

AUXILIARY-LEVEL-ASSISTED OPERATIONS WITH CHARGE QUBITS IN SEMICONDUCTORS

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We present a new scheme for rotations of a charge qubit associated with a singly ionized pair of donor atoms in a semiconductor host. The logical states of such a qubit proposed recently by Hollenberg et al. [16] are defined by the lowest two energy states of the remaining valence electron localized around one or another donor. We show that an electron located initially at one donor site can be transferred to another donor site via an auxiliary molecular level formed upon the hybridization of the excited states of two donors. The electron transfer is driven by a single resonant microwave pulse in the case where the energies of the lowest donor states coincide or by two resonant pulses in the case where they differ from each other. Depending on the pulse parameters, various one-qubit operations, including the phase gate, the NOT gate, and the Hadamard gate, can be realized in short times. Decoherence of an electron due to the interaction with acoustic phonons is analyzed and shown to be weak enough for coherent qubit manipulation being possible, at least in the proof-of-principle experiments on one-qubit devices.

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1. INTRODUCTION

Solid-state systems are of great interest in searching for a scalable quantum computer technology. Several schemes for solid-state quantum information processing have been proposed [1–3]. For example, the coherent control of superconducting qubits [4] and their coupling [5] have been demonstrated, the qubits being encoded in the states of a Cooper-pair box. One promising area of current investigation is concerned with the semiconductor-based devices. In Kane's proposal [6], the qubits are defined by long-lived nuclear spins of phosphorous dopants in a silicon host. They are manipulated by external surface gates and radio-frequency magnetic fields. While long coherence times of nuclear spins make the Kane scheme very promising, the single-spin measurement remains a significant challenge [7]. This also concerns an alternative Si:P architecture that uses electron spin states as qubits [8].

Along with spin-based qubits, the charged-based qubits in semiconductors are currently discussed as well. The logical states of a charge semiconductor qubit may be formed by, e.g., the ground state and the excited state of the electron in a single quantum dot [1]

or the spatially separated states of the electron in two different quantum dots [9–13]. Although decoherence of the charge-based qubits is rather strong [14, 15], the charge qubits are nevertheless believed to be realizable at the present technological level due to their short operation times [16]. One of the obstacles to the practical realization of scalable quantum computation in the system of quantum dots is that it is extremely difficult, if at all possible, to manufacture a set of quantum dots with identical or at least predetermined characteristics each. This complicates the issue, introducing the errors into the operations with qubits [17] and resulting in a need for numerous ancillary corrective gates. In this respect, it would be more reasonable to use natural atoms (instead of «artificial» ones) as the localization centers for the electrons carrying the quantum information. Recent advances in manipulation with single atoms on the solid surface [18] and atomically precise placement of single dopants in semiconductors [19, 20] allow constructing rather complex solid-state atomic architectures.

Recently, Hollenberg et al. proposed a two-atom charge-qubit scheme [16] and reported the first results on its fabrication and characterization [20] in the case

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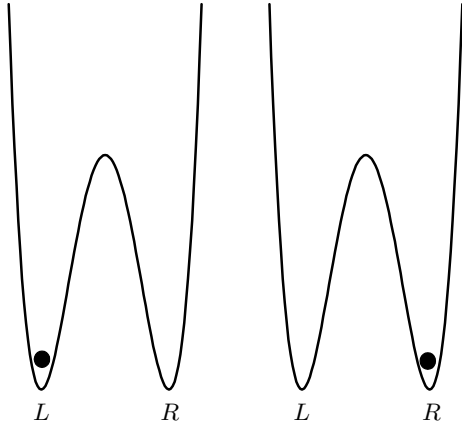


Fig. 1. The logical states $|0\rangle = |L\rangle$ and $|1\rangle = |R\rangle$ of the buried donor charge qubit

of phosphorous dopants in silicon. In that scheme, the buried donor charge qubit consists of two dopant atoms about 50 nm apart in a semiconductor host. One of the donors is singly ionized. The logical states are formed by the lowest two energy states of the remaining valence electron localized at the left or the right donor, $|0\rangle = |L\rangle$ and $|1\rangle = |R\rangle$, see Fig. 1. The qubit is controlled by the surface electrodes through adiabatic variations of the donor potentials. Initialization and read-out of the qubit are facilitated by a single-electron transistor. The coupling of such qubits via the Coulomb interaction, in principle, allows realizing the conditional two-qubit gates [16].

It was shown in Ref. [16] that although the coherence time $\tau_{coh} \sim 1$ ns for charge-based qubits is much shorter than for their spin-based counterparts, the corresponding gate operations times are also shorter, of the order of $\tau_{op} \sim 50$ ps. We note, however, that the ratio $\tau_{op}/\tau_{coh} \sim 10^{-1}$ seems to be insufficiently small for the fault-tolerant scalable quantum computation being possible [21]. In this paper, we propose an alternative scheme for operations with buried donor charge qubits, instead of applying biases to the surface gates. Our scheme is based on the effect of electron transfer between the lowest states localized at different donors upon the influence of a resonant pulse [9] or two resonant pulses [22]. Such a transfer occurs via an excited molecular level of the double-donor system and allows implementation of different one-qubit rotations. The operation times can be made orders of magnitude shorter than in the original proposal [16].

The paper is organized as follows. In Sec. 2, we describe a three-level model for the resonant electron transfer between the donors and briefly discuss the rele-

vant one-electron states of a P_2^+ molecular ion in Si. We next present the analytical solution for the unitary electron evolution under the influence of microwave pulses. In Sec. 3, we show that in the $P_2^+ : Si$ system, it is possible to realize various one-qubit operations, including the NOT gate, the phase gate, and the Hadamard transformation. Decoherence due to the electron interaction with acoustic phonons is studied in Sec. 4. Discussion of the results is given in Sec. 5.

2. MODEL FOR THE RESONANT ELECTRON TRANSFER

We consider a singly ionized pair of phosphorous atoms embedded in silicon. The remaining valence electron is described by the Hamiltonian

$$\hat{H}_0 = \sum_n E_n |\chi_n\rangle \langle \chi_n|, \quad (1)$$

where E_n and $|\chi_n\rangle$ are the respective one-electron eigenenergies and eigenstates of the molecular ion $P_2^+ : Si$. In general, to calculate the energy spectrum and the wave functions $\langle \mathbf{r} | \chi_n \rangle$ of the single-electron/double-donor system beneath the surface, one should account for the conduction-band anisotropy, the intervalley terms, the surface effects, the potentials induced in the substrate by the gate voltages, etc. This necessarily requires numerical calculations, see, e.g., Ref. [23]. We note that although the conduction-band edge of bulk silicon has six degenerate minima, it has been shown both experimentally [24] and theoretically [25] that substitutional impurities break the translational symmetry of the crystal lattice, thus lifting the degeneracy. The spacing between energy levels in the ground-state and excited-state multiplets may be further increased by appropriately choosing the gate potentials. Anyway, to quantify the structure of the $P_2^+ : Si$ energy spectrum and wave functions, one should make sophisticated numerical calculations for a specific donor configuration. In this paper, however, we restrict ourselves to a semiquantitative consideration based on an isotropic effective mass approximation [26] that allows an explicit analytical solution. The problem then reduces to that for a hydrogen-like molecular ion with the effective Bohr radius $a_B^* \approx 3$ nm and the effective Hartree unit of energy $E^* = e^2/\epsilon a_B^* \approx 40$ meV, where $\epsilon = 11.7$ is the dielectric constant for silicon¹⁾.

¹⁾ We note that the isotropic effective mass approximation gives the value $E = -E^*/2 \approx -20$ meV for the ground-state energy of a single phosphorous donor in silicon, which is about half the experimentally observed value $E = -45.5$ meV (see, e.g. [27]).

The energy spectrum of the H_2^+ ion for different atomic separations is known with high accuracy [28].

We approximate the Hamiltonian \hat{H}_0 in Eq. (1) by the reduced three-level Hamiltonian

$$\hat{H}_r = E_1|\chi_1\rangle\langle\chi_1| + E_2|\chi_2\rangle\langle\chi_2| + E_{TR}|\chi_{TR}\rangle\langle\chi_{TR}|, \quad (2)$$

where $|\chi_1\rangle$ and $|\chi_2\rangle$ are the lowest molecular states $1s\sigma_g$ and $2p\sigma_u$, whose respective wave functions are, respectively, symmetric and antisymmetric about the midpoint of the line joining the two donors (Fig. 2), and $|\chi_{TR}\rangle$ is one of the excited molecular states discussed below. It is convenient to pass from the states $|\chi_1\rangle$ and $|\chi_2\rangle$ delocalized over the $\text{P}_2^+:\text{Si}$ ion to the states

$$|L\rangle = \frac{|\chi_1\rangle + |\chi_2\rangle}{\sqrt{2}} \quad \text{and} \quad |R\rangle = \frac{|\chi_1\rangle - |\chi_2\rangle}{\sqrt{2}}$$

localized at the left and the right donor, respectively. For donor separations $R_d \gg a_B^*$, the wave functions $\langle\mathbf{r}|L\rangle$ and $\langle\mathbf{r}|R\rangle$ are almost indistinguishable from the one-electron $1s$ orbitals of the corresponding donor atoms.

The states $|L\rangle$ and $|R\rangle$ form the respective qubit logical states $|0\rangle$ and $|1\rangle$. These states are well defined if the thermal energy $k_B T$ is much lower than the differences $\Delta E_{31} = E_3 - E_1$ and $\Delta E_{32} = E_3 - E_2$ between the energy E_3 of the excited molecular state $|\chi_3\rangle$ and the respective energies E_1 and E_2 . At $R_d \gg a_B^*$, we have $E_1 \approx E_2 \approx -E^*/2$ and $E_3 \approx -E^*/8$, and therefore $\Delta E_{31} \approx \Delta E_{32} \approx 3E^*/8 \approx 15$ meV. Because the states $|L\rangle$ and $|R\rangle$ are not the exact eigenstates of the Hamiltonian \hat{H}_r , the initial qubit state $|\Psi(0)\rangle = \alpha|L\rangle + \beta|R\rangle$ evolves with time in the absence of external fields as

$$|\Psi(t)\rangle = \exp\left(-\frac{i\hat{H}_r t}{\hbar}\right)|\Psi(0)\rangle = \exp\left(-\frac{iE_1 t}{\hbar}\right) \times \\ \times \left\{ |\Psi(0)\rangle + i(\beta - \alpha) \exp\left(-\frac{i\Delta E_{21} t}{2\hbar}\right) \times \right. \\ \left. \times \sin\left(\frac{\Delta E_{21} t}{2\hbar}\right) [|L\rangle - |R\rangle] \right\}, \quad (3)$$

where $\Delta E_{21} = E_2 - E_1$. We note that at $t \ll t_0 = \hbar/\Delta E_{21}$, the initial qubit state remains almost unchanged (not counting the common phase). Because the value of ΔE_{21} is exponentially small at $x = R_d/a_B^* \gg 1$ [29, 30],

$$\frac{\Delta E_{21}}{E^*} = 4xe^{-x-1} \left[1 + \frac{1}{2x} + O\left(\frac{1}{x^2}\right) \right], \quad (4)$$

the period $t_0 \sim \hbar/\Delta E_{21}$ that it takes for the qubit state to change is rather long, $t_0 > 1 \mu\text{s}$ at $R_d > 60$ nm.

In what follows, we consider the processes occurring in time intervals much shorter than t_0 and hence ignore the off-diagonal term $[-(\Delta E_{21}/2)|L\rangle\langle R| + \text{H.c.}]$ in \hat{H}_r that gives rise to the electron tunneling $|L\rangle \leftrightarrow |R\rangle$. Then Hamiltonian (2) takes the form

$$\hat{H}_r \approx \frac{E_1 + E_2}{2} \left[|L\rangle\langle L| + |R\rangle\langle R| \right] + \\ + E_{TR}|\chi_{TR}\rangle\langle\chi_{TR}|, \quad (5)$$

where $(E_1 + E_2)/2 \approx E_1 \approx E_2$ at $R_d \gg a_B^*$. In the general case where the qubit is biased by gate voltages, the energies E_L and E_R of the respective lowest states localized at the left and the right donor differ from each other. In this case, the localized states are all the better approximations to the energy eigenstates, and the Hamiltonian \hat{H}_r becomes

$$\hat{H}_r \approx E_L|L\rangle\langle L| + E_R|R\rangle\langle R| + E_{TR}|\chi_{TR}\rangle\langle\chi_{TR}|. \quad (6)$$

We now let the buried donor charge qubit interact with an external electromagnetic field $\mathbf{E}(t)$. Then the Hamiltonian becomes

$$\hat{H}(t) = \hat{H}_r + \hat{V}(t), \quad (7)$$

where the interaction term $\hat{V}(t)$ is

$$\hat{V}(t) = \mathbf{E}(t) \left[\mathbf{d}_L|\chi_{TR}\rangle\langle L| + \mathbf{d}_R|\chi_{TR}\rangle\langle R| + \text{H.c.} \right], \quad (8)$$

with $\mathbf{d}_L = \langle\chi_{TR}| - e\mathbf{r}|L\rangle$ and $\mathbf{d}_R = \langle\chi_{TR}| - e\mathbf{r}|R\rangle$ being the electric dipole moments for the transitions $|L, R\rangle \leftrightarrow |\chi_{TR}\rangle$ between the respective localized states $|L\rangle$ and $|R\rangle$ and one of the excited molecular states $|\chi_{TR}\rangle$ delocalized over the double-donor system. For definiteness, we choose this state to be the third one-electron state $|\chi_3\rangle$ of the molecular ion $\text{P}_2^+:\text{Si}$. At $E_L = E_R$ and $R_d/a_B^* > 6$, this is the $3d\sigma_g$ state whose wave function $\langle\mathbf{r}|\chi_3\rangle$ is symmetric about the midpoint of the line joining the two donors and has its maxima at the donor locations [31], see Fig. 2. If the donors are arranged along the x axis, the state $|\chi_3\rangle$ is formed upon the hybridization of $|2S\rangle_{L,R}$ and $|2P_x\rangle_{L,R}$ atomic states of the donors, and the wave function $\langle\mathbf{r}|\chi_3\rangle$ in the vicinity of the left/right donor is equal to $[\langle\mathbf{r}|2S\rangle_{L,R} \mp \langle\mathbf{r}|2P_x\rangle_{L,R}]/2$ at $R_d \gg a_B^*$. We note that for such a choice of the state $|\chi_3\rangle$, the electric field should have a nonzero x component in order that $\mathbf{d}_{L,R} \neq 0$.

We consider two cases: (a) $E_L = E_R \approx E_1$ and (b) $E_L \neq E_R$, the desired value of the difference $E_R - E_L$

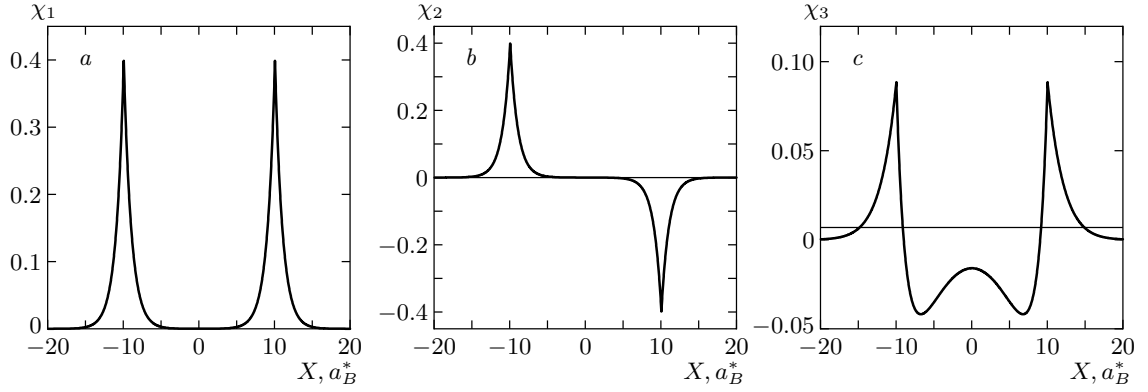


Fig. 2. One-electron wave functions of the lowest two states, $1s\sigma_g$ (a) and $2p\sigma_u$ (b), and the excited state $3d\sigma_g$ (c) of the molecular ion $\text{P}_2^+:\text{Si}$ in the isotropic effective mass approximation. The coordinate x is along the line joining the two donors. The donor separation is $R_d = 20a_B^*$. The symmetric and antisymmetric linear superpositions of the $1s\sigma_g$ and $2p\sigma_u$ states correspond to the respective $1s$ atomic states $|L\rangle$ and $|R\rangle$ localized at the left and the right donor. They form the qubit logical states $|0\rangle = |L\rangle$ and $|1\rangle = |R\rangle$. The excited state $3d\sigma_g$ is an auxiliary («transport») state needed to transfer an electron between $|L\rangle$ and $|R\rangle$ states under the influence of the external electromagnetic field

being discussed below. In case (a), we suppose $\mathbf{E}(t)$ to oscillate at a frequency $\omega = (E_{TR} - E_{L,R})/\hbar$,

$$\mathbf{E}(t) = \mathbf{E}_0(t) \cos \omega t, \quad (9)$$

where $\mathbf{E}_0(t)$ is the slowly varying envelope of the field. Using of the resonant approximation²⁾, i. e., omitting the rapidly oscillating terms with the frequencies $\pm(\omega + E_{TR}/\hbar - E_{L,R}/\hbar)$ from the Hamiltonian, we have

$$\hat{V}(t) = \frac{1}{2} e^{-i\omega t} \left[\lambda_L(t) |\chi_{TR}\rangle \langle L| + \lambda_R(t) |\chi_{TR}\rangle \langle R| \right] + \text{H.c.}, \quad (10)$$

where $\lambda_{L,R}(t) = \mathbf{E}_0(t) \mathbf{d}_{L,R}$. In case (b), the field $\mathbf{E}(t)$ has two components oscillating at the frequencies $\omega_L = (E_{TR} - E_L)/\hbar$ and $\omega_R = (E_{TR} - E_R)/\hbar$,

$$\mathbf{E}(t) = \mathbf{E}_{01}(t) \cos(\omega_L t) + \mathbf{E}_{02}(t) \cos(\omega_R t + \phi), \quad (11)$$

where ϕ is the phase shift between the two components. In the resonant approximation (see footnote 2), we have

²⁾ The resonant approximation is valid if the absolute value of the detuning from resonance, $\hbar\delta = \hbar\omega - (E_{TR} - E_{L,R})$, is small compared to the spacing between the energy E_{TR} of the state $|\chi_{TR}\rangle$ and the energy E' of the state $|\chi'\rangle$ nearest to $|\chi_{TR}\rangle$. In the case where there are two components in $\mathbf{E}(t)$, the absolute values of both $\hbar\delta_L = \hbar\omega_L - (E_{TR} - E_L)$ and $\hbar\delta_R = \hbar\omega_R - (E_{TR} - E_R)$ should be small compared to $|E' - E_{TR}|$.

$$\hat{V}(t) = \frac{1}{2} \exp(-i\omega_L t) \lambda_L(t) |\chi_{TR}\rangle \langle L| + \frac{1}{2} \exp(-i\omega_R t - i\phi) \lambda_R(t) |\chi_{TR}\rangle \langle R| + \text{H.c.}, \quad (12)$$

where $\lambda_{L,R}(t) = \mathbf{E}_{01,2}(t) \cdot \mathbf{d}_{L,R}$. In this paper, we restrict ourselves to the rectangular pulse shape, and therefore $\mathbf{E}_0(t)$ in Eq. (9) and both $\mathbf{E}_{01}(t)$ and $\mathbf{E}_{02}(t)$ in Eq. (11) are constant at $0 < t < \tau_{op}$ and zero elsewhere.

It is straightforward to solve the nonstationary Schrödinger equation for the state vector $|\Psi(t)\rangle$,

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \hat{H}(t) |\Psi(t)\rangle, \quad (13)$$

with the Hamiltonian $\hat{H}(t)$ in Eq. (7) given by Eqs. (5) and (10) in case (a) or Eqs. (6) and (12) in case (b), and to find the coefficients $C_L(t)$, $C_R(t)$, and $C_{TR}(t)$ in the expansion of $|\Psi(t)\rangle$ in terms of the states $|L\rangle$, $|R\rangle$, and $|\chi_{TR}\rangle$,

$$|\Psi(t)\rangle = C_L(t) \exp\left(-\frac{iE_L t}{\hbar}\right) |L\rangle + C_R(t) \exp\left(-\frac{iE_R t}{\hbar}\right) |R\rangle + C_{TR}(t) \exp\left(-\frac{iE_{TR} t}{\hbar}\right) |\chi_{TR}\rangle, \quad (14)$$

provided that $|\Psi(0)\rangle = \alpha|L\rangle + \beta|R\rangle$, where $|\alpha|^2 + |\beta|^2 = 1$. In case (a), we have

$$\begin{aligned}
C_L(t) &= \alpha \left[1 - \frac{2|\lambda_L|^2}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2 \Omega t \right] - \\
&\quad - \beta \frac{2\lambda_L^* \lambda_R}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2 \Omega t, \\
C_R(t) &= -\alpha \frac{2\lambda_L \lambda_R^*}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2 \Omega t + \\
&\quad + \beta \left[1 - \frac{2|\lambda_R|^2}{|\lambda_L|^2 + |\lambda_R|^2} \sin^2 \Omega t \right], \\
C_{TR}(t) &= -i \frac{\alpha \lambda_L + \beta \lambda_R}{\sqrt{|\lambda_L|^2 + |\lambda_R|^2}} \sin 2\Omega t,
\end{aligned} \tag{15}$$

where

$$\Omega = \frac{\sqrt{|\lambda_L|^2 + |\lambda_R|^2}}{4\hbar}. \tag{16}$$

In case (b), the coefficients $C_L(t)$, $C_R(t)$, and $C_{TR}(t)$ are also given by Eqs. (15) and (16) with the only exception that λ_R must be replaced by $\lambda_R \exp(-i\phi)$. From Eqs. (15) and (16), we can see that at $t = \tau_{op} = \pi k/2\Omega$ (hereafter, k is a positive integer), the coefficient C_{TR} vanishes, and hence the state vector $|\Psi(t)\rangle$ remains in the qubit subspace $\{|L\rangle, |R\rangle\}$ and $|C_L(\tau_{op})|^2 + |C_R(\tau_{op})|^2 = 1$. In particular, if $C_L(0) = 1$ and $C_R(0) = 0$, then $C_L(\tau_{op}) = 0$ and $C_R(\tau_{op}) = \pm 1$ at $\lambda_L = \mp \lambda_R$ and odd k , i. e., there is a complete population transfer $|L\rangle \rightarrow |R\rangle$, see Ref. [9]. Thus, the auxiliary excited state $|\chi_{TR}\rangle$ plays the role of the «transport» state, in that it assists the qubit evolution by means of the electron transfer between the states $|L\rangle$ and $|R\rangle$ as the pulse is on but remains unpopulated after the pulse is off.

3. QUBIT ROTATIONS

In this section, we show that the auxiliary-state-assisted electron transfer between the two donors allows various qubit rotations. In case (a), where the two donors in the molecular ion $P_2^+ : \text{Si}$ are equivalent, i. e., $E_L = E_R$ and $|\lambda_L| = |\lambda_R|$, the qubit state $|\Psi(t)\rangle$ at the operation time τ_{op} remains unchanged,

$$|\Psi(\tau_{op})\rangle = \exp\left(-\frac{iE_L\tau_{op}}{\hbar}\right) |\Psi(0)\rangle, \tag{17}$$

if $\tau_{op} = \pi k/\Omega$, or changes into

$$|\Psi(\tau_{op})\rangle = \pm \exp\left(-\frac{iE_L\tau_{op}}{\hbar}\right) [\beta|L\rangle + \alpha|R\rangle] \tag{18}$$

if $\tau_{op} = \pi(2k-1)/2\Omega$ and $\lambda_L = \mp \lambda_R$, see Eqs. (14) and (15). The latter corresponds to the quantum NOT operation.

Case (b) seems to be more realistic because of the different local atomic surroundings of the donors in the

pair due to both the uncontrollable damage of the host upon ion implantation and the probabilistic variations in the path taken through the substrate by each implanted ion [20]. Besides, the surface gates can be used to intentionally tune E_L and E_R to the predetermined values. Moreover, one can change the values of λ_L and λ_R separately by changing the electric field amplitudes E_{01} and E_{02} . It follows from Eqs. (14) and (15) that the relative phase shift operation is implemented at $\tau_{op} = \pi k/\Omega$,

$$\begin{aligned}
|\Psi(\tau_{op})\rangle &= \exp\left(-\frac{iE_L\tau_{op}}{\hbar}\right) \times \\
&\quad \times \left[\alpha|L\rangle + \beta \exp\left[-\frac{i(E_R - E_L)\tau_{op}}{\hbar}\right] |R\rangle \right], \tag{19}
\end{aligned}$$

while the value of $\tau_{op} = \pi(2k-1)/2\Omega$ corresponds to realization of the quantum NOT operation,

$$|\Psi(\tau_{op})\rangle = \pm \exp\left(-\frac{iE_L\tau_{op}}{\hbar} - i\phi\right) [\beta|L\rangle + \alpha|R\rangle], \tag{20}$$

if $\lambda_L = \mp \lambda_R$ and $\phi = \pi n + (E_R - E_L)\tau_{op}/2\hbar$ (hereafter, n is an integer), or to the Hadamard transformation,

$$\begin{aligned}
|\Psi(\tau_{op})\rangle &= \pm \exp\left(-\frac{iE_L\tau_{op}}{\hbar}\right) \times \\
&\quad \times \left[\frac{\alpha + \beta}{\sqrt{2}} |L\rangle + \frac{\alpha - \beta}{\sqrt{2}} |R\rangle \right], \tag{21}
\end{aligned}$$

if $(E_R - E_L)\tau_{op}/\hbar = 2\pi m$ (where m is a positive integer). Here, the plus sign corresponds to the values of $\phi = 2\pi n$ and $\lambda_L = -\lambda_R(\sqrt{2}-1)$ or $\phi = \pi(2n+1)$ and $\lambda_L = \lambda_R(\sqrt{2}-1)$, and the minus sign corresponds to the values of $\phi = 2\pi n$ and $\lambda_L = \lambda_R(\sqrt{2}+1)$ or $\phi = \pi(2n+1)$ and $\lambda_L = -\lambda_R(\sqrt{2}+1)$.

Therefore, various one-qubit operations can be implemented on the buried donor charge qubit through appropriate choices of the pulse frequency, phase, amplitude, and duration. Let us estimate the value of the operation time

$$\tau_{op} \sim 1/\Omega \sim \hbar/|\lambda_{L,R}| \sim \hbar/ea_B^*E_0,$$

see Sec. 2. For the field amplitude $E_0 \sim 1$ V/cm, we have $\tau_{op} \sim 1$ ns. An increase in the pulse intensity causes the value of τ_{op} to decrease to the picosecond time scale, such that the value of τ_{op} can be made orders of magnitude shorter than the period t_0 that it takes for the qubit state to change due to the direct electron tunneling $|L\rangle \leftrightarrow |R\rangle$, see Sec. 2, as well as the operation times in the case where the qubit is manipulated by adiabatically varying the potentials of the

surface gates [16]. We note that in case (b), the energies E_L and E_R should be sufficiently different from each other in order that all these operations could be implemented in short times to avoid decoherence, as discussed below. For example, at $\tau_{op} \sim 1$ ps, we should have $E_R - E_L \sim 3$ meV.

4. DECOHERENCE EFFECTS

An uncontrolled interaction of the quantum system with its environment leads to entanglement between the states of the system and the environmental degrees of freedom. This disturbs the unitary evolution of the system and results in the loss of coherence. There are various sources of decoherence in solids. For the charge qubit considered in this paper, the decoherence due to the phonon emission/absorption processes was studied in Refs. [16, 26] and was found to be much weaker than the decoherence due to both Nyquist–Johnson voltage fluctuations in the surface electrodes and the $1/f$ noise from the background charge fluctuations. We note, however, that there are two mechanisms of the phonon-induced decoherence, which are caused by either the energy relaxation processes or the virtual-phonon dephasing processes. Which one of those mechanisms is dominant depends on the specific parameters of the quantum system and its environment, as well as on the operation times. Here, we show that the dephasing processes play a decisive role in limiting the fault tolerance of the buried donor charge qubit. For simplicity, we consider the qubit at zero temperature and assume isotropic acoustic phonons with the linear dispersion law $\omega_{\mathbf{q}} = sq$, where s is the speed of sound.

We first recall some general concepts concerning the transition probability for an electron moving in a time-dependent potential. If the electron, being initially in a state $|i\rangle$ of the discrete energy spectrum, interacts with the harmonic field

$$\hat{V}(t) = \hat{F}e^{-i\omega t} + \hat{F}^\dagger e^{i\omega t}, \quad (22)$$

then the probability amplitude to find it in a state $|f\rangle$ at a time t is given by the following expression that results from the first-order perturbation theory [32]³⁾:

$$a_{i \rightarrow f}(\omega, t) = F_{fi} \frac{\exp[-i(\omega_{if} + \omega)t] - 1}{\hbar(\omega_{if} + \omega)} + F_{if}^* \frac{\exp[-i(\omega_{if} - \omega)t] - 1}{\hbar(\omega_{if} - \omega)}, \quad (23)$$

³⁾ We note that Eq. (23) is applicable as long as $|a_{i \rightarrow f}(\omega, t)| \ll 1$.

where $\omega_{if} = (E_i - E_f)/\hbar$. The common approach is to ignore the first term in Eq. (23) and use the expression

$$\lim_{t \rightarrow \infty} \frac{\sin^2(\epsilon t)}{\pi t \epsilon^2} = \delta(\epsilon), \quad (24)$$

thus arriving at the so-called Fermi golden rule for the transition probability,

$$\begin{aligned} W_{i \rightarrow f}(\omega, t) &= |a_{i \rightarrow f}(\omega, t)|^2 \approx \\ &\approx |F_{if}|^2 \frac{4 \sin^2[(\omega_{if} - \omega)t/2]}{\hbar^2(\omega_{if} - \omega)^2} \approx \\ &\approx \frac{2\pi}{\hbar} |F_{if}|^2 \delta(\hbar\omega_{if} - \hbar\omega)t \equiv \Gamma_{i \rightarrow f}(\omega)t, \end{aligned} \quad (25)$$

where $\Gamma_{i \rightarrow f}(\omega)$ is the time-independent transition rate. The δ -function reflects the energy conservation, $\hbar\omega_{if} = \hbar\omega$, for such a transition.

The electron–phonon coupling in confined systems is described by the Hamiltonian

$$\hat{H}_{el-ph} = \sum_{\mathbf{q}} \lambda(\mathbf{q}) \hat{\rho}(\mathbf{q}) \left[\hat{b}_{\mathbf{q}}^\dagger + \hat{b}_{-\mathbf{q}} \right], \quad (26)$$

where $\hat{b}_{\mathbf{q}}^\dagger$ and $\hat{b}_{\mathbf{q}}$ are the respective operators of creation and annihilation of a phonon with the wave vector \mathbf{q} , $\hat{\rho}(\mathbf{q}) = \int d\mathbf{r} \exp(i\mathbf{q} \cdot \mathbf{r}) \hat{\rho}(\mathbf{r})$ is the Fourier transform of the electron density operator $\hat{\rho}(\mathbf{r}) = \sum_{mn} \Psi_m^*(\mathbf{r}) \Psi_n(\mathbf{r}) |m\rangle \langle n|$, and $\lambda(\mathbf{q})$ is the microscopic electron–phonon interaction matrix element, which can be expressed in terms of the deformation potential D and the density of the crystal ρ as

$$\lambda(\mathbf{q}) = qD \sqrt{\frac{\hbar}{2\rho\omega_{\mathbf{q}}v}}, \quad (27)$$

with v being the normalizing volume. If harmonic field (22) is associated with a deformation phonon having the frequency $\omega_{\mathbf{q}}$, then, taking into account that the deformation fields produced by the phonons with different wave vectors are not correlated, we have the total transition rate [33]⁴⁾

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} \sum_{\mathbf{q}} |F_{if}(\mathbf{q})|^2 \delta(\hbar\omega_{if} - \hbar\omega_{\mathbf{q}}), \quad (28)$$

where

$$F_{if}(\mathbf{q}) = \lambda(\mathbf{q}) \langle i | e^{i\mathbf{q} \cdot \mathbf{r}} | f \rangle. \quad (29)$$

⁴⁾ We note that at $T = 0$, there are no phonons in the sample, and hence only the second term in Eq. (22) is relevant for the electron–phonon interaction because the initial and final phonon states, $|i_{ph}\rangle$ and $|f_{ph}\rangle$, are the respective states $|0_{\mathbf{q}}\rangle \exp(-iE_0 t)$ and $|1_{\mathbf{q}}\rangle \exp[-i(E_0 + \omega_{\mathbf{q}})t]$, where $E_0 = \sum_{\mathbf{q}} (\hbar\omega_{\mathbf{q}}/2)$, and hence $\langle f_{ph} | \hat{b}_{\mathbf{q}}^\dagger | i_{ph} \rangle = \exp(i\omega_{\mathbf{q}} t)$.

4.1. Decoherence during adiabatic variations of the surface gate potentials

In the case where the buried donor charge qubit is controlled by the surface gates [16], such that the state vector $|\Psi(t)\rangle$ remains in the qubit subspace $\{|L\rangle, |R\rangle\}$ during the operation and the overlap $\langle L|R\rangle$ is negligibly small, Hamiltonian (26) can be written in the spin-boson form [34]

$$\hat{H}_{el-ph} = \hat{\sigma}_z \sum_{\mathbf{q}} g(\mathbf{q}) [\hat{b}_{\mathbf{q}}^\dagger + \hat{b}_{-\mathbf{q}}], \quad (30)$$

where $\hat{\sigma}_z = |L\rangle\langle L| - |R\rangle\langle R|$ and

$$g(\mathbf{q}) = \frac{\lambda(\mathbf{q})}{2} [\langle L|e^{i\mathbf{q}\mathbf{r}}|L\rangle - \langle R|e^{i\mathbf{q}\mathbf{r}}|R\rangle]. \quad (31)$$

Since $\langle \mathbf{r}|L, R\rangle = (\pi a_B^*{}^3)^{-1/2} \exp(-|\mathbf{r} - \mathbf{r}_{L,R}|/a_B^*)$ for $1s$ -orbitals, where $\mathbf{r}_{L,R}$ are the donor coordinates, we have [14]

$$g(\mathbf{q}) = -i\lambda(\mathbf{q}) \frac{\sin(q_x R_d/2)}{[1 + (qa_B^*)^2/4]}, \quad (32)$$

where q_x is the component of the phonon wave vector along the line joining the two donors, and we chose the origin of the coordinates in between the donors, such that $\mathbf{r}_{L,R} = \mp(R_d/2)\mathbf{e}_x$.

Fedichkin and Fedorov [14] have shown that at $T = 0$, decoherence upon implementing the phase operation emerges as pure dephasing, the electron density matrix being given by the general expression [35, 36]

$$\begin{pmatrix} \rho_{LL}(0) & \rho_{LR}(0) \exp\left[-B^2(t) + i\frac{(E_R - E_L)t}{\hbar}\right] \\ \rho_{RL}(0) \exp\left[-B^2(t) - i\frac{(E_R - E_L)t}{\hbar}\right] & \rho_{RR}(0) \end{pmatrix} \quad (33)$$

with the spectral function

$$B^2(t) = \frac{8}{\hbar^2} \sum_{\mathbf{q}} \frac{|g(\mathbf{q})|^2}{\omega_{\mathbf{q}}^2} \sin^2 \frac{\omega_{\mathbf{q}} t}{2}. \quad (34)$$

There is no relaxation in this case because for the phase operation to be implemented, the energies E_L and E_R must be sufficiently different from each other [14], so that the basis $\{|L\rangle, |R\rangle\}$ coincides with the energy basis of the electron in the double donor system and electron term (6) commutes with interaction term (30) in the Hamiltonian. As a result, the diagonal elements of the density matrix remain unchanged. On the other hand, decoherence upon implementing the quantum NOT operation (where $E_L = E_R$ and the energy basis of the electron is formed by the states $|\chi_{1,2}\rangle = [|L\rangle \pm |R\rangle]/\sqrt{2}$, see Sec. 2) was suggested to be caused by relaxation [14], such that both off-diagonal and diagonal elements of the density matrix decrease exponentially with time, the relaxation rate $\Gamma_{2\rightarrow 1}$ (see Eq. (28)) being [14, 26]

$$\Gamma_{2\rightarrow 1} = \frac{D^2}{4\pi\rho\hbar s^2} \frac{q_{21}^3}{[1 + (q_{21}a_B^*)^2/4]^4} \times \left(1 - \frac{\sin(q_{21}R_d)}{q_{21}R_d}\right), \quad (35)$$

where $q_{21} = \Delta E_{21}/s\hbar$, see Eq. (4).

We note, however, that approximation (25) for $W_{i\rightarrow f}(\omega, t)$ and, accordingly, Eq. (28) for $\Gamma_{i\rightarrow f}$ are valid if the time t is sufficiently long, see Eq. (24). To quantify the applicability of this approximation, we analyze the more general expression for $W_{i\rightarrow f}(t)$ that follows from Eq. (25),

$$W_{i\rightarrow f}(t) = \frac{4}{\hbar^2} \sum_{\mathbf{q}} |F_{if}(\mathbf{q})|^2 \frac{\sin^2[(\omega_{if} - \omega_{\mathbf{q}})t/2]}{(\omega_{if} - \omega_{\mathbf{q}})^2}. \quad (36)$$

We can roughly distinguish two phonon contributions to $W_{i\rightarrow f}(t)$, one being from the «resonant component», i. e., from the δ -function-like peak of $\sin^2[(\omega_{if} - \omega_{\mathbf{q}})t/2]/(\omega_{if} - \omega_{\mathbf{q}})^2$ as a function of q at $q = q_{if} = \omega_{if}/s$, with the height $t^2/4$ and the width $\sim 1/st$, and the other from the remaining «nonresonant background» of the phonon spectrum. The former can be estimated as

$$W_{i\rightarrow f}^{(1)}(t) \sim \frac{vq_{if}^2}{\hbar^2 s} |F_{if}(q_{if})|^2 t, \quad (37)$$

and the latter as

$$W_{i\rightarrow f}^{(2)}(t) \sim \frac{v\Delta q}{\hbar^2 s^2} |F_{if}(q_{max})|^2 \quad (38)$$

at $q_{if} \ll q_{max}$ and

$$W_{i\rightarrow f}^{(2)}(t) \sim \frac{v\Delta q}{\hbar^2 s^2} \left(\frac{q_{max}}{q_{if}}\right)^2 |F_{if}(q_{max})|^2 \quad (39)$$

at $q_{if} \gg q_{max}$, where q_{max} is the wave vector at which the function $|F_{if}(q)|^2$ has a maximum and Δq is a characteristic width of $|F_{if}(q)|^2$ in the maximum. The specific values of Δq , q_{max} , and $F_{if}(q_{max})$ depend on the specific type of wave functions $\langle \mathbf{r}|i\rangle$ and $\langle \mathbf{r}|f\rangle$ in the matrix element $\langle i|\exp(i\mathbf{q}\cdot\mathbf{r})|f\rangle$. Next, if, e.g., $q_{if} \ll q_{max}$ and we are interested in the transition probability $W_{i\rightarrow f}(t)$ at a moment of time t such that $s q_{if}^2 |F_{if}(q_{if})|^2 t \ll \Delta q |F_{if}(q_{max})|^2$, then $W_{i\rightarrow f}^{(1)}(t) \ll W_{i\rightarrow f}^{(2)}(t)$, and hence the Fermi golden rule appears to be broken [37, 38]. This is due to the violation of the energy conservation at short times [32].

Inspection of the phonon-induced transitions between the states $|\chi_{1,2}\rangle = [|L\rangle \pm |R\rangle]/\sqrt{2}$ of the double-donor system with $E_L = E_R$ and the donor separation $R_d \gg a_B^*$ (these transitions are relevant for decoherence during the implementation of the NOT operation [14]) provides an illustrative example of the departure from the Fermi golden rule. In this case,

$$\langle 2|e^{i\mathbf{q}\cdot\mathbf{r}}|1\rangle = [\langle L|e^{i\mathbf{q}\cdot\mathbf{r}}|L\rangle - \langle R|e^{i\mathbf{q}\cdot\mathbf{r}}|R\rangle]/2,$$

and hence $F_{21}(\mathbf{q}) = g(\mathbf{q})$, see Eq. (32), and the resonant component of the transition probability is $W_{2\rightarrow 1}^{(1)}(t) \sim q_{21}^3 D^2 t / \rho \hbar s^2$, in accordance with the value of the relaxation rate $\Gamma_{2\rightarrow 1}$ given by Eq. (35). Since the value of $q_{21} = \Delta E_{21} / \hbar s$ decreases exponentially with R_d , see Eq. (4), the value of $\Gamma_{2\rightarrow 1}$ decreases exponentially as well, going below 10^3 s^{-1} at $R_d/a_B^* > 10$ (see Fig. 5 in Ref. [26]). On the other hand, since $q_{21} \ll q_{max} \sim 1/a_B^*$, we have $W_{2\rightarrow 1}^{(2)}(t) \sim D^2 / \rho \hbar s^3 a_B^{*2}$ from Eq. (38). More accurate calculations result in $W_{2\rightarrow 1}^{(2)}(t) = B^2(t)/2$, see Eq. (34). If the operation time τ_{op} is long compared to the phonon transit time, a_B^*/s ($\approx 0.3 \text{ ps}$ for $\text{P}_2^+:\text{Si}$), it follows from Eq. (34) (see Ref. [14]) that

$$B^2(\tau_{op}) = \frac{D^2}{3\pi^2 \rho \hbar s^3 a_B^{*2}}, \quad (40)$$

and therefore spectral function (34) appears to be a material constant, being about $6 \cdot 10^{-3}$ for the phosphorous donors in silicon [14], where $D = 3.3 \text{ eV}$, $s = 9 \cdot 10^5 \text{ cm/s}$, and $\rho = 2.33 \text{ g/cm}^3$. Hence, $W_{2\rightarrow 1}^{(2)}(t) \gg W_{2\rightarrow 1}^{(1)}(t)$ at $R_d/a_B^* = 10$ and $t \ll \tilde{t} \approx 3 \cdot 10^{-6} \text{ s}$, the time \tilde{t} being exponentially longer for larger values of R_d/a_B^* , and in any case longer than the operation time τ_{op} , see Sec. 3.

Therefore, contrary to suggestions [14, 26] that the phonon-induced decoherence in the case of the NOT operation is determined by the value of the relaxation rate $\Gamma_{2\rightarrow 1}$ given by Eq. (35), we see that at sufficiently short operation times, decoherence in the cases of both

phase and NOT operations is determined by the same spectral function $B^2(t)$, see Eq. (34). The distinction between the two cases is that the diagonal elements of the density matrix remain unchanged in the case of the phase operation because there is no relaxation, while they decay exponentially (along with the off-diagonal matrix elements) in the case of the NOT operation [14].

4.2. Decoherence during the auxiliary-state-assisted operations

Because the excited «transport» level $|TR\rangle$ becomes temporarily populated during the resonant-pulse operations on the $\text{P}_2^+:\text{Si}$ qubit, the phonon-induced electron transitions $|TR\rangle \leftrightarrow |L, R\rangle$ and $|TR\rangle \leftrightarrow |\chi_{1,2}\rangle$ can have a detrimental effect on the qubit evolution, along with the transitions $|L\rangle \leftrightarrow |R\rangle$ and $|\chi_1\rangle \leftrightarrow |\chi_2\rangle$ studied above. We now clarify which type of the phonon-induced electron transitions («resonant» or «nonresonant») is dominant in this case and estimate the transition probability. We follow the line of reasoning outlined above and start with calculations of the matrix elements $\langle TR|\exp(i\mathbf{q}\cdot\mathbf{r})|L, R\rangle$. For our choices of the «transport» state $|TR\rangle = |\chi_3\rangle$ and the double donor orientation, see Sec. 2, at $R \gg a_B^*$, we have $|TR\rangle \approx [|2S\rangle_L - |2P_x\rangle_L + |2S\rangle_R + |2P_x\rangle_R]/2$, where

$$\begin{aligned} \langle \mathbf{r}|2S\rangle_{L,R} &= \\ &= \frac{1}{\sqrt{8\pi a_B^{*3}}} \left(1 - \frac{|\mathbf{r} - \mathbf{r}_{L,R}|}{2a_B^*} \right) \exp\left(-\frac{|\mathbf{r} - \mathbf{r}_{L,R}|}{2a_B^*} \right), \end{aligned}$$

$$\langle \mathbf{r}|2P_x\rangle_{L,R} = \frac{1}{\sqrt{32\pi a_B^{*5}}} (x - x_{L,R}) \exp\left(-\frac{|\mathbf{r} - \mathbf{r}_{L,R}|}{2a_B^*} \right).$$

Neglecting the exponentially small overlap between the localized atomic-like orbitals centered at different donors, we have

$$\begin{aligned} \langle TR|e^{i\mathbf{q}\cdot\mathbf{r}}|L, R\rangle &= \\ &= 2\sqrt{2} \frac{(qa_B^*)^2 \mp 3i(q_x a_B^*)/2}{[9/4 + (qa_B^*)^2]^3} \exp\left(\mp \frac{iq_x R}{2} \right). \quad (41) \end{aligned}$$

Depending on the relative values of E_L and E_R , the lowest energy eigenstates of $\text{P}_2^+:\text{Si}$ are either $|L\rangle$ and $|R\rangle$ (if $E_L \neq E_R$) or χ_1 and χ_2 (if $E_L = E_R$), and therefore, in order to find the probability $W_{TR}(t)$ of the electron escape from the «transport» state at $T = 0$, we must add the respective probabilities of the $|TR\rangle \rightarrow |L\rangle$ and $|TR\rangle \rightarrow |R\rangle$ or $|TR\rangle \rightarrow |\chi_1\rangle$ and $|TR\rangle \rightarrow |\chi_2\rangle$ electron transitions. If the value of $E_R - E_L$ is much less than the difference between E_{TR} and $E_{L,R}$, then we have the same result in both cases, and hence $W_{TR}(t)$ is

given by Eq. (36), where now $\omega_{if} \approx \Delta E_{31}/\hbar \approx 3E^*/8\hbar$ is independent of R_d at $R_d \gg a_B^*$, and

$$|F_{if}(\mathbf{q})|^2 = 16 \frac{(qa_B^*)^4 + 9(q_x a_B^*)^2/4}{[9/4 + (qa_B^*)^2]^6} |\lambda(\mathbf{q})|^2. \quad (42)$$

Taking into account that

$$q_{if} a_B^* = \frac{\omega_{if} a_B^*}{s} \approx \frac{3e^2}{8\varepsilon \hbar s} \approx 8 \gg q_{max} a_B^* \sim 1$$

and using Eq. (36), it is straightforward to derive the following expressions for the respective probabilities of the «resonant» and «nonresonant» transitions:

$$W_{TR}^{(1)}(t) \approx \frac{8D^2}{\pi \rho \hbar s^2 a_B^{*3}} (q_{if} a_B^*)^5 \frac{3/4 + (q_{if} a_B^*)^2}{[9/4 + (q_{if} a_B^*)^2]^6} t \quad (43)$$

and

$$W_{TR}^{(2)}(t) \approx \frac{176D^2}{3645\pi^2 \rho \hbar s^3 (a_B^*)^2 (q_{if} a_B^*)^2}. \quad (44)$$

It follows from Eqs. (43) and (44) that $W_{TR}^{(1)}(t) = \Gamma_{TR} t$, where $\Gamma_{TR} \approx 3 \cdot 10^7 \text{ s}^{-1}$, and $W_{TR}^{(2)}(t) \approx 10^{-5}$, and hence the «resonant» transitions are dominant at $t > 0.3 \text{ ps}$.

We now check what states among those involved in the auxiliary-state-assisted qubit evolution are most sensitive to phonon-induced decoherence. As we have seen above, decoherence of the low-energy states $|L\rangle$ and $|R\rangle$ (or $|\chi_1\rangle$ and $|\chi_2\rangle$) is quantified by the error rate [14], i. e., the error generated during the operation time, $D(t) = B^2(t)/2 \approx 3 \cdot 10^{-3}$. This value is greater than $W_{TR}^{(2)}(t)$ but less than $W_{TR}^{(1)}(t)$ at $t > 10^{-10} \text{ s}$, where the processes of the spontaneous phonon emission by an electron temporarily occupying the «transport» level become prevailing. Hence at $\tau_{op} < 100 \text{ ps}$, the error rate does not exceed the value of $D(\tau_{op}) \approx 3 \cdot 10^{-3}$.

5. DISCUSSION

Fast auxiliary-state-assisted evolution of the double-donor charge qubit driven by the resonant electromagnetic field allows implementation of various one-qubit rotations in very short operation times $\tau_{op} < 100 \text{ ps}$, thus minimizing the unwanted decoherence effects. At such times, the error rate due to acoustic phonons is $D(\tau_{op}) \approx 3 \cdot 10^{-3}$ at $T = 0$. At finite temperatures, such that $k_B T > \hbar \omega_0$, where $\hbar \omega_0 = \hbar s/a_B^* \approx 2 \text{ meV}$ for dephasing processes and «nonresonant» emission/absorption transitions, and $\hbar \omega_0 = |E_i - E_f|$ for the «resonant» $|i\rangle \leftrightarrow |f\rangle$ transitions, the error rate increases by a factor of $\sim k_B T/\hbar \omega_0$.

The strongest increase in the error rate at $T \neq 0$ occurs if the two donors in the molecular ion $\text{P}_2^+:\text{Si}$ are

equivalent, because the energies E_L and E_R of the lowest localized states $|L\rangle$ and $|R\rangle$ are then equal to each other, and the difference $E_2 - E_1$ between the eigenenergies of the two lowest delocalized molecular states $|\chi_1\rangle$ and $|\chi_2\rangle$ is exponentially small at large donor separations, e.g., $E_2 - E_1 \approx 10^{-6} \text{ meV}$ at $R = 60 \text{ nm}$, see Eq. (4). To weaken the decoherence, it would be reasonable to use the surface gates in order to increase the difference $E_R - E_L$ up to $E_R - E_L \sim 1 \text{ meV}$ such that the energy basis of the electron be formed by the states $|L\rangle$ and $|R\rangle$ instead of the states $|\chi_1\rangle$ and $|\chi_2\rangle$. In this case, the electromagnetic field should have two components driving the electron transitions $|L\rangle \leftrightarrow |TR\rangle$ and $|R\rangle \leftrightarrow |TR\rangle$ between the states $|L, R\rangle$ and the auxiliary «transport» state $|TR\rangle$.

At $T \neq 0$, the processes of the phonon absorption by an electron temporarily occupying the transport state also contribute to decoherence. For our choice of the transport state, $|TR\rangle = |\chi_3\rangle$, the state nearest to it in energy is the state $|\chi_4\rangle$. In the case where the two donors are equivalent and $R/a_B^* > 15$, this is the $4f\sigma_u$ state $|\chi_4\rangle \approx [2S\rangle_L - |2P_x\rangle_L - |2S\rangle_R - |2P_x\rangle_R]/2$, whose wave function $\langle \mathbf{r} | \chi_4 \rangle$ is antisymmetric about the midpoint of the line joining the two donors [31]. At $x = R_d/a_B^* \gg 1$, the energy separation [30]

$$E_4 - E_3 = E^* \frac{x^3}{4} \exp\left(-\frac{x}{2} - 2\right) \left[1 + O\left(\frac{1}{x}\right)\right]$$

is small but greatly exceeds the value of $E_2 - E_1$, e.g., $E_4 - E_3 \approx 0.3 \text{ meV}$ at $R_d = 60 \text{ nm}$. The donor asymmetry in the presence of gate potentials results in a further increase in $E_4 - E_3$, and therefore the phonon absorption processes does not contribute much to decoherence at sufficiently low temperatures $T < 10 \text{ K}$.

Thus, the error rate due to phonon-induced decoherence is $D(\tau_{op}) \approx 3 \cdot 10^{-3}$ at $\tau_{op} < 100 \text{ ps}$ and $T < 10 \text{ K}$. This value is to be compared to the error rates due to other sources of decoherence. The lowest bounds for the decoherence times associated with the Johnson noise from the gates and the environmental charge fluctuations are [16, 20, 26], respectively, $\tau \sim 1 \mu\text{s}$ and $\tau \sim 1 \text{ ns}$, and hence the corresponding error rates [14] $D(\tau_{op}) = 1 - \exp(-\tau_{op}/\tau)$ do not exceed that due to phonons at $\tau_{op} < (1-10) \text{ ps}$. Hence, the performance of the buried donor charge qubit appears to be limited primarily by the electron-phonon interaction. In this paper, we concentrated on the phosphorous donors in silicon. Since spectral function (34) that ultimately determines the error rate for one-qubit operations is a material constant, it would be worthwhile to search for other materials and/or doping elements

for the buried donor charge qubit, in order to weaken the decoherence effects.

Although we restricted ourselves to rectangular shapes of the resonant pulses, our consideration can be generalized to other pulse shapes [39]. The results obtained can also be applied to quantum-dot structures and Josephson three-level gates [39–42]. Finally, once a fundamental possibility of the auxiliary-state-assisted operations has been demonstrated, it is straightforward to organize the coupling of $P_2^+ : \text{Si}$ qubits for conditional quantum operations [16, 20].

In summary, we have proposed a scheme for fast rotations of the buried donor charge qubit through an auxiliary-state-assisted electron evolution under the influence of resonant microwave pulses. This scheme allows implementing one-qubit operations in times as short as $\tau_{op} \sim 1$ ps. With the example of the $P_2^+ : \text{Si}$ qubit, we have shown that dephasing and «nonresonant» relaxation due to acoustic phonons are the main sources of decoherence. The error rate at $T < 10$ K and operation times $\tau_{op} = (1-10)$ ps is about $3 \cdot 10^{-3}$, i. e., greater than the fault-tolerance threshold for quantum computation but sufficiently low to investigate the small-scale devices and thus to demonstrate the experimental feasibility of the scheme.

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REFERENCES

1. A. Barenco, D. Deutsch, A. Ekert, and R. Jozsa, *Phys. Rev. Lett.* **74**, 4083 (1995).
2. A. Shnirman, G. Schon, and Z. Hermon, *Phys. Rev. Lett.* **79**, 2371 (1997).
3. D. Loss and D. P. DiVincenzo, *Phys. Rev. A* **57**, 120 (1998).
4. Y. Nakamura, Yu. A. Pashkin, and J. S. Tsai, *Nature* **398**, 786 (1999).
5. Yu. A. Pashkin, T. Yamamoto, O. Astafiev et al., *Nature* **421**, 823 (2003).
6. B. E. Kane, *Nature* **393**, 133 (1998).
7. B. E. Kane, N. S. McAlpine, A. S. Dzurak et al., *Phys. Rev. B* **61**, 2961 (2000).
8. R. Vrijen, E. Yablonovitch, K. Wang et al., *Phys. Rev. A* **62**, 012306 (2000).
9. L. A. Openov, *Phys. Rev. B* **60**, 8798 (1999).
10. L. Fedichkin, M. Yanchenko, and K. A. Valiev, *Nanotechnology* **11**, 387 (2000).
11. T. Tanamoto, *Phys. Rev. A* **61**, 022305 (2000).
12. J. H. Oh, D. Ahn, and S. W. Hwang, *Phys. Rev. A* **62**, 052306 (2000).
13. T. Hayashi, T. Fujisawa, H. D. Cheong et al., *Phys. Rev. Lett.* **91**, 226804 (2003).
14. L. Fedichkin and A. Fedorov, *Phys. Rev. A* **69**, 032311 (2004).
15. J. R. Petta, A. C. Johnson, C. M. Marcus et al., E-print archives, cond-mat/0408139.
16. L. C. L. Hollenberg, A. S. Dzurak, C. Wellard et al., *Phys. Rev. B* **69**, 113301 (2004).
17. A. V. Tsukanov and L. A. Openov, *Fiz. Tekh. Poluprovodn.* **38**, 94 (2004) [*Semiconductors* **38**, 91 (2004)].
18. D. M. Eigler and E. K. Schweizer, *Nature* **344**, 524 (1990).
19. S. R. Schofield, N. J. Curson, M. Y. Simmons et al., *Phys. Rev. Lett.* **91**, 136104 (2003).
20. A. S. Dzurak, L. C. L. Hollenberg, D. N. Jamieson et al., E-print archives, cond-mat/0306265.
21. D. P. DiVincenzo, *Forsch. Phys.* **48**, 771 (2000).
22. L. A. Openov and A. V. Tsukanov, *Pis'ma v Zh. Eksp. Teor. Fiz.* **80**, 572 (2004); L. A. Openov, *Phys. Rev. B* **70**, 233313 (2004).
23. L. M. Kettle, H.-S. Goan, S. C. Smith et al., *Phys. Rev. B* **68**, 075317 (2003).
24. R. L. Aggarwal, *Sol. St. Comm.* **2**, 163 (1964).
25. A. Baldereschi, *Phys. Rev. B* **1**, 4673 (1970).
26. S. D. Barrett and G. J. Milburn, *Phys. Rev. B* **68**, 155307 (2003).
27. S. T. Pantelides and C. T. Sah, *Phys. Rev. B* **10**, 621 (1974).
28. D. R. Bates and R. H. G. Reid, *Adv. At. Mol. Phys.* **4**, 13 (1968).
29. N. Bardsley, T. Holstein, B. R. Junker, and S. Sinha, *Phys. Rev. A* **11**, 1911 (1975).
30. T. C. Scott, A. Dalgarno, and J. D. Morgan, III, *Phys. Rev. Lett.* **67**, 1419 (1991).
31. S. Fujinaga, *Molecular Orbitals Method*, Mir, Moscow (1983) [translated from Japanese to Russian].

- 32.** L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, Nauka, Moscow (1974), Ch. VI.
- 33.** U. Bockelmann and G. Bastard, *Phys. Rev. B* **42**, 8947 (1990).
- 34.** T. Brandes and T. Vorrath, *Phys. Rev. B* **66**, 075341 (2002).
- 35.** N. G. van Kampen, *J. Stat. Phys.* **78**, 299 (1995).
- 36.** D. Mozyrsky and V. Privman, *J. Stat. Phys.* **91**, 787 (1998).
- 37.** F.-S. Liu, K.-D. Peng, and W.-F. Chen, *Int. J. Theor. Phys.* **40**, 2037 (2001).
- 38.** L. A. Openov, *Phys. Rev. Lett.* **93**, 158901 (2004).
- 39.** E. Paspalakis, Z. Kis, E. Voutsinas, and A. F. Terzis, *Phys. Rev. B* **69**, 155316 (2004).
- 40.** Z. Kis and E. Paspalakis, *Phys. Rev. B* **69**, 024510 (2004).
- 41.** C.-P. Yang, S.-I. Chu, and S. Han, *Phys. Rev. A* **67**, 042311 (2003).
- 42.** M. H. S. Amin, A. Yu. Smirnov, and A. M. van den Brink, *Phys. Rev. B* **67**, 100508 (2003).