

## Error rate of a charge qubit coupled to an acoustic phonon reservoir

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We analyze decoherence of an electron in a double dot due to the interaction with acoustic phonons. For large tunneling rates between the quantum dots, the main contribution to decoherence comes from the phonon emission relaxation processes, while for small tunneling rates, the virtual-phonon, dephasing processes dominate. Our results show that in common semiconductors, such as Si and GaAs, the latter mechanism determines the upper limit for the double-dot charge qubit performance measure.

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Recently, there has been a lot of interest in implementation of quantum logic gates by manipulating two-level electron systems in semiconductor quantum dots (artificial atoms) [1]. Several designs for coherent solid-state quantum information processing have been suggested [2-4]. Quantum-dot architecture of a quantum computer is very attractive because it is possibly scalable and the most compatible with the recent microelectronics technology. However, it is a great challenge to maintain a satisfactory level of coherence of an electron in semiconductor to perform even elementary quantum gates [5]. Hopefully, coherence can be enhanced by encoding of the logical qubit states into a subspace of the electron states in a large quantum-dot array (artificial crystal) [6]. It is also noted that in a gate-engineered structure of two coupled identical quantum dots one can control decoherence rates by several orders of magnitude [3]. Recent advances in technology of fabrication of double-dot [7,8] and double-donor [4] qubits have been reported. Coherent oscillations in double-dot qubit are observed [9]. It has been demonstrated that scattering by phonons can significantly influence electron transport through double-dot system [10] and qubit dynamics during measurement [11]. In this work, we analyze decoherence of an electron in a double-dot potential due to acoustic phonons during one qubit gate cycle.

We consider a single electron in the double-well potential shown schematically in Fig. 1. Such a structure can be fabricated as two gate-engineered quantum dots [7-9], whose geometry is determined by the pattern of external metallic gates and electric potential at them, or by the coupling the two nearby phosphorus donors embedded in silicon [4]. The resulting qubit is supposed to evolve in the basis spanned by the states  $|0\rangle$  and  $|1\rangle$  which describe the electron localized around the left and right minima of the potential, respectively. We assume that the parameters of the double-dot qubit structure are selected appropriately and the temperature is low enough such that the effects of the electron transitions to the higher energy levels can be neglected. Investigation of decoherence due to acoustic phonons is the primary goal of our work. Below, we will present the model and describe the two main mechanisms of decoherence. We will introduce the appropriate approximations schemes, quantify the overall error rate, and discuss the ways to minimize it.

The Hamiltonian of the electron and the phonon bath is

$$H = H_e + H_p + H_{ep}. \quad (1)$$

Here qubit term in Hamiltonian is

$$H_e = -\frac{1}{2}\varepsilon_A(t)\sigma_x - \frac{1}{2}\varepsilon_P(t)\sigma_z, \quad (2)$$

where  $\sigma_x$  and  $\sigma_z$  are the Pauli matrices. The parameters  $\varepsilon_A$  and  $\varepsilon_P$  are controlled by the external metallic gates and can be used to perform on demand single-qubit rotations. These parameters determine the splitting  $\varepsilon$  between the ground state and the first excited state of the electron in the energy basis. This splitting is given by  $\varepsilon = \sqrt{\varepsilon_A^2 + \varepsilon_P^2}$ . The phonon term in the Hamiltonian is

$$H_p = \sum_{\mathbf{q},\lambda} \hbar s \mathbf{q} b_{\mathbf{q},\lambda}^\dagger b_{\mathbf{q},\lambda}, \quad (3)$$

where  $b_{\mathbf{q},\lambda}^\dagger$  and  $b_{\mathbf{q},\lambda}$  are the creation and annihilation operators of the phonons with the wave vector  $\mathbf{q}$  and polarization  $\lambda$ . For simplicity we consider isotropic acoustic phonons with the linear dispersion law. The electron-phonon interaction term is [12]

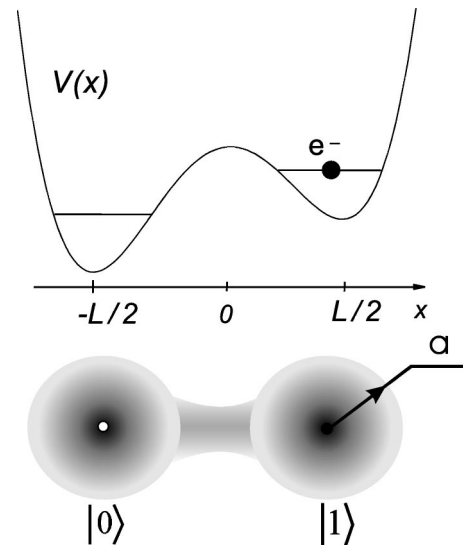


FIG. 1. Sketch of the qubit: single electron within double-well potential.

$$H_{ep} = \sum_{\mathbf{q},\lambda} \sigma_z (g_{\mathbf{q},\lambda} b_{\mathbf{q},\lambda}^\dagger + g_{\mathbf{q},\lambda}^* b_{\mathbf{q},\lambda}), \quad (4)$$

where  $g_{\mathbf{q},\lambda}$  is the coupling constant, which depends on the specific configuration of the system and the type of the interaction. Both the distance  $L$  between quantum-dots centers and their finite size  $a$  will cutoff the effect of the electron-phonon interaction at the tails of the phonon spectrum.

One can show that for the interaction of an electron bound in a gate-engineered Gaussian-shaped double dot with deformation phonons, the coupling constant is

$$g_{\mathbf{q}} = iq\Xi \left( \frac{\hbar}{2\rho q s V} \right)^{1/2} e^{-i\mathbf{q}\cdot\mathbf{R} - a^2 q^2/4} \sin(\mathbf{q} \cdot \mathbf{L}/2), \quad (5)$$

where  $\Xi$  is the deformation potential,  $s$  is the speed of sound,  $\rho$  is the density of the crystal,  $V$  is normalizing volume, and  $\mathbf{R}$  is the coordinate of the middle point of the double dot. For crystal structures with inversion symmetry, such as Si, there is no additional interaction due to the piezopotential. For crystals of the symmetry class  $T_d$ , such as GaAs, the piezoelectric phonon coupling is

$$g_{\mathbf{q},\lambda} = - \left( \frac{\hbar}{2\rho q s V} \right)^{1/2} M e^{-i\mathbf{q}\cdot\mathbf{R} - a^2 q^2/4} \times (\xi_1 e_2 e_3 + \xi_2 e_1 e_3 + \xi_3 e_1 e_2) \sin(\mathbf{q} \cdot \mathbf{L}/2), \quad (6)$$

where  $e_i = q_i/q$ ,  $\xi$  is the polarization vector, and  $M$  is the piezoconstant of the substrate.

For a double-donor system composed of two coupled hydrogen-like dopant impurity states, e.g., for two phosphorus atoms embedded in silicon, the following expression for the coupling constant with the deformation phonons was obtained

$$g_{\mathbf{q}} = iq\Xi \left( \frac{\hbar}{2\rho q s V} \right)^{1/2} \frac{e^{-i\mathbf{q}\cdot\mathbf{R}}}{(1 + a^2 q^2/4)^2} \sin(\mathbf{q} \cdot \mathbf{L}/2). \quad (7)$$

The interaction term (4) leads to decoherence of the qubit. The resulting loss of coherence is some functional of  $\varepsilon_A(t)$  and  $\varepsilon_P(t)$ . Here we consider two representative cases of the single-qubit gate functions and derive estimates for the error rate due to phonons. First, we consider the relaxation of an electron during the NOT gate ( $\sigma_x$ ), implemented by setting  $\varepsilon_A(t) = \varepsilon \equiv \text{const}$  and  $\varepsilon_P(t) = 0$  in the Hamiltonian (2), for the time interval (cycle time of the quantum computer)  $\Delta t = \pi\hbar/\varepsilon$ . Second, we consider the decoherence of an electron during the  $\pi$ -phase-rotation gate ( $\sigma_z$ ), implemented by setting  $\varepsilon_A(t) = 0$  and  $\varepsilon_P(t) = \varepsilon \equiv \text{const}$  for the same time interval  $\Delta t = \pi\hbar/\varepsilon$ .

To evaluate the relaxation of a double-dot qubit due to acoustic phonons, we will follow [3,10,13]. We assume that the temperature is low compared to energy gaps of the system. Therefore we consider the qubit at zero temperature. The major parameter of dots influencing the interaction with phonons is their size  $a$ . For gate-engineered quantum dots the actual shape of wave function of confined electron can vary. We consider Gaussian-shaped dots in which electron wave function is Gaussian ( $\Psi(\mathbf{r}) \sim \exp[-r^2/(2a^2)]$ ). With

these assumptions, the following result for the relaxation rate due to the interaction with deformation phonons can be obtained,

$$\Gamma_{DA} = \frac{\Xi^2 k^3}{4\pi\rho s^2 \hbar} \exp(-a^2 k^2/2) \left( 1 - \frac{\sin(kL)}{kL} \right), \quad (8)$$

where  $k = \varepsilon/(s\hbar)$  is the wave vector of the emitted phonon. For the piezoelectric type of interaction, we get

$$\Gamma_{PA} = \frac{M^2}{20\pi\rho s^2 \hbar L^5 k^4} \exp(-a^2 k^2/2) ((kL)^5 + 5kL[2(kL)^2 - 21]\cos(kL) + 15[7 - 3(kL)^2]\sin(kL)). \quad (9)$$

In double phosphorus dopant structures in silicon, the relaxation rate due to the deformation phonons for the hydrogen-like impurity states is

$$\Gamma_{IDA} = \frac{\Xi^2}{4\pi\rho s^2 \hbar} \frac{k^3}{(1 + a^2 k^2/4)^4} \left( 1 - \frac{\sin(kL)}{kL} \right). \quad (10)$$

If the wavelength of the phonon to be emitted is high enough compared to the size of dots,  $a$ , and the distance between the dots,  $L$ , i.e.,

$$ak \ll 1; \quad Lk \ll 1, \quad (11)$$

which is often the case in present-day heterostructures, then the following approximate expressions are valid:

$$\Gamma_{DA} = \Gamma_{IDA} = \frac{\Xi^2 L^2 \varepsilon^5}{24\pi\rho s^7 \hbar^6} \quad (12)$$

and

$$\Gamma_{PA} = \frac{M^2 L^2 \varepsilon^3}{120\pi\rho s^5 \hbar^4}. \quad (13)$$

Right after the implementation of the NOT gate the density matrix in the energy basis  $\{|+\rangle, |-\rangle\}$ , where  $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$ , will be [14]

$$\begin{pmatrix} 1 - \rho_{--}(0)e^{-\Gamma\Delta t} & \rho_{+-}(0)e^{-(\Gamma/2 - i\varepsilon/\hbar)\Delta t} \\ \rho_{-+}(0)e^{-(\Gamma/2 + i\varepsilon/\hbar)\Delta t} & \rho_{--}(0)e^{-\Gamma\Delta t} \end{pmatrix}, \quad (14)$$

where  $\rho_{\pm\pm}(0)$  are the elements of the electron density matrix before the implementation of the NOT gate and the parameter  $\Gamma$  should be taken from Eqs. (8) to (10), respectively.

We now consider the implementation of the phase gate. In this case, decoherence emerges as pure dephasing. There is no relaxation because the interaction term (4) commutes with the electron term in the Hamiltonian (2). The basis  $\{|0\rangle, |1\rangle\}$  coincides with the energy basis of the electron. For evaluation of the dephasing rate we used the general analytical expression for the density operator of the electron in the boson bath given in [15,16],

$$\rho = \begin{pmatrix} \rho_{00}(0) & \rho_{01}(0)e^{-B^2(\Delta t) + i\varepsilon\Delta t/\hbar} \\ \rho_{10}(0)e^{-B^2(\Delta t) - i\varepsilon\Delta t/\hbar} & \rho_{11}(0) \end{pmatrix}. \quad (15)$$

Thus, the evolution of the system is determined by the spectral function  $B(t)$  [15,17], which in our case is expressed as

$$B^2(t) = \frac{8}{\hbar^2} \sum_{\mathbf{q}, \lambda} \frac{|g_{\mathbf{q}, \lambda}|^2}{s^2 q^2} \sin^2 \frac{sqt}{2}. \quad (16)$$

By performing the summation in Eq. (16), we get the spectral functions determining the density matrices after the  $\pi$ -phase rotation of both the qubits made of double dots with deformation and piezoelectric electron-phonon interaction, and of double-impurity qubit states, respectively,

$$B_{DA}^2 = \frac{\Xi^2}{2\pi^2 \rho s^3 a^2 \hbar}, \quad (17)$$

$$B_{PA}^2 = \frac{M^2 L^2 \left[ 1 - \exp\left(-\frac{a^2 \pi^2}{2L^2}\right) + \frac{3a^2}{L^2} E_1\left(\frac{a^2 \pi^2}{2L^2}\right) \right]}{60\pi^2 \rho s^3 a^2 \hbar}, \quad (18)$$

$$B_{IDA}^2 = \frac{\Xi^2}{3\pi^2 \rho s^3 a^2 \hbar}. \quad (19)$$

Here  $E_1(z) = \int_z^\infty t^{-1} e^{-t} dt$ . Expressions (17)–(19) were obtained by using an additional observation that the duration of the qubit phase rotation is large compared to the phonon transit time  $\Delta t \gg a/s$ . This condition holds for the GaAs and Si structures considered.

To analyze the double-dot qubit architecture with respect to the fault-tolerant quantum computing criteria [18], one should be able to estimate the error generated during the “clock” time of the quantum computer  $\Delta t$ . To quantify the error due to decoherence, we use the approach of Ref. [19]. We consider the norm of the deviation operator  $\sigma$ ,

$$\sigma(t) = \rho(t) - \rho_{\text{ideal}}(t), \quad (20)$$

where the “ideal” evolution is defined as that at zero interaction with the environment,

$$\rho_{\text{ideal}}(t) = e^{-iH_e t/\hbar} \rho(0) e^{iH_e t/\hbar}. \quad (21)$$

The error is characterized [19] by the value

$$D(t) = \sup_{\rho(0)} (\|\sigma(t, \rho(0))\|_\lambda), \quad (22)$$

which is the maximal norm of the deviation operator over all the possible initial density operators of the electron  $\rho(0)$ . For fault-tolerant computation we need to satisfy the condition  $D(\Delta t) \leq O(10^{-4})$  [18]. For the density operators after the NOT and phase gates given by Eqs. (14) and (15), the corresponding errors  $D_A, D_P$  can be expressed in a compact and elegant form as

$$D_A(\Delta t) = 1 - e^{-\Gamma \Delta t}, \quad (23)$$

$$D_P(\Delta t) = \frac{1}{2}(1 - e^{-B^2(\Delta t)}). \quad (24)$$

To evaluate the single-gate error rate we take the maximum of the two gate errors considered which are typical single-qubit gates in quantum algorithms. The error rate per each step can be estimated as the largest of the above errors

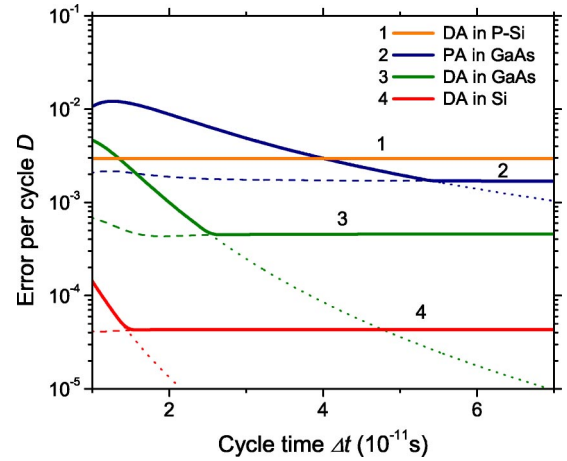


FIG. 2. Error rate estimate per cycle due to electron-phonon interaction as a function of the cycle time  $\Delta t (\Delta t = \pi \hbar / \epsilon)$ . The distance between the dot centers was  $L = 50$  nm for all the cases considered. For all the gate-engineered quantum dots, the effective radius was  $a = 25$  nm. The parameters for the GaAs dots were  $\Xi = 7$  eV,  $s = 5.14 \times 10^3$  m/s,  $\rho = 5.31$  g/cm<sup>3</sup>,  $M = ee_{14}/(\epsilon_0 \kappa)$ , where  $e_{14} = 0.16$  C/m<sup>2</sup>,  $\kappa = 12.8$  [20]. As in Ref. [13], for silicon the following parameters were used:  $a = 3$  nm for phosphorus impurity states, effective deformation potential  $\Xi = 3.3$  eV,  $s = 9.0 \times 10^3$  m/s,  $\rho = 2.33$  g/cm<sup>3</sup>. The results are shown as follows: (1) the double-donor structure in silicon; (2) decoherence in GaAs due to piezointeraction; (3) the contribution to decoherence due to deformation interaction in GaAs; (4) the gate-engineered dots in Si. The dashed lines denote  $D_A$ , the dotted lines denote  $D_P$ , and the solid lines are  $D$ . The relaxation rate for the double-donor structure in silicon is not seen because it is very small in the given range of times.

$$D(\Delta t) = \max(D_A(\Delta t), D_P(\Delta t)). \quad (25)$$

The obtained error rates for GaAs and Si quantum dots are shown in Fig. 2. It should be noted that dephasing appears to be the limiting factor of fault tolerance of this type of qubits. For a qubit made of impurity states, the corresponding spectral function (19) determining its dephasing rate is, in fact, material constant and cannot be changed significantly. Still, phonon decoherence can be reduced by the change of phonon spectrum with the help of phonon cavities [7,21]. Gate-engineered quantum dots show better coherence. Moreover, their performance can be improved because their geometric parameters are flexible.

In conclusion, we evaluated error rates in semiconductor charge qubits. The error rates were quantified by the maximal operator norm of qubit density matrix deviation. Our results show that the expected error rate due to acoustic phonons may be a major factor limiting qubit performance. For double-phosphorus impurity states in silicon it is of the order of the fault-tolerance threshold for quantum computation. Larger gate-engineered double quantum dots both in Si and GaAs, with parameters close to those in modern experiments [4,8,9], can be controlled more coherently. Realization

of those qubits would be a significant step toward the implementation of a full-scale solid-state quantum computer.

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