In this corrigendum to the paper by Livadaru et al (2010 New J. Phys. 12 083018) we point out an omission in one of the equations describing the decoherence analysis for silicon dangling bond qubit systems due to electron–phonon interactions. We also provide a corrected version of the equation and of the subsequent calculations and results in the paper and discuss the implications for the overall decoherence rate in DB charge qubits.

The omission of a factor of $c_s$, in the denominator of equation (23) was found. Thus, the correct form of the rate of acoustic phonon emission is

$$\Gamma_{c \rightarrow \text{ph}} = \frac{64D^2q^3\sin^2 \theta n_B(E, \Theta) + 1}{\pi \rho \hbar c_s^3 [(q \Delta)^2 + 4]} \left( 1 - \frac{\sin qd}{qd} \right),$$

where $c_s$ is the longitudinal sound velocity in silicon, $\rho$ is the density, $D$ is the deformation potential, $d$ is the dot separation, $q$ the phonon wavevector, $E$ the phonon energy, $a_B$ the renormalized Bohr radius, $\Theta$ the lattice temperature, $n_B$ the Bose occupation distribution, and $\theta = \tan^{-1}(0.5 \Delta / \varepsilon)$, with $\Delta$ and $\varepsilon$ the tunnel splitting and the applied bias on the qubit. We also corrected the value of $\rho$ used in our initial calculation.

In figure 1 we plot the corrected decoherence rate as a function of intra-qubit dot separation together with the bare tunneling rates of the qubit and the decoherence rate due to the Johnson–Nyquist voltage fluctuations. For DB separations of 3.84 Å and 7.68 Å, the tunneling rates (4.67 $\times$ 10$^{14}$ s$^{-1}$ and 1.33 $\times$ 10$^{14}$ s$^{-1}$, respectively) are denoted by circles, and tunneling rates for greater DB separations are calculated by the Wentzel–Kramers–Brillouin (WKB) method. The chosen values of inter-dot separation correspond to allowed DB–DB spacing on the H–Si(100)2 × 1 surface. Dashed lines joining different inter-dot separations facilitate direct comparison.

The most important consequence of this correction for our DB qubit is that the above decoherence rate $\Gamma_{c \rightarrow \text{ph}}$ is much lower than previously calculated and no longer the dominant rate. In fact, for separation less than 20 Å, $\Gamma_{c \rightarrow \text{ph}}$ is less than 10$^6$ s$^{-1}$, namely \{3.12, 3.70, 4.48, 5.47, 8.25\} $\times$ 10$^5$ s$^{-1}$, respectively for separations of \{3.84, 7.68, 11.52, 15.36, 19.20\} Å. These rates are calculated for $T = 4$ K, but the results are very weakly varying with temperature and are virtually unchanged at 77 K and just 5% higher at 300 K. Thus, in the absence of control and readout apparatus and other environmental perturbations, the $T_1$ times for the above separations are \{3.20, 2.70, 2.22, 1.83, 1.21\} $\times$ 10$^{-6}$ s.

Here, as in the original paper, s$^{-1}$ is shorthand for rad s$^{-1}$. 

© 2017 IOP Publishing Ltd and Deutsche Physikalische Gesellschaft
We also need to correct a typo in equation (11) giving the expression of decoherence rates due to Johnson–Nyquist noise. The denominator in the last fraction there should have been $\frac{E_k}{Q e}$ instead of $\frac{E_k}{e}$, so the correct formula is

$$\Gamma_{\text{JN}} = \frac{1}{2} \frac{\sqrt{\pi} \hbar \Delta^2}{1 + \frac{\hbar c \beta}{\sqrt{E_k} k T}} \exp\left(\frac{E_k}{\sqrt{E_k} k T}\right).$$

(2)

Our original calculations were not affected by this typo, as the correct formula was used to generate the original results.

The corrected $\Gamma_{\text{e-ph}}$ rates are much lower than the decoherence rates due to Johnson–Nyquist noise in the electrodes, $\Gamma_{\text{JN}}$. Thus, in a regime of interest, $d < 16 \, \text{Å}$, we now identify $\Gamma_{\text{JN}}$ as the dominant decoherence rate with values of $1.30 \times 10^8 \, \text{s}^{-1}$ at $T = 1 \, \text{K}$, $5.24 \times 10^8 \, \text{s}^{-1}$ at $T = 4 \, \text{K}$, and $1.00 \times 10^9 \, \text{s}^{-1}$ at $T = 77 \, \text{K}$. Furthermore, $\Gamma_{\text{JN}}$ decreases with increasing separation (see figure 1). We stress that the essential fact for our DB qubit is that, at low $T$, decoherence still occurs over several nanoseconds whereas the tunneling period for the DB–DB pair with a few Å separation is close to 10 fs, which enables many coherent qubit oscillations before decoherence sets in.

The consequences of this correction for quantum computing gates using DB qubits are as follows. The overall decoherence rates in the presence of control electrodes have not changed significantly, yielding error probabilities of the order of $10^{-6}$ for the single-qubit gate and $10^{-5}$ for two-qubit gate, at low $T$. These are well within the tolerance required by standard quantum error correction protocols.

**Acknowledgments**

This project has been supported by NRC, NSERC, AITF, QuantumWorks, iCORE. PX acknowledges support from the Natural Science Foundation of China (Grant Nos. 11474049 and 11674056) and the Natural Science Foundation of Jiangsu Province (Grant No. BK20160024).

**ORCID iDs**

Barry C Sanders https://orcid.org/0000-0002-8326-8912
Dangling-bond charge qubit on a silicon surface

To cite this article: Lucian Livadaru et al 2010 New J. Phys. 12 083018

View the article online for updates and enhancements.

Related content
- Tutorial
  Veronica Cerletti, W A Coish, Oliver Gywat et al.
- Time-dependent single-electron transport
  Toshimasa Fujisawa, Toshiaki Hayashi and Satoshi Sasaki
- Group IV solid state proposals for quantum computation
  P S Fodor and J Levy

Recent citations
- Toward multimodal inquiry: opportunities, challenges and implications of multimodality for research and scholarship
  Ioana Literat et al
- Atomic White-Out: Enabling Atomic Circuity through Mechanically Induced Bonding of Single Hydrogen Atoms to a Silicon Surface
  Taleana Rochelle Huff et al
- Two-probe STM experiments at the atomic level
  Marek Kolmer et al
Dangling-bond charge qubit on a silicon surface

Lucian Livadaru\textsuperscript{1,2,5}, Peng Xue\textsuperscript{3,4}, Zahra Shaterzadeh-Yazdi\textsuperscript{3}, Gino A DiLabio\textsuperscript{1}, Josh Mutus\textsuperscript{2}, Jason L Pitters\textsuperscript{1}, Barry C Sanders\textsuperscript{3} and Robert A Wolkow\textsuperscript{1,2}

\textsuperscript{1} National Institute for Nanotechnology, National Research Council of Canada, Edmonton, Alberta, T6G 2M9, Canada
\textsuperscript{2} Department of Physics, University of Alberta, Edmonton, Alberta, T6G 2J1, Canada
\textsuperscript{3} Institute for Quantum Information Science, University of Calgary, Alberta, T2N 1N4, Canada
\textsuperscript{4} Department of Physics, Southeast University, Nanjing 211189, People's Republic of China
E-mail: lucian@ualberta.ca

\textit{New Journal of Physics} \textbf{12} (2010) 083018 (15pp)
Received 14 April 2010
Published 9 August 2010
Online at \url{http://www.njp.org/}
doi:10.1088/1367-2630/12/8/083018

\textbf{Abstract.} Two closely spaced dangling bonds (DBs) positioned on a silicon surface and sharing an excess electron are revealed to be a strong candidate for a charge qubit. Based on our study of the coherent dynamics of this qubit, its extremely high tunneling rate $\sim 10^{14}$ \textit{s}$^{-1}$ greatly exceeds the expected decoherence rates for a silicon-based system, thereby overcoming a critical obstacle of charge qubit quantum computing (QC). We investigate possible configurations of DB qubits for QC devices. A first-order analysis of coherent dynamics of DBs shows promise in this respect.
1. Introduction

Quantum computing (QC) enables certain problems to be solved much faster than by known classical algorithms [1], and certain quantum algorithms are believed to speed up exponentially, solving other problems such as factorization [2]. Semiconductor solid-state implementations, especially in silicon, are particularly attractive because of the advanced state of silicon technology and the desire to integrate standard silicon-chip computing with quantum computation. Silicon-based qubits could be manifested as nuclear spin [3], electron spin [4]–[7] and charge qubits [8, 9]. Although charge qubits have been successfully created in superconducting Cooper pair boxes [10, 11], realizations of semiconductor charge qubits are difficult because of strong decoherence effects. Electron-spin qubits offer an alternative approach but face severe challenges such as readout: in fact, a promising approach to reading spin qubits first converts them to charge qubits [12]. Thus, semiconductor charge qubits are important either as quantum information carriers or as intermediaries for spin-qubit readout.

The charge qubit is manifested as a quantum dot pair such that having an excess electron on the ‘left’ (or ‘right’) dot corresponds to the logical state $|0\rangle$ (or the orthogonal state $|1\rangle$). Coherent tunneling between the two quantum dots with a tunneling frequency $\Delta$ yields superpositions of $|0\rangle$ and $|1\rangle$. These states correspond to position encoding, whereas the symmetric and antisymmetric qubit states correspond to energy encoding.

Here we show that a pair of quantum dots, with a dot corresponding to a silicon-surface dangling bond (DB), should be an excellent semiconductor charge qubit with low decoherence. Such pairs of coupled DBs have recently been fabricated [13]. As previously proposed, semiconductor charge qubits critically suffer from large decoherence [6, 14]. It appears worth investigating whether this obstacle can be tackled by shrinking the scale of the constituent quantum dots, concomitantly with the spacing between them. The motivation for shrinking the size is that the tunneling rate increases exponentially with decreasing inter-dot separation, whereas, as shown below, decoherence is expected to scale weakly with inter-dot separation. Therefore, decreasing separation allows many coherent oscillations before the onset of significant decoherence.
Implementing such a strategy involves abandoning heterostructure quantum dots and instead adopting DB quantum dots on an H-terminated Si surface. As this quantum dot size is of atomic dimensions, commensurately close spacing of dots is enabled [13]. Pairs of appropriately separated DBs at low temperature share precisely one excess electron per pair (denoted DB–DB$^-$), yielding coherent tunnel coupling between the two DBs [13]. This fact strongly motivates opening up a new area of interest, namely coherent dynamics of tunnel-coupled DBs on a silicon surface with the potential for exploiting them in quantum information processing.

The novelty of our qubit consists in its extremely high tunneling rate $\Delta \sim 4.7 \times 10^{14} \, \text{s}^{-1}$, compared to a maximum order of magnitude of $10^{12} \, \text{s}^{-1}$ in previously proposed charge qubits of atomic scale [6]. Another novel feature is the relative ease of fabrication, as already demonstrated [13]. DB quantum dots can be separated by subnanometer distances, are almost physically identical and, as surface entities, are directly amenable to measurement and control. Furthermore, unlike the case for quantum dots composed of atoms buried in bulk media, the silicon-based scheme proposed here trades the extraordinarily difficult requirement of precisely positioned single dopant atoms with the challenging but attainable requirement that single H atoms be removed by a scanned probe. These DB–DB$^-$ charge qubits could form the basic units of a quantum computer, the dynamics of which we describe with the extended Hubbard model [15].

The outline of our paper is as follows. In section 2, we describe the physical characteristics of the silicon DBs and we show that all DB–DB$^-$ pairs can be initialized such that each excess electron is in either the ‘left’ or the ‘right’ DB of each pair; subsequently, the potential landscape can be tilted so that all are initialized in the ‘left’ state. In section 3, we formulate the quantum dynamics of a system of DBs in the frame of an extended Hubbard model. In section 4, we analyze the decoherence effects on the quantum dynamics of the DB system due to its interaction with external factors such as thermal noise in conductors and phonons in the silicon substrate. Without undertaking a full analysis, we mention in section 5 how these DB–DB$^-$ pairs could find applicability in a quantum computer circuit, for example the flying-qubit circuit model based on a bulk-silicon electron-spin qubit version [16] or on measurement-based one-way QC [17]. The complete fulfillment of the DiVincenzo criteria is not being explicitly addressed because it exceeds the scope of this paper.

2. Dangling bond (DB) pairs as charge qubits

A neutral DB hosts a bound electron within the Si 1.1 eV bulk band gap. The itinerant electrons available in a doped semiconductor can provide a second electron of opposite spin to the DB, thus rendering it a DB$^-$. If two DBs are sufficiently close together ($\leq 16 \, \text{Å}$), Coulomb repulsion ensures that a doubly-charged DB$^-–DB^-\, \text{pair cannot form}$ [13]. Hence, a closely spaced DB pair shares one extra electron tunneling between two centers, suggesting its use as a charge qubit. Tunnel-coupled DBs, as shown in figure 1(a), have been created on an Si(100) surface by first passivating an Si(100) surface with a hydrogen monolayer and then using a scanning tunneling microscope (STM) tip to remove H atoms at selected sites [13]. The separation between the two DBs forming a pair has a strict lower bound of 3.84 Å, as determined by the lattice spacing of the Si(100) surface, whereas the upper bound for enabling a qubit is given by the tunneling range of about 16 Å. Distinct pairs are created farther apart than this limit to avoid inter-pair tunnel coupling. Here we claim that DB–DB$^-$ pairs exhibit coherent quantum dynamics and can serve as good charge qubits.
Figure 1. (a) Variably spaced qubits in an atom-resolved STM image (46 Å × 46 Å, 2V, 0.2 nA) created from pairs of DBs on an H-Si(100)2 × 1 surface, separated by 15.36 Å (qubit A) and 7.68 Å (qubit B). DBs appear as bright protrusions in the gray scale image. A schematic diagram (left) shows the position of DBs (red and green circles) on the Si surface. Black dashes represent silicon dimers. (b) A DB–DB− pair modeled as a double-well potential, with the extra electron at the left well immediately after initialization to |0⟩. (c) Relaxed ground state of the DB electrons after lattice relaxation is completed.

The localized nature of the DB wavefunction and its energy level in the band gap allows us to formulate an electron-confinement model corresponding to a potential well accounting for the effect of the environment. Such a potential well description must render the correct eigenstate energy and orbital size, and must allow for electron excitation into the bulk conduction band of the crystal. For a neutral DB, we calculate the binding energy of an electron to be about 0.77 eV [18]. In a highly doped n-type crystal, a high Fermi level of the crystal allows an extra electron to be localized at a DB, rendering the DB site negatively charged. Similarly, if the crystal is p-type, the DB can lose all its electrons, thereby becoming positively charged.

This localization has two important physical consequences:

- A 0.5 eV upward shift of the DB− energy level relative to that of a neutral DB to ~0.85 eV above the valence band edge (a change in the potential well resulting in weaker confinement and a lower ionization energy).
- A local lattice deformation whereby the host Si atom at a DB− is raised by 0.3 Å from the plane of the surface. After the electron tunnels out of a DB−, the lattice begins to relax.

In figures 1(b) and (c), we depict a DB pair as an effective double-well potential with (b) an excess electron at the left well immediately after release from a biasing external field, as required for qubit initialization, and (c) after complete lattice equilibration when the potential landscape becomes symmetrical. Due to the localized extra charge, the double-well in case (b) does not exhibit the symmetry of case (c), and the DB energy is shifted upward at the left site. Consequently, during lattice relaxation, the coherent oscillation between the two DBs takes place between two wells of slightly different shapes, resulting in a periodic oscillation that is biased towards the ‘left’ (excess electron spends more time on the left than on the ‘right’). Slow relaxation of the lattice will modify the electron oscillation and cause weak decoherence, commensurate with the ratio of relaxation rate to oscillation rate.

We calculate tunneling rates in a DB–DB− pair for various separations by two different methods. For DB separations of 3.84 and 7.68 Å, tunnel splitting is determined to be 307.7 and 87.8 meV, respectively, by time-dependent density-functional theory on cluster models [18].

New Journal of Physics 12 (2010) 083018 (http://www.njp.org/)
These correspond to tunneling rates of $4.67 \times 10^{14}$ and $1.33 \times 10^{14} \text{s}^{-1}$, respectively. For greater separations, the size of the silicon cluster model becomes prohibitively expensive for this computation, and we resort to simpler approximations, namely the Wentzel–Kramers–Brillouin (WKB) method. The results are plotted in figure 3.

3. Quantum dynamics of the DB system

3.1. Hamiltonian dynamics

Our estimated decoherence rates (section 4) are orders of magnitude smaller than tunneling rates, for chosen intra-qubit DB separations. Therefore, the dynamics of DBs on the surface can be described by a Hamiltonian $\hat{H}$ that acts upon the Hilbert space spanned by zero, one or two electrons at each DB upon the silicon surface. On-site energy, electron tunneling (hopping), intra- and inter-DB Coulomb repulsion between electrons and potential differences across the surface are all incorporated into $\hat{H}$.

We consider any number of DBs on the surface, with $i$ labeling the DB site. Let $E_{os}$ be the on-site energy of an electron at any DB, which includes a constant surface chemical potential offset, and let $\eta_i$ be a site-dependent energy correction due to local field effects. The slow lattice deformation due to the excess electron and the potential well deformation due to external biasing fields can be incorporated into this $\eta_i$ parameter. The hopping integral between sites $i$ and $j$ is $T_{ij} = \hbar \Delta_{ij}/2$, which depends on the separation $r_{ij}$ between the two DBs. $U_i$ denotes the energy cost of putting two electrons of opposite spin at the same site $i$, including the screening energy. The cost of putting one electron with spin $\sigma \in \{\uparrow, \downarrow\}$ at site $i$ and another electron of spin $\sigma'$ at site $j$ is denoted by $W_{i\sigma j\sigma'}$.

Tunneling between DB sites can be controlled by modifying the inter-site potential bias. For example, two sites $i$ and $j$ can have a time-dependent potential difference of $V_{ij}(t)$. For $\hat{c}_{i,\sigma}$ ($\hat{c}_{i,\sigma}^\dagger$) the annihilation (creation) operator for an electron with spin $\sigma$ at site $i$ and $\hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}$ the number operator for electrons of spin $\sigma$ at site $i$, the potential difference operator between sites $i$ and $j$ is

$$\hat{\mathcal{V}} \equiv \frac{1}{2} \sum_{i < j, \sigma} V_{ij}(\hat{n}_{i,\sigma} - \hat{n}_{j,\sigma}).$$

(1)

We now have all the terms required to express the Hamiltonian as an extended Hubbard model [15],

$$\hat{H} = \sum_{i,\sigma} (E_{os} + \eta_i) \hat{n}_{i,\sigma} - \sum_{i' < j} T_{ij} (\hat{c}_{i',\sigma}^\dagger \hat{c}_{j,\sigma} + \hat{c}_{j,\sigma}^\dagger \hat{c}_{i',\sigma}) + \sum_i U_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \sum_{i < j, \sigma, \sigma'} W_{i\sigma j\sigma'} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'} + \hat{\mathcal{V}}.$$  

(2)

As DB–DB$^-$ qubit tunneling is much faster than decoherence processes, Hamiltonian (2) is justified by working in a regime of coupled qubits with standard descriptions of Markovian qubit decoherence [19].

Typical values of system parameters are the Fermi level (or more exactly, the chemical potential) $E_F = 0.95 \text{ eV}$, for a medium-level n-type doped silicon sample; the neutral DB energy level $E_{DB} = 0.35 \text{ eV}$, the negative DB energy level $E_{DB^-} = 0.85 \text{ eV}$ (energy values given with respect to the silicon valence band edge). We extracted the Hubbard model parameters from
the results of our \textit{ab initio} calculations: $E_{os} = 0.6$ eV and $U = 1.00$ eV. For a DB separation of 3.84 Å, $T = 0.154$ eV and $W = 0.37$ eV.

3.2. Qubit dynamics

Hamiltonian (2) describes dynamics for quite general configurations of DBs on the silicon surface. For QC, we need to generate entanglement by applying time-dependent gate potentials for specific qubit separation and relative orientation on the Si surface. A highly ordered pattern of DBs, corresponding to grouping DBs into pairs of nearby DBs, and well-chosen separations between pairs, greatly simplifies (2). For DBs on the silicon surface, electron spin is preserved so it can be neglected. Hence the ‘left’ state $|0\rangle$ and ‘right’ state $|1\rangle$ form a qubit basis with conjugate (energy) basis corresponding to $|\pm\rangle = (|0\rangle \pm |1\rangle) / \sqrt{2}$. In fact, the wave functions corresponding to ‘left’ and ‘right’ occupation are not completely orthogonal, but the overlap is negligibly small for the case of two DBs separated by several angstroms.

For $N$ DB–DB$^-$ pairs, the Hamiltonian can be conveniently rewritten in the qubit basis as a linear combination of quantum gates and tensor products thereof:

$$\hat{H}_q(t) = \kappa \mathbf{1} + \sum_{i=1}^{N} \left[ T \hat{X}_i + \frac{1}{2} \Delta V_i(t) \hat{Z}_i + \frac{1}{2} \sum_{j<i} W_{ij} \hat{Z}_i \otimes \hat{Z}_j \right].$$  \hspace{1cm} (3)

Intra-qubit separation is constant for all qubits with $U_0$ and $W_0$ on-site and inter-site Coulomb interactions within each DB–DB$^-$ qubit, and $W_{ij}$ is the inter-qubit Coulomb repulsion $W_{ij} = W_{ij}^x + W_{ij}^z$ and $W_{ij}^x$ ($W_{ij}^z$) is the inter-site Coulomb interaction between the same (cross) sites of two DB–DB$^-$ pairs $i$ and $j$. Then

$$\kappa = N (3E_{os} + 3\eta + U_0 + 2W_0) + \frac{9}{2} \sum_{i<j} W_{ij}^x.$$  \hspace{1cm} (4)

Qubit-specific time-dependent potential-landscape tilting $\Delta V_i(t)$ is incorporated into $\hat{H}_q(t)$, with $T$ being the intra-qubit tunnel splitting energy.

4. Decoherence analysis for DB–DB$^-$ qubit systems

For a DB–DB$^-$ qubit on a H-Si(001) surface, we treat the decoherence mechanism due to various interactions with the environment within the spin-boson model. The spin-boson model is a well-established simplified model for a few-level quantum system interacting with a bath of harmonic oscillators, and for a two-level system, spin-boson dynamics has been extensively studied [20]. The spin-boson model has previously been employed for the treatment of decoherence in the P–P$^+$ charge qubit in bulk silicon [6]. Based on earlier studies of silicon systems [6, 21], we estimate that the main sources of decoherence for our system are (i) the voltage fluctuations on the gate electrodes and (ii) the interaction between the qubit electron and phonons in silicon bulk and at the surface. We discuss these sources below and calculate the corresponding decoherence rates for a DB–DB$^-$ qubit. Other decoherence sources, such as control errors, are not included in this analysis, as they depend on a specific architecture of the device. Decoherence due to stray charges in the system is also believed to be small [13], as the
spacing between DBs in a qubit is much smaller than distances to the nearest trapped charges in the semiconductor.

The spin–boson Hamiltonian [20] for a single qubit interacting with its environment is given by

\[ \tilde{H}_{\text{sb}} = \tilde{H}_{\text{qb}} + \tilde{H}_{\text{bath}} + \tilde{H}_{\text{int}} \]  

for \( \tilde{H}_{\text{qb}} \) and \( \tilde{H}_{\text{bath}} \) separate qubit and bath Hamiltonians, respectively, and \( \tilde{H}_{\text{int}} \) the interaction term. The latter is given by

\[ \tilde{H}_{\text{int}} = \frac{1}{2} \hbar \hat{Z} \sum_i \lambda_i (\hat{a}_i + \hat{a}_i^\dagger) = \frac{1}{2} \hbar \sum_i c_i \hat{x}_i, \]  

where \( \lambda_i \) denotes a harmonic oscillator mode with frequency \( \omega_i \), and \( \hat{a}_i \) and \( \hat{a}_i^\dagger \) are the creation and anihilation operators for mode \( i \) within the second quantization formalism, and \( \lambda_i \) is the coupling coefficient between the qubit and mode \( i \). In this model, the coupling between the qubit and the bath depends linearly on the coordinate of the qubit and those of the harmonic oscillator modes. This is obvious in the expression in equation (6), where \( d \) is the distance between the localized qubit states, \( \hat{x}_i \) is the spatial coordinate of mode \( i \), and \( c_i \) is the coupling strength between the qubit and mode \( i \).

Earlier studies show that, for any system characterized by the equilibrium statistical average over the initial and final states of the bath, the only physically relevant quantity in the spin-boson model is the so-called spectral density function of the bath [20],

\[ J(\omega) = \frac{\pi}{2} \sum_i \delta(\omega - \omega_i) \frac{c_i^2}{m_i \omega_i}. \]  

A large class of open systems can be characterized by a spectral function of the form

\[ J(\omega) = \alpha \omega^s \exp(-\omega/\omega_c), \]  

where \( \omega_c \) is a cutoff frequency and \( \alpha \) and \( s \) empirically-fitted constants. For \( s = 1 \), the bath is said to be ohmic. In our study, we assume the spectral density to be of the form (8), for which we will specify appropriate parameters \( \alpha, s \) and \( \omega_c \).

The spin-boson model, although one of the simplest dissipative two-state systems, does not have a general analytic solution. The dynamical behavior of this model essentially depends on the ratios between the parameters \( \Delta, \omega_c \) and \( k \Theta \) (where \( k \) is the Boltzmann constant and \( \Theta \) is the temperature). For practical purposes, the most common solutions are perturbative ones (in which the weakest term in the total Hamiltonian plays the role of the perturbation) and path integral techniques. For example, in the adiabatic limit, \( \Delta \gg \omega_c \), the bath evolves quite slowly and has an almost classical behavior, whereas in the non-adiabatic limit, \( \Delta \approx \omega_c \), the golden rule offers a reliable solution. Other limiting cases also involving \( k \Theta \) and other energy scales are well understood [22, 23].

As the bare tunneling rate in a qubit increases, fluctuations in the tunneling splitting can play an important role in the coupling with the environment. This can be described as terms in the interaction Hamiltonian proportional to \( \sigma_x \) and \( \sigma_y \), which do not explicitly appear in the spin-boson Hamiltonian. However, it was shown in early studies on the spin-boson model [20] that this effect can still be accommodated by the spin-boson model via renormalizing the bare tunneling rate and the applied bias. The only condition is that the tunneling rate be much less than the classical oscillation frequency \( \omega_0 \) corresponding to electron confinement in an isolated

*New Journal of Physics* 12 (2010) 083018 (http://www.njp.org/)
DB. As the confinement energy in a DB is about 0.52 eV, this condition is generally fulfilled for all qubit configurations, with the exception of the qubit with a separation of 3.84 Å. Therefore, we must bear in mind that, in this limit, the accuracy of the spin-boson model may be unreliable.

4.1. Decoherence due to Johnson–Nyquist voltage fluctuations

Johnson–Nyquist noise (also known as Johnson noise) is due to random thermal fluctuations of the charge carriers in a conductor or semiconductor. For the purpose of calculating its effect on the coherent oscillations in a charge qubit, we employ the spin–boson model with the qubit being the two-level system and the gate electrode being the bath. In order to obtain a reliable estimate of the decoherence effect, we need to look at how the power spectrum of the bath compares to the bare tunneling frequency of the qubit.

The Johnson noise stretches uniformly in the frequency range from zero to the quantum limit of \(k \Theta / \hbar\), which practically means up to about 10\(^{11}\)–10\(^{13}\) s\(^{-1}\). In particular, we can see that, for a temperature \(\Theta = 4\) K, the spectrum has a cutoff frequency \(\omega_c = 5.2 \times 10^{11}\) s\(^{-1}\). As the bare tunneling frequency of the charge qubit in our DB implementation has a value \(\Delta \approx 10^{14}\) s\(^{-1}\) \(\gg \omega_c \approx 10^{12}\) s\(^{-1}\), we can safely regard the effect of the bath on the qubit as being approximately adiabatic (potential energy changes experienced by a qubit electron due to fluctuations in the bath vary slowly in time compared to the bare tunneling frequency of the qubit).

To proceed, we assume ohmic dissipation corresponding to \(s = 1\) in equation (8), so the spectral function in the spin–boson model has the form

\[
G(\omega) = \alpha_{\text{JN}} \omega \exp(-\omega/\omega_c)
\]  

(9)

for

\[
\alpha_{\text{JN}} = \frac{\eta d}{2\pi \hbar},
\]

(10)
a dimensionless dissipation/coupling function of the distance between the two charge centers \(d\) and viscosity coefficient \(\eta\).

One of the simplifying features of the spin–boson Hamiltonian is that, in the limit of weak qubit–bath coupling, the decoherence times \(T_1\) (describing population decay) and \(T_2\) (describing coherence decay) are equal to second order in the coupling [20], which allows us to characterize the system by a single decoherence rate \(\Gamma = 1/T_1\). In the adiabatic limit \((\Delta \gg \omega_c)\), and for the case when \(\omega_c \gg \Gamma\) (which can be verified \textit{a posteriori}), the decoherence rate for the qubit can be determined according to [22, 23],

\[
\Gamma_{\text{JN}} = \frac{1}{2} \sqrt{\pi} \hbar \Delta^2 \exp(-\frac{E_r}{\hbar kT})
\]

(11)

with \(E_r\) being the bath reorganization energy,

\[
E_r = \int_0^\infty d\omega \frac{G(\omega)}{\omega},
\]

(12)

which can be calculated from equation (9) to yield

\[
E_r = 2\alpha_{\text{JN}} \hbar \omega_c.
\]

(13)

For a typical charge–qubit gating [6],

\[
\alpha_{\text{JN}} = \frac{e^2 \beta^2 R_g}{4\hbar},
\]

(14)
Figure 2. Sketch of the gating geometry for our proposed DB–DB$^-$ qubit on the silicon surface. DBs are indicated as red circles and are indexed L and R corresponding to their locations. The electrodes (based on STM tips) are indicated in blue and have fixed potentials $V_1$ and $V_2$, with $V_{12} = V_1 - V_2$. The radius of the electrode at the apex is $a$.

where $R_g$ is the resistance of the gate circuit, and

$$\beta = \frac{\delta V_{LR}}{\delta V_{12}}$$

is another dimensionless parameter that depends solely on the system geometry. Here, $V_{LR}$ is the difference between the electrostatic potentials at the L and R sites and $V_{12}$ the difference between the applied voltage on the two electrodes.

A simple approximation (but yielding a good order-of-magnitude estimate) for the electrostatic problem (figure 2) yields

$$\delta V_{LR} = \left( \frac{a}{r_1} - \frac{a}{r_2} \right) (V_1 - V_2),$$

whence we obtain

$$\beta_{JN} = a \left( \frac{1}{\sqrt{c^2 + (a+b)^2}} - \frac{1}{\sqrt{(c+d)^2 + (a+b)^2}} \right).$$

Plugging in reasonable estimates for the parameters, $a = b = c = 2$ nm, $d = 0.772$ nm, we find $\beta = 0.036$. Further, assuming $R_g = 50 \Omega$ and using equation (14) yields $\alpha_{JN} = 6.364 \times 10^{-7}$.

Finally, we can calculate the decoherence rate due to Johnson–Nyquist noise for a DB–DB$^-$ charge-qubit implementation depicted in figure 2 with typical parameters $\Delta = 1.33 \times 10^{14} \text{s}^{-1}$, $\omega_c = 1.31 \times 10^{11} \text{s}^{-1}$ ($\Theta = 1$ K). From equation (11) we obtain

$$\Gamma_{JN} = 1.30 \times 10^8 \text{s}^{-1},$$

which is much less than $\omega_c$, thereby showing that our approximations are consistent. Note that, as discussed above, the spin–boson model is less reliable for high qubit-tunneling rates, which
means that its results are unreliable for the closest DB separation of 3.84 Å. Nonetheless, the
decoherence for all other DB separations can be accurately treated by this model because the
corresponding tunnel-splitting energy is much less than the binding energy 0.52 eV.

Based on the above analysis, we claim that our decoherence rate is much smaller than the
bare tunneling frequency of the qubit, a very favorable fact for implementing reliable quantum
gates. This also compares well with the decoherence rate due to Johnson noise in the P–P+
charge qubit implementation proposed in previous studies [6, 24]. Note, however, that the
treatment of decoherence due to Johnson–Nyquist noise in our DB system is quite different from
the P–P+ system. This is due to the fact that, in the latter system, the bare tunneling frequency
$\Delta$ is actually much smaller than the cutoff frequency of the bath $\omega_c$, which requires different
approximations to be employed when calculating decoherence rates.

4.2. Decoherence due to electron–phonon interaction

Previous studies of electron–phonon scattering in reduced-dimension systems have found that,
for zero-dimensional systems, the scattering rates are smaller by at least an order of magnitude
than in 1D and 2D systems [25]. This is due to the fact that, for a given initial state of the
electron, the number of final states is greatly reduced in the zero-dimensional case. For our
system, if the DB–DB$^-$ charge qubit is in the anti-symmetric state $|-\rangle$, only the (symmetric)
ground state $|+\rangle$ is lower in energy, thereby drastically reducing coupling to phonons.

Nonetheless, for our system, the interaction between electrons and phonons can be a
serious source of decoherence and we anticipate that, in our system, it dominates all other
forms. From previous experimental and theoretical studies [26] on phonons in the Si(001)
crystal, we know that the phonon spectrum can extend up to about 70 meV, corresponding to
a frequency of $1.06 \times 10^{14} \text{s}^{-1}$. This rate is comparable to the bare tunneling frequency for the
charge qubit, which means that the adiabatic approximation used in the previous section fails.
A different approach is required and, as in previous theoretical analyses of the electron–phonon
interaction, we calculate the rates of electron–phonon scattering within the frame of the first-
order perturbation theory via the Fermi golden rule [25],

$$\Gamma_{e-ph} = \frac{2\pi}{\hbar} \sum_{q, f} \alpha^2(q) \left| \langle \psi_f | e^{\pm i q \cdot r} | \psi_i \rangle \right|^2 \delta(E_f - E_i \mp E_q) \left[ n_B(E_q, \Theta) + \frac{1}{2} \mp \frac{1}{2} \right], \quad (19)$$

where $i$ and $f$ are indices for the initial and final electronic states, $q$ the phonon wavevector, $E_q$
the phonon energy, $\alpha(q)$ a coupling function and $n_B$ the Bose occupation distribution, and the
upper/lower signs correspond to absorption/emission of a phonon by the qubit.

Below, we quantify the coupling of the charge qubit with the acoustic phonons only. The
coupling of electrons to the longitudinal-optical (LO) phonons is also possible. However, optical
phonons have a more discrete-like energy spectrum (a set of distinct spectral lines), and this fact
prevents any first-order coupling to electrons, unless the energy matching condition

$$\hbar \omega_{LO} = E_f - E_i \quad (20)$$

is fulfilled. Condition (20) can be avoided in our system by judiciously choosing the inter-dot
distance and the amplitude of the applied bias.

If the coupling is given via a deformation potential, $D$, then the coupling function above
can be shown to be

$$\alpha^2(q) = \frac{D^2}{2 \rho c_s^2 \Omega} \hbar c_s^2 q, \quad (21)$$
where $c_s^2$ is the longitudinal sound velocity, $\rho$ is the density and $\Omega$ is a normalization volume. Piezoelectric coupling to acoustic phonons is also possible, but in general it is much weaker (by an order of magnitude [25]) than the coupling via a deformation potential. After appropriate manipulation, the expression for the scattering rate can be reduced to [27]

$$\Gamma_{\text{e-ph}} = \frac{D^2 q_{if}^3}{8\pi^2 \hbar \rho c_s^2} \left[ n_B(E_q, \Theta) + \frac{1}{2} \mp 1 \right] \int \Omega_q \left| \langle \psi_f | e^{\pm i q \cdot r} | \psi_i \rangle \right|^2,$$

where $q_{if} = E_{if} / \hbar c_s$ for $E_{if}$ the energy difference between the $i$ and $f$ states and $\Omega_q$ is the solid angle element in $q$-space.

As in previous studies [6, 21], we assume that a DB can be modeled as a 1s hydrogen-like orbital with a renormalized Bohr radius, $a_B$, and we fit this parameter so that the tunnel splitting of a DB pair derived from the hydrogen-like model reproduces the value predicted by our ab initio calculations for a DB separation of 7.68 Å. Then it can be shown that the rate of phonon emission is given by

$$\Gamma_{\text{e-ph}} = \frac{64D^2 q^3 \sin^2 \theta}{\pi \hbar \rho c_s} \left[ n_B(E, \Theta) + 1 \right] \left[ (qa_B)^2 + 4 \right]^4 \frac{1 - \sin q d}{q d},$$

where $\theta = \tan^{-1}(\hbar \Delta / \epsilon)$, $\epsilon$ is the applied bias on the qubit and $d$ is the dot separation. Note that the results for $\Gamma_{\text{e-ph}}$ are of the same order of magnitude for any other form of the isolated dot wavefunction exhibiting exponential decay, as long as the decay rate is similar.

The decoherence rate as a function of dot separation is plotted in figure 3 together with the bare tunneling rates for different intra-qubit DB separation. For DB separations of 3.84 and 7.68 Å, the tunneling rates ($4.67 \times 10^{14}$ and $1.33 \times 10^{14}$ s$^{-1}$, respectively) are denoted by circles and tunneling rates for greater DB separations are calculated by the WKB method. A continuous line corresponding to interpolation between calculated tunneling rates for different inter-dot separations allows direct comparison.
Table 1. Estimates of the single-qubit and two-qubit gate times for chosen DB configurations. $s_{i,j}^{\text{inter}}$ is the distance between the two identical and parallel qubits, $d_{\text{DB–DB}}^{\text{intra}}$ is the intra-qubit DB–DB distance, and $W_{i,j}^{s}$ and $W_{i,j}^{c}$ are the Coulomb interactions, as explained in the text.

| $s_{i,j}^{\text{inter}}$ (Å) | $d_{\text{DB–DB}}^{\text{intra}}$ (Å) | 1-QB gate time (s) | $W_{i,j}^{s}$ (eV) | $W_{i,j}^{c}$ (eV) | 2-QB gate time (s) |
|-----------------------------|----------------------------------|-------------------|-----------------|-----------------|------------------|
| 15.36                       | 7.68                             | $4.72 \times 10^{-14}$ | 0.1268          | 0.1141          | $3.24 \times 10^{-13}$ |
| 15.36                       | 3.84                             | $1.35 \times 10^{-14}$ | 0.1268          | 0.1232          | $1.15 \times 10^{-12}$ |
| 19.20                       | 7.68                             | $4.72 \times 10^{-14}$ | 0.1025          | 0.0954          | $5.84 \times 10^{-13}$ |

The black dashed line joining the calculated points shows an interpolation of the results obtained by the two methods, whereas, for comparison, the red curve in figure 3 shows the calculated decoherence rate due to electron interaction with LA phonons in the silicon crystal.

Note that, for our DB system, the above rate $\Gamma_{\text{e-phon}}$ is greater than the decoherence rate due to Johnson noise in the electrodes, $\Gamma_{\text{JN}}$, calculated in the previous section. Thus we identify $\Gamma_{\text{e-phon}}$ as the dominant decoherence rate. We note an important fact for our qubit: relaxation via this mode occurs over several nanoseconds, whereas the tunneling period for the DB-DB$^-$ pair with a few angstroms separation is close to 10 fs, which enables many coherent qubit oscillations before decoherence sets in.

Other phonon modes both in bulk and at the surface [26] are less likely to couple to electron tunneling due to their discrete-like energy spectrum. Without considering all the selection rules, at least for DB separations of 3.84 and 7.68 Å, there are no phonon modes to match the tunnel splitting energy, as the highest phonon energy is about 70 meV. A more detailed analysis of the qubit coupling to the optical phonon modes is beyond the scope of this paper. Overall, we estimate that, for our closely spaced qubits, Rabi-type oscillations will take place over many periods before the onset of critical decoherence, illustrating the advantage of closely spaced quantum dots.

5. Applications to quantum computation

For our DB–DB$^-$ pair to be an effective charge qubit, initialization to a simple pure state and qubit-specific readout are critical, as two of DiVincenzo’s five criteria [28] (the other criteria are scalability, a universal set of gates, long coherence times, with coherence time addressed in the previous section). Complete fulfillment of DiVincenzo’s five criteria is beyond the scope of this work, but here we briefly discuss coherence times, initialization and readout.

As shown in the sections above, the single-qubit gate time is of the order of $10^{-14}$ s, whereas the two-qubit gate time can be estimated as $\hbar/(W_{i,j}^{s} - W_{i,j}^{c})$. Estimated values for the two-qubit gate times are given in table 1 for chosen DB configurations. For example, for the first DB configuration in that table, the expected decoherence time is $2 \times 10^{-8}$ s, thereby yielding an error probability of $2.3 \times 10^{-6}$ ($1.6 \times 10^{-5}$) for the single-qubit (two-qubit) gate, well within the tolerance demanded by standard quantum error correction protocols.

Qubits are initialized in the $|0\rangle$ state by applying an electrostatic potential $\Delta V_r(t)$, so that the left DB is lower in energy, thus attracting the pair’s excess electron [6]. When initialization is complete, the electrostatic bias is eliminated and tunneling between the two DBs commences.
A lattice deformation due to charge localization as in figure 1(b) is present during subsequent tunneling, but is expected to relax at a much lower rate than $\Delta$ (by a few orders of magnitude), hence having a small decoherence effect. Application of a static potential has shown polarization to be achievable [13]. In the same experiment, steps towards qubit-specific readout were achieved by STM detection of the excess charge preferentially localized at one site in a DB-DB$^-$ pair. This experiment thus shows that both state preparation on one side and readout of $|0\rangle$ versus $|1\rangle$ state is feasible. Fast readout would be desirable, not only for error correction but also to measure decoherence. One approach to fast readout is to couple the charge qubit to single electron transistor (SET) and detect the changes in its output when the qubit is in the $|0\rangle$ as opposed to the $|1\rangle$ state. The charging state of a DB was shown to affect the STM current through a nearby molecule attached to the surface [29]: the molecule’s electronic structure can be Stark-shifted by the DB’s excess electron.

The Hamiltonian $H_q$ enables a universal set of gates [30]. Single- and two-qubit gates are effected by varying the inter-dot tunneling rate by tilting the potential landscape and then rapidly turning off the tilting. Such a fast and spatially precise control is beyond the current capability of standard electronics, but is in principle conceivable by placing a suitable pattern of metallic nanowires near the surface and irradiating it with a laser pulse. The resulting electromagnetic field, created via plasmonic action [31], can bias the surface with a temporal control comparable to the duration of the pulse, which can be as short as femtoseconds. The laser carrier frequency should be low enough to avoid charging and discharging of DBs through excitation processes, thereby causing qubit losses. Different gates could be effected by time-varying biases achieved by controlled laser pulses.

Scalability of our surface charge-qubit quantum computer follows the same arguments as for those cases, but, of course, better understanding of small-scale devices is required to assess scalability to many-qubit devices. An important feature in our DB system is that qubit cross-talk is minimized by screening effects in the semiconductor. At this early stage, bearing in mind that many implementation details are in need of development, possible computing schemes appear to be a four-rail flying qubit model analogous to the one for electron–spin qubits in bulk silicon [16], or a one-way quantum computer [17], where the qubits are stationary.

6. Summary and outlook

We show that closely separated DB–DB$^-$ pairs on the silicon surface behave as charge qubits, with excellent coherence properties following the extreme miniaturization of qubits, indeed to the atomic realm. This is a consequence of the fact that the tunneling rate is extremely high due to atomic-scale proximity of DBs, whereas the major source of decoherence scales weakly with separation. The scaling advantage comes at the price of having to achieve rapid gating control. As far as we can see, such a scheme entails some technical objectives to be achieved: scaling down the nanowire network needed for biasing qubits; accurate control of the amplitudes of the pulsed fields; ways to incorporate readout during the computation for the purpose of quantum error correction.

A logical step forward would be to further develop QC implementations using our DB–DB$^-$ qubits, with the need to address all DiVincenzo’s criteria for such architectures, which will require much elaboration. Near-future efforts will be concentrated on developing ways to investigate experimentally a small number of DBs. In the first instance, experimental characterization of the decoherence for these charge qubits is of paramount importance.
Whereas time-domain control is ultimately required, decoherence can be studied in the near term by fluorescence techniques: charge qubits are dipoles that will fluoresce in the THz regime, and decoherence can be extracted from linewidths.

In addition to weak decoherence, our scheme has another important advantage over other semiconductor charge qubit proposals: the charge qubits are on the surface rather than in the bulk medium, thus enabling more direct preparation, control and readout. Some of the required DB quantum dot dynamics have already been demonstrated. We believe that the findings outlined here could reinvigorate charge qubit prospects for QC.

Acknowledgments

This project has been supported by NSERC, MITACS, Quantum Works and iCORE. RAW and BCS are CIFAR Fellows. PX acknowledges support from the National Natural Science Foundation of China, grant no. 10944005, and the Southeast University Startup Fund.

References

[1] Grover L K 1997 Quantum mechanics helps in searching for a needle in a haystack Phys. Rev. Lett. 79 325–8
[2] Shor P W 1994 Algorithms for quantum computation: discrete log and factoring Proc. 35th Annu. Symp. on Foundations of Computer Science (Citeseer) pp 124–34
[3] Kane B E 1998 A silicon-based nuclear spin quantum computer Nature 393 133–8
[4] Loss D and DiVincenzo D P 1998 Quantum computation with quantum dots Phys. Rev. A 57 120–6
[5] Vrijen R, Yablonovitch E, Wang K, Jiang H W, Balandin A, Roychowdhury V, Mor T and DiVincenzo D 2000 Electron-spin-resonance transistors for quantum computing in silicon-germanium heterostructures Phys. Rev. A 62 12306
[6] Barrett S D and Milburn G J 2003 Measuring the decoherence rate in a semiconductor charge qubit Phys. Rev. B 68 155307
[7] Sanders B C, Hollenberg L C L, Edmundson D and Edmundson A 2008 Visualizing a silicon quantum computer New J. Phys. 10 125005
[8] Hayashi T, Fujisawa T, Cheong H D, Jeong Y H and Hiyaraya Y 2003 Coherent manipulation of electronic states in a double quantum dot Phys. Rev. Lett. 91 226804
[9] Gorman J, Hasko D G and Williams D A 2005 Charge-qubit operation of an isolated double quantum dot Phys. Rev. Lett. 95 90502
[10] Nakamura Y, Pashkin Yu A and Tsai J S 1999 Coherent control of macroscopic quantum states in a single-Cooper-pair box? Nature 398 786
[11] Wallraff A, Schuster D I, Blais A, Frunzio L, Majer J, Devoret M H, Girvin S M and Schoelkopf R J 2005 Approaching unit visibility for control of a superconducting qubit with dispersive readout Phys. Rev. Lett. 95 060501
[12] Elzerman J M, Hanson R, Willems van Beveren L H, Witkamp B, Vandersypen L M K and Kouwenhoven L P 2004 Single-shot read-out of an individual electron spin in a quantum dot Nature 430 431–5
[13] Haider M B, Pitters J L, DiLabio G A, Livadaru L, Matus J Y and Wolkow R A 2009 Controlled coupling and occupation of silicon atomic quantum dots at room temperature Phys. Rev. Lett. 102 46805
[14] Fujisawa T, Hayashi T and Hiyaraya Y 2004 Controlled decoherence of a charge qubit in a double quantum dot J. Vac. Sci. Technol. B 22 2035
[15] Hubbard J 1978 Generalized Wigner lattices in one dimension and some applications to tetracyanoquinodimethane (TCNQ) salts Phys. Rev. B 17 494–505
[16] Hollenberg L C L, Greentree A D, Fowler A G and Wellard C J 2006 Two-dimensional architectures for donor-based quantum computing Phys. Rev. B 74 45311
[17] Raussendorf R and Briegel H J 2001 A one-way quantum computer Phys. Rev. Lett. 86 5188–91
[18] Frisch M J et al 2004 Gaussian 03 Revision C.02 (Wallingford, CT: Gaussian)
[19] Caldeira A O and Leggett A J 1981 Influence of dissipation on quantum tunneling in macroscopic systems Phys. Rev. Lett. 46 211–4
[20] Leggett A J, Chakravarty S, Dorsey A T, Fisher M P A, Garg A and Zwerger W 1987 Dynamics of the dissipative two-state system Rev. Mod. Phys. 59 1–85
[21] Andresen S E S, Brenner R, Wellard C J, Yang C, Hopf T, Escott C C, Clark R G, Dzurak A S, Jamieson D N and Hollenberg L C L 2007 Charge state control and relaxation in an atomically doped silicon device Nano Lett. 7 2000–3
[22] Garg A, Onuchic J N and Ambegaokar V 1985 Effect of friction on electron transfer in biomolecules J. Chem. Phys. 83 4491
[23] Hornbach M J and Dakhnovskii Y 1999 Electron transfer in a slow relaxation bath: coherence and nonexponential kinetics J. Chem. Phys. 111 5073
[24] Hollenberg L C L, Dzurak A S, Wellard C, Hamilton A R, Reilly D J, Milburn G J and Clark R G 2004 Charge-based quantum computing using single donors in semiconductors Phys. Rev. B 69 113301
[25] Bockelmann U and Bastard G 1990 Phonon scattering and energy relaxation in two-, one-, and zero-dimensional electron gases Phys. Rev. B 42 8947–51
[26] Tütüncü H M, Jenkins S J and Srivastava G P 1997 Theoretical studies of atomic vibrations on the Si (001)(2 × 1) surface Phys. Rev. B 56 4656–64
[27] Benisty H 1995 Reduced electron-phonon relaxation rates in quantum-box systems: theoretical analysis Phys. Rev. B 51 13281–93
[28] DiVincenzo D P 2000 The physical implementation of quantum computation Fortschr. Phys. 48 771–83
[29] Piva P G, DiLabio G A, Pitter J L, Zikovsky J, Rezeq M, Dogel S, Hofer W A and Wolkow R A 2005 Field regulation of single-molecule conductivity by a charged surface atom Nature 435 658–61
[30] Barenco A, Bennett C H, Cleve R, DiVincenzo D P, Margolus N, Shor P, Sleator T, Smolin J A and Weinfurter H 1995 Elementary gates for quantum computation Phys. Rev. A 52 3457–67
[31] Maier S A and Atwater H A 2005 Plasmonics: localization and guiding of electromagnetic energy in metal/dielectric structures J. Appl. Phys. 98 011101