Quantum control of spin qubits in silicon

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Motivation

A silicon-based nuclear spin quantum computer

Quantum computers promise to exceed the computational efficiency of ordinary classical machines because quantum algorithms allow the execution of certain tasks in fewer steps. But practical implementation of these machines poses a formidable challenge. Here I present a scheme for implementing a quantum-mechanical computer. Information is encoded onto the nuclear spins of donor atoms in doped silicon electronic devices. Logical operations on individual spins are performed using externally applied electric fields, and spin measurements are made using currents of spin-polarized electrons. The realization of such a computer is dependent on future refinements of conventional silicon electronics.

Qubits are the $^{31}\text{P}$ nuclear spins $I=1/2$.

Quantum computation with a $^{31}\text{P}$ array in silicon

The strength of the hyperfine interaction is proportional to the probability density of the electron wavefunction at the nucleus. In semiconductors, the electron wavefunction extends over large distances through the crystal lattice. Two nuclear spins can consequently interact with the same electron, leading to electron-mediated or indirect nuclear spin coupling. Because the electron is sensitive to externally applied electric fields, the hyperfine inter-
“Elementary gates for quantum computation”
Barenco et al PRA (1995)

Combinations of two qubits eXclusiveOR + all single qubit operations may perform any unitary operation on arbitrarily many qubits, i.e., any operation in a QC.

\[ H_S(t) = J(t) \vec{S}_1 \cdot \vec{S}_2 \rightarrow \text{Transient Heisenberg coupling} \]

Evolution:
\[ \Psi(t) = U_S(t)\Psi(0) = T \exp\{-i\int_0^t H_S(t')dt'\}\Psi(0) \]
\[ \int_0^{\tau_S} J(t)dt = J_0\tau_S = \pi (\text{mod } 2\pi) \implies U_S(\tau_S) = U_{SWAP} \]

**spin qubits \rightarrow exchange gate**
Loss & DiVincenzo PRA (1998)
Kane Nature (1998)

**XOR-GATE:**
\[ U_{XOR} = \exp\{i(\pi / 2)S_1^z\} \exp\{-i(\pi / 2)S_2^z\} U^{1/2}_S(\tau_S) \exp\{i(\pi / 2)S_1^z\} U^{1/2}_S(\tau_S) \]
Spin interactions in Si$^{31}$P

1-qubit operations

\[ H_{e-n} = \mu_B B \sigma_z^e - g_n \mu_n B \sigma_z^n + A \sigma^e \cdot \sigma^n \]

2-qubits operations

\[ H(R) = H(B) + A_1 \sigma^{1e} \cdot \sigma^{1n} + A_2 \sigma^{2e} \cdot \sigma^{2n} + J(R) \sigma^{1e} \cdot \sigma^{2e} \]
Why Si:$^{31}$P?

- Lifetimes of P-bound electron and nuclear spin are extremely long in silicon*.
- Availability of the state-of-the-art crystal growth, processing, and isotope engineering technologies.
- Well understood physical properties.
- Possible integration with currently used Si devices.

### Si

*Stable isotopes* | Nuclear spin
--- | ---
$^{28}$Si | 92.2% → 0
$^{29}$Si | 4.7% → ½
$^{30}$Si | 3.1% → 0

### GaAs

*Stable isotopes* | Nuclear spin
--- | ---
$^{69}$Ga | 60.1% → 3/2
$^{71}$Ga | 39.9% → 3/2
$^{75}$As | 100% → 3/2
Experimental status (spin coherence)

- Coherence times of **60 ms** for donor electron spin and of **65 ms to 1.75 s** for donor nuclear spin have been measured for donors in Si.


Experimental status (STM bottom-up)

• “Towards the fabrication of P qubits for a Si quantum computer”  

• “Atomically precise placement of single dopants in Si”  

~1 nm accuracy positioning of single P atoms in Si demonstrated
Top-down fabrication: ion implant

As modeled by SRIM, a 14 keV $^{31}$P$^+$ ion implanted into Si with 5 nm SiO$_2$ surface layerd has a mean depth of 20 nm with lateral and longitudinal straggles of 8 and 11 nm, respectively.

Spin read-out

PHYSICAL REVIEW B 80, 081307(R) (2009)

Architecture for high-sensitivity single-shot readout and control of the electron spin of individual donors in silicon

A. Morello,1,6 C. C. Escott,1 H. Huebl,1,4 L. H. Willems van Beveren,1 L. C. L. Hollenberg,2 D. N. Jamieson,2 A. S. Dzurak,1 and R. G. Clark1

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Successful experimental implementation on ion-implanted samples reported in Silicon Qubit Workshop – Berkeley August 24 to 26, 2009
Outline

- Bulk Si
  - Shallow donors (P, As) in Si
  - 2-qubit Exchange gate
  - Doped photonic-crystal Silicon cavity
Bloch states in Si

Lattice potential periodicity → Translational symmetry: $\varepsilon_n(\mathbf{k})$

FCC lattice
Diamond structure

$\mathbf{k} \in 1^{st}$ Brillouin zone

$\mathbf{k} = 0$ filled states

$\mathbf{k}$ empty states
Conduction-band edge

6 equivalent minima

$\vec{k}_\mu \ (\mu = 1, 2, ..., 6) = (0, 0, \pm k_0); (0, \pm k_0, 0); (\pm k_0, 0, 0)$

$k_0 = 0.85 \cdot 2\pi/a$

Eigenfunctions: 6 Bloch states:

$$\phi_{\mu} (\vec{r}) = \exp[i\vec{k}_\mu \cdot (\vec{r} - \vec{\phi}_\mu)] u_\mu (\vec{r})$$

Planewave part (free electron-like)

Periodic part (atomic-like)
Bloch states in Si conduction band-edge: Electronic probability density

Bloch state at $\vec{k} = \vec{k}_x$

$$|\phi_{k_x}|^2 = 1 \times |u_{k_x}|^2$$

$p_x$-like symmetry with lattice periodicity

Any superposition of degenerate Bloch states is also an eigenstate (not in Bloch’s form). Example:

$$\phi(\vec{r}) = \frac{1}{\sqrt{6}} \sum_{\mu=1,6} \phi_{\vec{k}_\mu}(r - \vec{R}_0) \Rightarrow |\phi(\vec{r})|^2$$

Interference pattern:
- oscillatory
- incommensurate
Outline

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• 2-qubit Exchange gate

• Doped photonic-crystal Silicon cavity
Hydrogenic model for P in Si

\[ \psi(r) = \left(\frac{1}{\sqrt{\pi}a^*^3}\right) \exp\left(-\frac{r}{a^*}\right), \quad a^* = a_0 \varepsilon (m_0 / m^*) \approx 30 \text{ Å} \]

Asymptotic exchange coupling of two hydrogen atoms
(Herring & Flicker, 1964)

donor pair exchange:

\[ J(R) \propto \left(\frac{R}{a^*}\right)^5 \exp\left(-2\frac{R}{a^*}\right) \]
Lowest energy levels for As in Si
Single substitutional donor at $R_0$

$$V(\vec{r}) = -\frac{e^2}{\epsilon |\vec{r} - \vec{R}_0|}$$

Kohn-Luttinger electronic ground state (A$_1$ symmetry)

$$\psi_{\vec{R}_0}(\vec{r}) = \frac{1}{\sqrt{6}} \sum_{\mu=1,6} F_{\mu}(\vec{r} - \vec{R}_0) u_{\mu}(\vec{r}) e^{i \vec{k}_{\mu} \cdot (\vec{r} - \vec{R}_0)}$$

ENVELOPE FUNCTIONS (variational): deformed 1S hydrogenic orbitals centered at donor site

PLANEWAVE PHASES PINNED AT DONOR SITE
The oscillatory behavior of the donors wavefunctions in Si is well established. This behavior has no consequences for the conventional applications of n-doped Si. What is the impact of this behavior in the proposed Si-based quantum computer operations?

Koiller, Capaz, Hu & Das Sarma
PRB 70, 115207 (2004).
Outline

• Bulk Si

• Shallow donors (P) in Si

➤ 2-qubit exchange gate

• Doped photonic-crystal Silicon cavity
Donor pair exchange coupling
Heitler-London approach

\[ J(\vec{R}_A - \vec{R}_B) = \frac{1}{36} \sum_{\mu\nu} J_{\mu\nu} (\vec{R}_A - \vec{R}_B) \cos \left[ (\vec{k}_\mu - \vec{k}_\nu) \cdot (\vec{R}_A - \vec{R}_B) \right] \]

- Strongly dependent on inter-donor distance
- No lattice periodicity
- Anisotropic
- Oscillatory behavior

Koiller, Hu & Das Sarma
PRL 88, 027903 (2002)
PRB 66, 115201 (2002)
Donor pair exchange coupling
Exchange anisotropy and oscillatory behavior

For donors exactly aligned along the [100] crystal axis, the oscillatory behavior may be ignored in practice.
Inter-donor positioning uncertainties

1st donor

[100]

2nd donor within a sphere with given uncertainty radius, centered at target point.

Distributions of exchange coupling

R_{uncertainty}

Small displacements form the target relative position. On the order of atomic neighbor distances.

Peaked at $J \sim 0$ (very $\neq J_{\text{target}}$!!)
Inter-donor positioning uncertainties

1st donor

[100]

2nd donor within a sphere with given uncertainty radius, centered at target point.*

Distributions of exchange coupling

Peaked at $J \sim 0$ (very $\neq J_{\text{target}}$!!)

Exchange gates control: Nanofabrication challenge!

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awi)

awi)
Can we build a large-scale quantum computer using semiconductor materials?

“... scalable quantum computing in semiconductors may only be possible at the end of the road of Moore’s Law Scaling: when devices are engineered and fabricated at the atomic level.”

B.E. Kane
MRS BULLETIN, FEB 2005

... or, new ideas are needed!
Outline

• Bulk Si

• Shallow donors (P) in Si

• 2-qubit Exchange gate

➢ Doped photonic-crystal silicon cavity
Basic elements:

• Doped photonic-crystal Silicon cavity;
• Donor impurities placed at the antinodes of a cavity mode;
• Electrodes placed above donors, gated to produce electrical field at each donor position;
• Laser beams;
• Uniform magnetic field;
• Operating temperature \( \approx 7K \).

\[\delta r\]

• Robust against small donor displacements.
Substitutional Donors in Si: Solid-state analogue of the H atom

Relevant energy levels for Si:As

Generating well defined electron spin qubits from 1S(A1)

- Electronic spin state not well-defined due to hyperfine interaction.
  - Solution: apply magnetic field strong enough to decouple nuclear and electronic spin states

- Qubits encoded in the subspace \( \{ |\downarrow>, |\uparrow> \} \).
Spin interactions in Si:As
Optical cavity

1-qubit operations

Raman-coupling of qubit states through off-resonant excitation of transitions involving two laser beams.

Spin-orbit coupling

$|\uparrow\rangle \leftrightarrow |\downarrow\rangle$
Spin interactions in Si:As Optical cavity

**1-qubit operations**

Raman-coupling of qubit states through off-resonant excitation of transitions involving two laser beams.

**2-qubits operations**

Coupling between qubits mediated by cavity field.
2-qubits operations

\[ \delta_i = \delta_{i'} \neq \delta_j \]

\( j = \text{all other N-2 donors – except } i \text{ and } i' \).
Initialization and readout

**Initialization:** opt. pumping

At $T \approx 7K$ only manifold $1S(A1)$ is populated. Optical pumping of state $|\downarrow\downarrow\rangle$.

**Readout:** radiative decay

Readout by monitoring fluorescence light of a cycling transition.

No spin-orbit coupling: $\Delta S = 0$
Some numerical values

- Single-qubit rotations:
  - Remember Raman conditions: $\Delta \gg \Omega_{L1}, \Omega_{L2}, \Gamma_{2p}$
  - Upper bound for decay rate of level 2P⁺ in bulk silicon is $\Gamma_{2p} \approx 1 \text{GHz}$.
  - Decay rate could be reduced by more than one order of magnitude:
    - Spontaneous radiative decay suppressed due to the photonic band gap
    - Phonon-mediated decay can be suppressed by applying stress
  - Using $\Gamma_{2p} \approx 0.1 \text{GHz}$, we take $\frac{\Omega_{L1}}{2\pi} = \frac{\Omega_{L2}}{2\pi} = 2 \text{GHz}$ and $\Delta = 200 \text{GHz}$

$$\frac{\Omega_{\text{eff}}}{2\pi} = 20 \text{MHz}$$

$\epsilon_1 = 5 \times 10^{-4}$

- More than $10^6 \pi$-rotations in 60 ms.
Some numerical values

- **Two-qubit operations:**

  - We take $\frac{\Omega_L^i}{2\pi} \sim 5\text{GHz}$, $\frac{\Omega_c^i}{2\pi} \sim 30\text{MHz}$, $\Delta_L^i = 100\text{GHz}$, $\Delta_c^i = 99\text{GHz}$.

  - Since $\delta^i = 1\text{GHz}$, $\epsilon_2 = 1 \times 10^{-3}$ $\implies \Gamma_c \leq 1\text{MHz}$

  - This imposes strong limit on the cavity quality factor: $Q \geq 10^7$

    $\blacklozenge$ $Q \approx 10^6$ $\rightarrow$ Bong-Shik et al., Nature Materials 4, 207 (2005).

- Effective two-qubit coupling: $\frac{g_{ij}}{2\pi} \sim 2.25\text{KHz}$

  - More than $10^3 \sqrt{\text{SWAP}}$ operations in 60 ms.
Donor misplacements compatible with current nanofabrication capabilities present no problems here!

\[ \delta z = 100\text{Å} \]

Some numerical values

- Sensitivity to small donor misplacements

  Small deviation \( \delta_z \) from cavity field maximum introduces variation \( \Delta \Omega_c \) of cavity vacuum Rabi frequency.

- Error probability for \( \sqrt{SWAP} \) operation due misplacement:

  \[
  p \approx \left( \frac{\Delta g_{ij}}{g_{ij}} \right)^2 = \left( \frac{\Delta \Omega_c}{\Omega_c} \right)^2 \approx 1 \times 10^{-9}
  \]
Summary

- Theoretical investigations of the feasibility of 2-qubit operation based on donor-pair exchange coupling in Si, show fast oscillatory behavior of the coupling with interdonor position.

  Precisely controlling exchange gates for spin qubits in Si remains a nanofabrication challenge.

- We propose a scheme with donor-based electron spin qubits in Si THz cavities which combines the Si substitutional-donor quantum computing architecture with the optical initialization and manipulation processes (already demonstrated in ion traps and other atomic systems). 2-qubit operations are mediated by the vacuum field of the silicon material cavity, which couples to the donor states.

  The scheme is insensitive to small displacements of the donor impurities in the host.
Acknowledgments

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  Sankar Das Sarma – CMTC, U. Maryland
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