. We have chosen $V_{\rm rms}^0 = \sqrt{\omega_{\rm r}/cL}$, hence the coupling coefficient is the vacuum Rabi frequency $g = \frac{eC_{\rm g}}{2C_\Sigma}\sqrt{\frac{\omega_{\rm r}}{cL}}$.

At the charge energy degeneracy point (i.e. $n_g^{DC} = 1/2$ and $\theta = \pi/2$), with the rotating wave approximation, the effective Hamiltonian of the combined system is further simplified into

$$\hat{H}' = \omega_r\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \frac{\Omega}{2}\hat{\sigma}_z + g(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+). \quad (5)$$

The form of the Hamiltonian in Eq. (5) is identical to the well-known Jaynes–Cummings (JC) model.[35] The scheme which we describe therefore can be mapped to two-level atoms interacting with a cavity. This system can be used to prepare entangled states and to study quantum correlations. Furthermore, we can design a set of universal logical gates for quantum computation by using this model.

3. Implementation of a set of universal logical gates on charge qubits

In order to construct a quantum computer, analogous to the classical computer, it is necessary to realize a set of universal gate operations[22,36,37] on the qubits. Except for single-qubit logical gates including a NOT gate and a phase gate, we have implemented the two-qubit entangling gate $\sqrt{i\text{swap}}$ on two charge qubits by controlling the evolution time of the combined system.

3.1. Single-qubit gates

As discussed above, the dynamics of the combined system can be described by the JC model. In the case that the charge qubit is resonantly coupled to the resonator, i.e., $\delta = \Omega - \omega_r = 0$, by applying the unitary transformation $\hat{S}_0(t) = \exp[-\mathrm{i}(\omega_r\hat{a}^\dagger\hat{a} + \Omega\hat{\sigma}_z/2)t]$ to Eq. (5),[27,38] the Hamiltonian in Eq. (5) can be rewritten in the interaction picture as

$$\hat{V}_I = \hat{S}_0^{\ \dagger}\hat{H}'\hat{S}_0 - \mathrm{i}\hat{S}_0^{\ \dagger}\dot{\hat{S}}_0 = g(\hat{a}^\dagger\hat{\sigma}_- + \hat{a}\hat{\sigma}_+), \quad (6)$$

where $\dot{\hat{S}}_0 = \mathrm{d}\hat{S}_0(t)/\mathrm{d}t$. In the rotating frame, the time evolution operator is then given by

$$\begin{aligned} U_0(t) &= \exp(-i\hat{V}_I t) = \sum_{n=0}^{\infty}\frac{(-\mathrm{i}t\hat{V}_I)^n}{n!} \\ &= \cos(gt\sqrt{\hat{a}^\dagger\hat{a}+1})\,|1\rangle\langle 1| + \cos(gt\sqrt{\hat{a}^\dagger\hat{a}})\,|0\rangle\langle 0| \\ &\quad -\mathrm{i}\,\frac{\sin(gt\sqrt{\hat{a}^\dagger\hat{a}+1})}{\sqrt{\hat{a}^\dagger\hat{a}+1}}\hat{a}\,|1\rangle\langle 0| \\ &\quad -\mathrm{i}\sin(gt\sqrt{\hat{a}^\dagger\hat{a}})\frac{\hat{a}^\dagger}{\sqrt{\hat{a}^\dagger\hat{a}}}\,|0\rangle\langle 1|\,. \end{aligned} \quad (7)$$

Then the state of the combined system evolves over time to

$$\begin{aligned} &U_0(t)\,|\psi(0)\rangle \\ &= U_0(t)(\alpha\,|0,n+1\rangle + \beta\,|1,n\rangle) \\ &= \alpha\left[\cos(gt\sqrt{n+1})\,|0,n+1\rangle - \mathrm{i}\sin(gt\sqrt{n+1})\,|1,n\rangle\right] \\ &\quad +\beta\left[\cos(gt\sqrt{n+1})\,|1,n\rangle - \mathrm{i}\sin(gt\sqrt{n+1})\,|0,n+1\rangle\right]. \end{aligned} \quad (8)$$

Here we have assumed an arbitrary initial state of the combined system $|\psi(0)\rangle = \alpha\,|0,n+1\rangle + \beta\,|1,n\rangle$, with n denoting the number of photons in the cavity at $t = 0$ and $|\alpha|^2 + |\beta|^2 = 1$. By choosing $gt = 3\pi/(2\sqrt{n+1})$, the final state of the combined system is $|\psi(t)\rangle \propto \alpha\,|1,n\rangle + \beta\,|0,n+1\rangle$, and the evolution operator corresponds to the NOT gate $\hat{\sigma}_x$ on the charge qubit. In the dispersive regime $\delta = \Omega - \omega_r \gg g$, that is the charge qubit is off-resonantly coupled to the stripline resonator, by applying the unitary transformation $\hat{S}_1 = \exp\left[g/\delta(\hat{a}\hat{\sigma}_+ - \hat{a}^\dagger\hat{\sigma}_-)\right]$ and expanding to the second order of the coupling coefficient g, the Hamiltonian in Eq. (5) in the rotating frame turns into

$$\hat{S}_1\hat{H}'\hat{S}_1^{\ \dagger} = \left(\omega_r + \frac{g^2}{\delta}\hat{\sigma}_z\right)\hat{a}^\dagger\hat{a} + \frac{1}{2}\left(\Omega + \frac{g^2}{\delta}\right)\hat{\sigma}_z. \quad (9)$$

Here we only consider the evolution of the term describing the interaction between the charge qubit and the resonator in Eq. (9)

$$\begin{aligned} U_1(t) &= \exp\left(-\mathrm{i}\frac{g^2}{\delta}\hat{a}^\dagger\hat{a}\hat{\sigma}_z t\right) \\ &= \cos\left(\frac{g^2}{\delta}\hat{a}^\dagger\hat{a}t\right) - \mathrm{i}\hat{\sigma}_z\sin\left(\frac{g^2}{\delta}\hat{a}^\dagger\hat{a}t\right). \end{aligned} \quad (10)$$

Then the state of the combined system evolves over time to

$$\begin{aligned} &U_1(t)\,|\psi(0)\rangle \\ &= U_1(t)\,(\alpha\,|0,n+1\rangle + \beta\,|1,n\rangle) \\ &= \alpha\left[\cos\frac{g^2}{\delta}(n+1)t - \mathrm{i}\sin\frac{g^2}{\delta}(n+1)t\right]|0,n+1\rangle \\ &\quad +\beta\left[\cos\frac{g^2}{\delta}(n)t - \mathrm{i}\sin\frac{g^2}{\delta}(n)t\right]|1,n\rangle\,. \end{aligned} \quad (11)$$

Thus the final state of the combined system is $|\psi(t)\rangle \propto \alpha\,|0,n+1\rangle - \beta\,|1,n\rangle$, and the logical phase gate $\hat{\sigma}_z$ can be implemented on the charge qubit given in Eq. (11) by choosing an appropriate evolution time $t = \delta\pi/g^2$ with an odd number n of photons.

3.2. Two-qubit entangling gate $\sqrt{i\text{swap}}$

In order to realize quantum computation, universal two-qubit logical gates are more important. Considering two charge qubits interact with the cavity at the same time, the Hamiltonian of the whole system including two charge qubits and the resonator reads

$$\begin{aligned} \hat{H}_{2q} &= \omega_r\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) + \frac{\Omega}{2}(\hat{\sigma}_z^1 + \hat{\sigma}_z^2) + g(\hat{a}^\dagger\hat{\sigma}_-^1 + \hat{a}\hat{\sigma}_+^1) \\ &\quad +g(\hat{a}^\dagger\hat{\sigma}_-^2 + \hat{a}\hat{\sigma}_+^2), \end{aligned} \quad (12)$$

where the superscripts 1 and 2 denote the two qubits coupled with the same strength g to the cavity. Using the same approach on Eq. (9), we obtain the effective Hamiltonian of the whole system

$$\hat{H}'_{2q} = \left[\omega_r + \frac{g^2}{\delta}(\hat{\sigma}_z^1 + \hat{\sigma}_z^2)\right]\hat{a}^\dagger\hat{a} + \frac{1}{2}\left(\Omega + \frac{g^2}{\delta}\right)(\hat{\sigma}_z^1 + \hat{\sigma}_z^2) + \frac{g^2}{\delta}(\hat{\sigma}_+^1\hat{\sigma}_-^2 + \hat{\sigma}_-^1\hat{\sigma}_+^2). \quad (13)$$

The last term is the dipole–dipole interaction between the charge qubits induced by the cavity mode and couples the qubits through virtual excitations of the resonator.

Here we are only concerned about the interaction term of the two qubits in Eq. (13). In the rotating frame, we obtain the effective interaction Hamiltonian

$$\hat{H}_{2q}^{\prime\mathrm{int}} = \hat{S}_2^{\dagger}\hat{H}'_{2q}\hat{S}_2 - \mathrm{i}\hat{S}_2^{\dagger}\dot{\hat{S}}_2 = \frac{g^2}{\delta}(\hat{\sigma}_+^1\hat{\sigma}_-^2 + \hat{\sigma}_-^1\hat{\sigma}_+^2), \quad (14)$$

where

$$\hat{S}_2 = \exp\left\{-\mathrm{i}\left[\omega_r + \frac{g^2}{\delta}(\hat{\sigma}_z^1 + \hat{\sigma}_z^2)\right]\hat{a}^\dagger\hat{a}t - \frac{\mathrm{i}}{2}\left(\Omega + \frac{g^2}{\delta}\right)(\hat{\sigma}_z^1 + \hat{\sigma}_z^2)t\right\}.$$

The evolution operator is

$$\begin{aligned} U_2(t) &= \exp(-\mathrm{i}\hat{H}_{2q}^{\prime\mathrm{int}}t) \\ &= \exp\left[-\mathrm{i}\frac{g^2}{\delta}t(\hat{\sigma}_+^1\hat{\sigma}_-^2 + \hat{\sigma}_-^1\hat{\sigma}_+^2)\right] \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\frac{g^2}{\delta}t) & -\mathrm{i}\sin(\frac{g^2}{\delta}t) & 0 \\ 0 & -\mathrm{i}\sin(\frac{g^2}{\delta}t) & \cos(\frac{g^2}{\delta}t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \otimes I_r, \end{aligned} \quad (15)$$

where I_r is the identity operation on the Hilbert space of the resonator. With a proper evolution time $t = \pi\delta/(4g^2)$, the unitary operation U_2 corresponds to a two-qubit logical operation $\sqrt{i\mathrm{swap}}$ on the charge qubits

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{\sqrt{2}}{2} & -\mathrm{i}\frac{\sqrt{2}}{2} & 0 \\ 0 & -\mathrm{i}\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (16)$$

Up to single-qubit gates, this operation is equivalent to the controlled-NOT operation on the charge qubits. Together with single-qubit gates, the interaction $\hat{H}'_{2q}$ is therefore sufficient for universal quantum computation. Two-qubit logical gates on charge qubits in this setup can be controlled by individually tuning the qubits. Moreover, single- and two-qubit logical gates on different charge qubits and pairs of charge qubits can be realized simultaneously. Thus our scheme is one of the most promising candidates for quantum computation.

4. Conclusion

In summary, the DB pairs of silicon atoms can be modeled as charge qubits. By coupling the DB pairs to a stripline resonator and controlling the evolution time of the whole system, we can realize a set of universal logical gates including single-qubit NOT gate $\hat{\sigma}_x$, phase gate $\hat{\sigma}_z$, and two-qubit entangling gate $\sqrt{i\mathrm{swap}}$. The combined system has advantages in coherent control, entanglement, and readout of the charge qubits for QC.

Compared to the decay of the resonator $1/\kappa \sim 10^{-6}$ s,[16] the main source of decoherence[32,39] comes from the fluctuation of the electric field inside the resonator and the deformation when the excess electron tunnels between the DB pairs. For a single qubit presenting by the DB pairs separated 7.68 Å and two qubits with separation 15.36 Å,[32], the operation times for single- and two-qubit gates are $\sim 4.72\times10^{-13}$ s and $\sim 3.24\times10^{-12}$ s, respectively. Compared to the expected coherence lifetime of the charge qubit $\sim 2\times10^{-8}$ s,[32,33] it is long enough to achieve quantum computation through different combinations of the logical gates. In additional to the weak decoherence, our scheme has another advantage over other semiconductor QC proposals, the charge qubits are on the surface rather that in the bulk, thus enabling more direct control and readout. We believe that based on the advantages of our proposal, the QC with DB pairs coupled to a stripline resonator is one of the promising candidates to realize semiconductor quantum computation.

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