Quantum computing on long-lived donor states of Li in Si

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Abstract

We predict a gigantically long lifetime of the first excited state of an interstitial lithium donor in silicon. The nature of this effect roots in the anomalous level structure of the $1s$ Li manifold under external stress. Namely, the coupling between the lowest two states of the opposite parity is very weak and occurs via intervalley phonon transitions only. We propose to use these states under the controlled ac and dc stress to process quantum information. We find an unusual form of the elastic-dipole interaction between different donors. This interaction scales with the inter-donor distance $R$ as $R^{-3}$ or $R^{-5}$ for the transitions between the states of the same or opposite parity, respectively. The long-range $R^{-3}$ interaction provides a high fidelity mechanism for 2-qubit operations.

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A broad effort is currently underway to develop new techniques and systems for quantum information processing (QIP) that involves coherent manipulation and control of a large array of 2-level systems (qubits) for quantum storage and computing purposes. Implementation of the quantum computer (QC) as a solid-state device has a number of unique advantages related to scalability and the prospect of integration with state-of-the-art semiconductor device fabrication technology. One of the main challenges in developing a solid-state QC is the requirement of a relatively low qubit decoherence rate. The natural candidates in this respect are QC schemes based on spins as quantum bits, e.g. nuclear spins of $^{31}$P donors [1], or electron spins in semiconductor quantum dots [2]. While spins are relatively well isolated from the environment and characterized by long decoherence times, the implementation of the spin-based QC is complicated by a short-range character of exchange interaction. This provides additional difficulties to very challenging problems of a single spin measurement and control as well as nm-precision fabrication of a periodic qubit array. Additionally, the clock frequency for nuclear spin QC is relatively low. The optically enhanced RKKY mechanism for electron spin-exchange [3] in semiconductor quantum dots allows for greater inter-qubit distances, but it is not clear at present how to make this QC scheme scalable.

An interesting alternative to the spin-based qubits is provided by charge-based qubits formed by the two lowest states of a single-charged pair of quantum dots [4, 5], or donor atoms [6]. Those systems do not depend on the single-spin readout and rely on a long-range electric-dipole interaction between the qubits for performing quantum logic operations. The QC scheme proposed in [7] uses acceptors in silicon to encode qubits with a decoherence rate $\sim$ 1 KHz and relies on a long-range elastic-dipole interaction between qubits ($\sim R^{-3}$). A serious source of decoherence in all charge-based qubits is due to charge fluctuations in the surrounding environment [8]. In particular, relaxation of the charge traps can produce a shot noise signal leading to decoherence times that are significantly shorter than that in the spin-based QC [6].

In this Letter we exploit the multivalley nature of the Si conduction band and anomalous structure of the ground state of an interstitial Li donor to demonstrate that under certain conditions the first excited state of the single Li donor can have a lifetime comparable to that of a nuclear spin (in access of 1 sec). The two lowest $1s$ states of the Li donor in Si can be used to encode the qubit that is extremely well isolated from the electromagnetic fluctuations of the surrounding.
The conduction band of Si has six valley minima $\mathbf{k}$, located along six equivalent directions, $[\hat{x}, -\hat{x}, \hat{y}, -\hat{y}, \hat{z}, -\hat{z}]$ at about 85% of the distance $2\pi/a_{\text{Si}}$ to the Brillouin zone boundary (here $a_{\text{Si}}$ is a lattice constant for Si). In the framework of the effective mass theory (EMT) the ground state of a shallow donor electron is 6-fold degenerate. The valley-orbit interaction removes the degeneracy and gives rise to the splitting of the donor levels $\delta$. Excited states within the ground-state manifold are produced by splitting of the $1s$ hydrogenic energy levels and decay predominantly via emission of acoustic phonons. The donor electron wave function can be written in the standard form $|\Psi^\mu\rangle = \sum_{|j|=1}^3 \alpha_j^\mu \sum_{\mathbf{k},\mathbf{G}} A^j_{\mathbf{k}+\mathbf{G}} |\mathbf{k}\rangle$. Here $\mathbf{k}$ is a wave vector in the first Brillouin zone, $\mathbf{G}$ is a reciprocal lattice vector, $|\mathbf{k}\rangle$ are the Bloch functions and index $\mu$ labels the irreducible representations of the point group $T_d$ that are characterized by the coefficients $\alpha_j^\mu$. Also, $A^j_{\mathbf{k}}$ are the hydrogenic envelope functions in $k$–space that are strongly localized in the vicinity of the corresponding valley center $\mathbf{k}_j$ and the summation above is taken over all valleys $j = \pm 1, \pm 2, \pm 3$.

We now consider the acoustic phonon driven transition rate from a state $|\Psi^\mu\rangle$ to $|\Psi'^\mu\rangle$: $W_{\mu\mu'} = 2\pi/\hbar^2 \sum_{\mathbf{q},\nu} |V_{\mu\mu'}(\mathbf{q}\nu)|^2 \delta(\omega_{\mu'\mu} - \Omega_{\mathbf{q}\nu})$, where $\hbar \omega_{\mu'\mu}$ is the change in the donor energy during the transition, $\Omega_{\mathbf{q}\nu}$ is the frequency of an acoustic phonon mode $\nu$ with the wavevector $\mathbf{q}$, and $V_{\mu\mu'}(\mathbf{q}\nu)$ are the matrix elements of the electron-phonon interaction Hamiltonian, $\langle \Psi^\mu|H_{\text{el-ph}}|\Psi'^\mu\rangle = \sum_{\mathbf{q},\nu} V_{\mu\mu'}(\mathbf{q}\nu)(b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu})$, where

$$V_{\mathbf{q}\nu}^{\mu\mu'} = \sum_{|i|,|j|=1}^3 \alpha_i^{\mu*} \alpha_j^{\mu'} \sum_{\mathbf{k},\mathbf{G}} A^i_{\mathbf{k}} A^j_{\mathbf{k}+\mathbf{q}+\mathbf{G}} \mathcal{M}_{\mathbf{k}\mathbf{q}\nu}. \tag{1}$$

Here $\mathcal{M}_{\mathbf{k}\mathbf{q}\nu}$ is the matrix element of $H_{\text{el-ph}}$ between the Bloch functions $|\mathbf{k}\rangle$ and $|\mathbf{k}+\mathbf{q}\rangle$.

For the long-wavelength acoustic phonons, with $q \ll |\mathbf{k}_i - \mathbf{k}_j|$, the dominant contribution to (1) comes from the *intravalley* terms with $i = j$. The only other important terms correspond to the *intervalley umklapp* processes between the valleys $j$ and $-j$ centered at the band minima $\mathbf{k}_j$ and $\mathbf{k}'_{-j} = -\mathbf{k}_j + \mathbf{G}_j$, where $\mathbf{k}_{-j} = -\mathbf{k}_j$, $\mathbf{G}_j = (4\pi/a_{\text{Si}})\hat{k}_j$, and $\hat{k}_j = \mathbf{k}_j/k_j$. The points $\mathbf{k}_j$ and $\mathbf{k}'_{-j}$ lie on the opposite sides of the Brillouin zone boundary and correspond to the closest possible intervalley separation $\kappa_0 = 0.6\pi/a_{\text{Si}}$. All the other intervalley ($i \neq j$) and umklapp terms ($\mathbf{G} \neq 0$) are much smaller, since they are proportional to the overlap of the envelope functions from much farther separated valleys. For both the intravalley and intervalley ($j \to -j$) umklapp processes the sum over $\mathbf{k}$ in Eq. (1) is dominated by the small
vicinity of the valley centers, where \( \mathcal{M}_{\pm k, qv} \equiv M^i_{qv} \), and

\[
M^i_{qv} = \left( \frac{\hbar}{2 \rho V \Omega_{qv}} \right)^{1/2} \left[ \Xi_u (\hat{k}_j \cdot q) (\hat{k}_j \cdot \hat{e}_{qv}) + \Xi_d (q \cdot \hat{e}_{qv}) \right].
\]

Here \( \Xi_u \) and \( \Xi_d \) are the deformation potential constants, \( \hat{e}_{qv} \) is the polarization vector of a phonon mode \( qv \), \( \rho \) and \( V \) are the mass density and volume of the crystal, respectively. Finally, we obtain

\[
V^\mu\mu'_{qv} = \sum_{|j|=1}^{3} \sum_k M^i_{qv} \alpha_j^{\mu*} A_k^j \left[ \alpha_j^{\mu} A_k^j + \alpha_j^{\mu'} A_{-j}^k \right],
\]

The EMT donor eigenfunctions \( \Psi^\mu(r) \) have a certain parity which is equal to the parity of the multiples \( \alpha_j^{\mu} A_k^j \) under the operation \( k_j \rightarrow -k_j \). For example, the parity is even for the \( s \)-type singlet or doublet donor states belonging to the irreducible representations \( A_1 \) or \( E \), but it is odd for \( s \)-type triplet states belonging to \( T_2 \) etc. In the limit of small \( q \) the intervalley processes described by the second term in Eq. (3) give rather small contribution and presumably can be neglected. Then, as it follows from Eq. (2) and (3), the matrix elements between the states of the opposite parity, \( V^\mu\mu'_{qv} = 0 \), due to the cancellation of the intravally \( j \) and \( -j \) terms. Based on this observation one can expect that the probabilities of the even-odd transitions involving long-wave acoustic phonons are much smaller than those of the same parity transitions. Analogous symmetry arguments explain a strong suppression of the \( 1s(A_1) \rightarrow 1s(T_2) \) Raman transition in silicon donors \[11\]. One can also show that if the intervalley processes in (3) are neglected the transitions between the opposite-parity donor states are forbidden in all orders in \( V^\mu\mu'_{qv} \).

We now consider implications of this effect for the lithium donor in silicon. Li is an interstitial impurity with the \( T_d \)-site symmetry. It has an anomalous fivefold degenerate \( 1s(E + T_2) \) ground state while the fully symmetric state \( 1s(A_1) \) lies above, with the splitting between the states conventionally denoted as \( 6\Delta_c = 1.76 \) meV \[12\]. If a uniaxial compressive stress \( F_z \) is applied along the \( \langle 001 \rangle \) direction the site symmetry is reduced from \( T_d \) to \( D_{2d} \) and has a distinct mirror-rotation axis \( \hat{k}_3 \). Then the ground state level is split into three levels as shown in Fig. \[12, 13\]. The new ground state denoted as \( |0\rangle \) has an odd parity with the coefficients \( \alpha_j^{(0)} = (0, 0, 0, 0, 1, -1)/\sqrt{2} \). The first excited state, \( |1\rangle \), is a singlet, it has an even parity, \( \alpha_j^{(1)} = (b, b, b, a, a) \) where \( a = a(\varepsilon), b = b(\varepsilon) \). At small magnitude of the applied stress \( |F_z| \) one has \[13\]: \( a = (6 + \varepsilon)/6\sqrt{3}, b = (3 - \varepsilon)/6\sqrt{3} \), where

\[
\varepsilon = \Xi_u (s_{11} - s_{12}) F_z / 3 \Delta_c,
\]

\[4\]
and $s_{11}, s_{12}$ are elastic compliance constants. The second excited energy level is a triplet, it consists of an even parity state, $|2\rangle$, with $\alpha_j^{(2)} = \frac{1}{2}(1, 1, -1, -1, 0, 0)$ and two odd parity states.

From the above it follows that only the second term in Eq. (3) with $i = -j = \pm 3$ contributes to the phonon decay rate $W_{10}$ of the state $|1\rangle$. The decay rate calculated with the Kohn-Luttinger envelope functions $A^j_k$ reads

$$W_{10} \equiv \tau_{10}^{-1} = \frac{2}{35} \frac{a^2(\varepsilon)(a_\|\kappa_0)^2}{[1 + (a_\|\kappa_0/2)]^6} \frac{\Xi^2_\|\omega_{10}a_\|^2}{\pi \hbar u_t^4}.$$  

(5)

Here $u_t$ is the transverse speed of sound, $a_\|$ is the longitudinal Bohr radius for the $1s$ donor state in Si, and we assumed that $2\pi u_t/\omega_{10} \gg a_\|$. We emphasize a very fast decrease of the transition rate between the opposite parity states with the level separation, $W_{10} \propto \omega_{01}^5$. This is in contrast with the conventional dependence of the transition rate between the same parity states \[7, 14\]. For instance, $W_{21} \propto \omega_{21}^3$ for the transition $|2\rangle \rightarrow |1\rangle$. We note that the decay rate $\propto \omega^5$ was found in \[14\] for the electron transition in a singly-charged double-dot system between the antisymmetric excited state and symmetric ground state separated by the energy gap $\hbar\omega$. However, a key distinction of the expression (5) from the results of Ref. \[14\] is that it contains an additional small factor, $8a^2(\varepsilon)/35(a_\|\kappa_0/2)10 \approx 10^{-5}$, due to the overlap of the envelope functions from different valleys. It is the combination of these two small factors in (5) that gives rise to the giant lifetime of the state $|1\rangle$ at the low stress values (see Fig. 1). This is one of the central results of this work.

In addition to the energy decay there also exist the dephasing processes \[7\] due to quasi-elastic phonon scattering off donors. Detailed analysis shows that these are not important at low temperatures. For example, for $H_{el-ph}$ given by Eq. (3) the dephasing rate $\tilde{W}_{10} = \nu_0(T/T_0)^{11}$, with $\nu_0 \sim 2 \cdot 10^{14}$ Hz and $T_0 = \hbar u_t/a_\perp = 19$ K. Thus at $T=0.1$ K the dephasing rate is negligibly small. Finally, the dipole moment of $|0\rangle-|1\rangle$ transition is less then $10^{-3} e\AA$ and therefore its quantum phase is very robust against the charge noise.

The fact that electronic states of a Si:Li donor are extremely well-isolated from the environment provides an interesting possibility to consider this system for quantum information processing with a pair of states $|0\rangle, |1\rangle$ used to encode a qubit. In what follows we make use of the fact that by varying the local pressure $F_z$ on a given qubit one can change the frequencies $\omega_{\mu\mu'}$ and therefore lifetimes $\tau_{\mu\mu'}$ of the corresponding transitions. As seen in Fig. 1 there is a dramatic difference between the lifetimes of the even-odd and same-parity
operator $\hat{S}$ acting upon the qubit states $|0\rangle \equiv |\downarrow\rangle$ and $|1\rangle \equiv |\uparrow\rangle$. One can also apply a low-amplitude periodically modulated stress pulse $A_{\langle 001 \rangle} \cos \omega_{10} t$ of duration $\tau_{ac}$ in $\langle 001 \rangle$ direction. This pulse will resonantly drive the transition $|0\rangle \rightarrow |1\rangle$ of a given qubit. It will produce a pseudo-spin rotation around $x$-axis, $\hat{X}(\varphi) \equiv \exp[i \varphi \hat{S}_x / 2]$, $\varphi \equiv 2 \tau_1 \Omega_x$. An estimate for $\Omega_x$ in the rotating wave approximation gives

$$\Omega_x = \frac{128 A_{\langle 001 \rangle} \omega_{10} s_{11}}{u_1 \sqrt{6}} (\Xi_u + \Xi_d) \kappa_0 a^2. \quad (6)$$
Here \( u_t \) is the longitudinal speed of sound). With a modest ac stress amplitude \( A_{(001)} \simeq 10^5 \) dyn/cm\(^2\) and a driving frequency \( \omega_{10}/2\pi=10 \) GHz one gets \( \Omega_x/2\pi \simeq 630 \) MHz. Then the \( \pi \)-pulse \( \dot{X}(\pi) \) will have a duration \( \tau_1 \simeq 0.4 \) ns and a corresponding decoherence-induced error \( \sim \tau_1 W_{10} \) will be less then \( 10^{-9} \).

Another controlling option consists in applying pulses of the time-dependent electric field \( \mathbf{E}(t)||\langle 001 \rangle \) caused by the modulation of a bias voltage between the local electrodes (\( A, B \) in Fig. 3). The electric field will produce a quadratic Stark shift of \( \omega_{10} \) and will induce the Rabi oscillations between the qubit states \( |0\rangle \) and \( |1\rangle \) via the virtual transitions through the \( 2p_0 \) state. For an electric field amplitude \( E \sim 10^3 \) V/cm the period of the Rabi oscillations \( \tau_1 \propto E^{-2} \) is of the order of \( 0.1 \) ns.

Li donors in Si are coupled to each other via acoustic phonon field and behave as elastic dipoles. As in the case of the shallow acceptors in Si [7], this coupling can be used as a “data bus” to implement two-qubit logic gates. The matrix elements of the phonon-mediated coupling Hamiltonian, \( H_{ij} = \sum |\mu_i\mu_j\rangle G^{ij}_{\mu_i\mu'_i,\mu_j\mu'_j} \langle \mu'_i\mu'_j| + h.c. \), between a pair of donors at the sites \( \mathbf{R}_i \) and \( \mathbf{R}_j \) can be expressed as follows:

\[
G^{ij}_{\mu_i,\mu'_i,\mu_j,\mu'_j} = \frac{1}{\hbar} \sum_{q\nu} V^{\mu_i\mu'_i}_{q\nu} \left( V^{\nu_j\mu'_j}_{q\nu} \right)^* \frac{e^{i q (\mathbf{R}_i-\mathbf{R}_j)}}{\Omega_{q\nu}},
\]

where we assumed that \( \omega_{\mu\mu'}|\mathbf{R}_i-\mathbf{R}_j|/u_t \ll 1 \).

Consider first a resonant excitation transfer (RET) between donors \( i \) and \( j \) involving a pair of transitions, \( \mu \rightarrow \mu' \) on site \( i \) and \( \mu' \rightarrow \mu \) on site \( j \), that are in resonance with each other. The coupling constant corresponding to this process \( \hbar g^{ij}_{\mu\mu'} = G^{ij}_{\mu\mu',\mu'\mu} \). For the RET involving the even-odd transitions \( |0\rangle \leftrightarrow |1\rangle \) this coupling constant reads

\[
\frac{g^{10}_{ij}}{W_{10}} = \frac{315}{16} \left( 3 - \frac{u_t^2}{u_l^2} \right) \cdot \left( 4\sigma + 5 \right) \cdot \left( \frac{u_t}{\omega_{10} R_{ij}} \right)^5.
\]

Here \( \sigma = \Xi_d/\Xi_u \) and we assumed that \( \mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j \) lies in the plane normal to \( \langle 001 \rangle \). We note an unusually steep falloff of the coupling constant with the donor-donor separation. In fact, one can show that if the RET involves transitions between the states of the same parity, a conventional dependence \( g_{ij} \propto 1/R_{ij}^3 \) is recovered. In particular, the RET coupling constant for the \( |1\rangle \leftrightarrow |2\rangle \) transition in Si:Li is

\[
\frac{g^{21}_{ij}}{W_{21}} = \gamma (u_t/\omega_{21} R_{ij})^3
\]

where \( \gamma = (5/16)(2 + 7(1 - u_t^2/u_l^2)) \simeq 2.0 \). This long-range dipole interaction is due to the intravalley terms in \( V^{21}_{q\nu} \) that are absent in \( V^{10}_{q\nu} \). It can be used to selectively generate an
entanglement between two donors by tuning their energy levels into resonance with each other.

Consider now a diagonal part of the phonon-mediated donor-donor Hamiltonian generated by the diagonal matrix elements $V_{qq'}^{\mu\nu}$ in Eq. (7). This is an Ising-type dipole-dipole interaction resulting from the dependence of a polaron shift in the electron energy of a given donor on the electron states of the neighboring donors. The effective interaction Hamiltonian projected onto the states $\mu = 0, 1$ of $N$ donors located at $\mathbf{R}_j$ has the form:

$$H(t) = \frac{\hbar}{2} \sum_{i \neq j=1}^{N} [J_{ij}\hat{S}_iz\hat{S}_{jz} + g_{ij}\hat{S}_i^+\hat{S}_j^- + h.c.] + \sum_{j=1}^{N} H_j(t).$$  \hfill (10)

Here $\hat{S}_i^+$ and $\hat{S}_i^-$ are raising and lowering pseudo-spin operators for $j$th qubit, $H_j(t)$ is a single-qubit Hamiltonian, $g_{ij} \equiv g_{10}^{ij}$, and the Ising-exchange coupling constant $\hbar J_{ij} = G_{11,11}^{ij} + G_{00,00}^{ij} - 2G_{00,11}^{ij}$. Due to the symmetry of the problem, $J_{ij}$ does not depend on the in-plane orientation of $\mathbf{R}_{ij} \perp \langle 001 \rangle$. Using (2), (3), (7) and the form of the valley-orbit coefficients one can obtain

$$J_{ij} = \frac{\Xi^2}{32\pi\hbar\rho u_t^2 R_{ij}^3} \left(-1 + \frac{5}{3} \frac{u_r^2}{u_t^2}\right).$$  \hfill (11)

Here the $1/R_{ij}^3$ law is also due to the intravalley terms that are always present in the diagonal matrix elements $V_{qq'}^{\mu\nu}$. For $R_{ij} = 100$nm, $J_{ij}/\pi \simeq 10$ MHz while $g_{ij}/\pi = 0.4$ Hz. Because of the detuning of the donor transitions from resonance the RET frequency at $|0\rangle \rightarrow |1\rangle$ transition is further reduced and can always be neglected. Contrary to that, the dipole interaction in $H(t)$ always persists. It is a basic long-range 2-qubit interaction in the liquid-state NMR and also in the solid-state QC scheme based on magnetic-dipole coupling of donor spins in silicon [15]. The Hamiltonian (10) with $g_{ij} = 0$ is sufficient to execute any one- or two-qubit gates [15]. It serves as a basis of our QC scheme.

The QC scheme utilizing Ising-type dipole coupling has been described in Ref. [15]. It is based on the refocusing technique where an auxiliary set of $\pi$ pulses is applied to a group of qubits $j = 1 : n$. The $\pi$-pulses cancel the dipole interaction terms in (10) for all members of this group except for a selected pair of neighboring qubits. The error of two-qubit gates, caused by the non-exact cancellation, $p \sim (\tau_1/\tau_2)^6$ [15], where $\tau_1$ and $\tau_2 = \pi/J_{j,j+1}$ are characteristic time scales for one- and two-qubit gates, respectively. For $R_{j,j+1} = 100$ nm $\tau_2 = 10^{-7}$s and $\tau_1 \lesssim 10$ ns one has $p < 10^{-6}$. The error of two-qubit gates due to the
phonon-decay of the state $|1\rangle$ is extremely small. The corresponding quality factor $q$ for the two-qubit gate

$$q \equiv \frac{1}{\tau_2 W_{10}} = \frac{35 [1 + (a_{\parallel}\kappa_0/2)^2]^6}{64\pi a^2(\varepsilon)} \frac{u_2^5 (-1 + 5/3 (u_t/u_l)^2)}{(a\kappa_0)^2 R_{ij+1}^3 \omega_{10}^5 a_{\parallel}^2},$$

(12)
is probably greater then $10^7$ at $\omega_{10}=0.06$ meV/\(\hbar\).

We note that a frequency of resonant ac stress modulation $\omega \simeq \omega_{10}$ is typically limited by a high-frequency cutoff of the response function of a nano-scale piezoelectric transducer (cf. Fig. 3). One can show that for practically feasible cases this implies $\omega_{10} \lesssim 10^{10}$ rad/s. However one could keep the qubit energy difference at much higher levels, $\omega_{10} \simeq 10^{11}$ rad/s (0.1-0.06 meV), at all times, except the short time intervals when a given qubit is involved in a gate operation. Then the energy difference can be adiabatically reduced the smaller value $\omega_{10} \lesssim 10^{10}$ rad/s. If the time between gates involving a given qubit is $\gg W_{10}^{-1}$ the qubit energy levels will not be thermally repopulated and the working temperature of a quantum computer can be set to $T^* \simeq h\omega_{10}/k_B \simeq 50$-100 mK.

Similarly, one can use the adiabatic stress reduction in the alternative three-level QC scheme where a long-range RET, based on the donor transition $1 - 2$ (see above) with Rabi frequency $g_{21}^{ij}$ (Eq. 9), is used to execute 2-qubit gates. This process provides the most direct tool to generate entangled states $c|1_j0_{j+1}\rangle + c'|0_j1_{j+1}\rangle$ between a given pair of neighboring donors ($j, j+1$) whose energy levels are brought into resonance using locally applied stress pulses. To achieve high-fidelity 2-qubit gates within this scheme we need much smaller interlevel separation $h\omega_{21}$ than $h\omega_{21} = 0.12$ meV at $\varepsilon = 0.2$. Therefore whenever we need to execute a 2-qubit gate we will adiabatically reduce the stress $\varepsilon(t)$ from $\varepsilon_0 = 0.2$ to $\varepsilon_2 \simeq 0.002$ ($F_z \sim 1.3 \cdot 10^5$ dyn/cm$^2$) which will set the transition frequency to $\omega_{21}/2\pi \simeq 0.24$ GHz.

Within the three-level scheme the Rabi frequency $g_{21}^{i,i+1}$ defines the QC clock frequency. In analogy to the above we define the quality factor $q$ as the ratio of $g_{21}^{i,i+1}$ to the phonon decay rate of the state $|2\rangle$ at the finite temperature $T^*$:

$$q = \frac{g_{21}^{i,i+1}}{[n_{21}(T^*) + 1] W_{21}} = \frac{\gamma}{n_{21}(T^*) + 1} \left( \frac{u_t}{\omega_{21} R} \right)^3,$$

(13)

where $R \equiv R_{i,i+1}$ and $n_{21}(T^*) = [\exp(h\omega_{21}/k_B T^*) - 1]^{-1}$ is the Planck’s distribution function. Consider a particular example with $R = 50$ nm, $\varepsilon = 2 \cdot 10^{-3}$, and $T^* = 100$ mK. In this case the characteristic time for a 2-qubit gate, $2\pi/g_{12} \simeq 0.2$ µsec, is much shorter than the
FIG. 2: Quality factor for the 3-level quantum computing scheme: dependence of the operational temperature $T^\ast$ on the inter-qubit distance $R$ for different values of the quality factor $q$ and $F_z = 1.3 \cdot 10^5\text{dyn/cm}^2$ ($\hbar \omega_{12} = 0.001\text{ meV}$)

relaxation time $\tau_{21} \simeq 3\text{ msec}$ and therefore the donor electron levels will not be thermally repopulated during RET despite $k_B T^\ast/\hbar \omega_{12} \simeq 8$. As soon as the two-qubit gate is executed the qubits will be adiabatically returned into their high-stress state. With this choice of parameters the QC clock frequency is $g_{21}/2\pi \simeq 5.2\text{ MHz}$ and the quality factor of a 2-qubit gate $g_{21}/W_{21} \sim 10^5$. Solving Eq. (13) for $T^\ast$ we obtain the operational temperature as a function of desired quality factor $q$ and inter-qubit separation $R$:

$$T^\ast = -\hbar \omega_{21}/3k_B \ln \left(1 - \frac{q}{3\gamma} \cdot \frac{\omega_{21} R}{u_t}\right).$$ (14)

By lowering the operational temperature $T^\ast < 100\text{ mK}$ we can significantly increase the quality factor or/and increase the inter-qubit separation $R$ as shown in Fig. 2.

By varying the locally applied stress $F_z$ and voltage on the local electrodes (see Fig. 3) one can selectively shift the $1s(E + T_2) \rightarrow 2p_0$ transition frequencies of a given donor atom by $\hbar \Delta \omega \sim 0.3\text{ meV}$ without significantly affecting the qubit level separation $\hbar \omega_{10}$.

Then the donor excitation lines $1s(E + T_2) \rightarrow 2p_0$ can be selectively brought into resonance with a globally applied infrared radiation field since their homogeneous broadening ($\simeq 55\text{ MHz}$) is $\sim 500$ times smaller than the frequency shift $\Delta \omega$. Such a selective resonant excitation can
be used to perform a measurement of the qubit state. Indeed, according to the polarization selection rules [13], a linearly polarized electric field $\mathbf{E} \perp \mathbf{F}$ will resonantly excite the transitions from the state $|1\rangle$ to the states of the $2p_0$ manifold but will not affect the donor electron that was in the state $|0\rangle$ before the IR pulse arrived. Detection of the dipole moment of this state ($\sim 40 \text{ Å}e$) by means of a single electron transistor (SET) measurement will determine whether the state $|1\rangle$ was occupied prior to the excitation. The fabrication of the Si:Li QC.

FIG. 3: Schematic of the Si:Li-based quantum computer. An etched piezoceramic structure (blue), which is placed on the top Si layer (green), has a row of columns of a width $w \sim 20 \text{ nm}$ separated by arches. The columns are used to generate a local $\langle 001 \rangle$ pressure, controlled by the voltage biases between the pairs of $B$-$C$ electrodes. The decay factor of the local stress (and electric) field over the interqubit distance $d \sim 100 \text{ nm}$ is $\sim (w/2d)^2 = 10^{-2}$ [17]. The residual stress and electric field at each Li donor arising from the local control of the neighboring qubits can be compensated by the synchronized adjustment of voltages for all qubits.

will utilize very large electro-mobilities of Li ions in Si (at $T=400\text{K}$ and $E=10^6\text{V/cm}$ the drift velocity is 0.4 cm/s). By controlling the electric field between the electrodes $A$ and $B$ (Fig. 3) the Li ions, sequentially deposited on the surface of a super-pure Si layer (positions 1), will be dragged to their target positions 2 to form a subsurface array with the period $d \sim 100\text{nm}$. Subsequent lowering of the temperature to its operational value $T \sim 50$-100 mK will form a stable regular array of the neutral Li donors.

In conclusion, we have shown that the valley-orbit structure of the ground and first excited
states of the Si:Li donor gives rise to a gigantic lifetime of the excited state. We have found that the elastic dipole coupling between two donors scales with the inter-donor distance \( R \) as either \( 1/R^3 \) or \( 1/R^5 \), depending on their electronic states. We build on these findings and propose a QC scheme with the spinless stress-defined elastically coupled qubits. It is characterized by extremely small error rate (lesser then \( 10^{-6} \)), relatively large operational temperatures and interqubit separations that are 5 to 10 times greater then those used in the nuclear spin solid state QC.

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