Manipulating and characterizing spin qubits based on donors in silicon with electromagnetic field

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Challenging problems for classical computing:
• Search in big data
• Quantum chemistry simulation
• Network optimization
• Large number factorization
can be solved efficiently with quantum computing algorithms.

➤ Requires multiple coupled quantum bits (qubits)
e.g. 4 qubits to factorize a small number 143

Multiple coupled qubits are needed to perform quantum computing.
The next milestone is to realize two qubits

One qubit

Single spin operation driven by ac B-field

Experiment highlights:
• coherence time: 0.5 s
• control fidelity: 99.6%

J. Muhonen et al., Nature Nanotechnology 9, 986 (2014)
The next milestone is to realize two qubits.

One qubit

- Single spin operation driven by ac B-field

Two qubits

- Couple two qubits with exchange (J)

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J. Muhonen et al., Nature Nanotechnology 9, 986 (2014)

Kane, Nature 393, 133 (1998)
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One qubit

- Single spin operation driven by ac B-field

Two qubits

- Couple two qubits with exchange ($J$)

Multiple qubits

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- coherence time: 0.5 s
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- J. Muhonen et al., Nature Nanotechnology 9, 986 (2014)


A long way to go…
The next milestone is to realize two qubits

- **One qubit**
  - Single spin rotation driven by ac B-field

- **Two qubits**
  - Couple two qubits with exchange (J)

- **Multiple qubits**

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**Experiment highlights:**
- Coherence time: 0.5 s
- Control fidelity: 99.6%
- Readout fidelity: 97%

- J. Muhonen et al., Nature Nanotechnology 9, 986 (2014)
- Kane, Nature 393, 133 (1998)

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**Universal quantum computation with the exchange interaction**

- D. P. DiVincenzo, D. Bacon, J. Kempe, G. Burkard, & K. B. Whaley

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**Understand and design experimental two-qubit devices in silicon.**
The objectives of this work

A STM-patterned two-qubit device from our collaborator

- Characterization
  - Number of donors
  - Donor locations
  - Number of electrons

- Feasibility
  Prove that two-qubit operations can be realized

• Characterization of donor-cluster qubits with electron spin resonance (ESR) technique
  » ESR of a donor-cluster in silicon
  » Determine the configuration of a donor cluster using ESR
    ✓ Donor number
    ✓ Donor locations
    ✓ Electron number

• Feasibility: manipulation of two donor-cluster qubits with ESR
  » Two-qubits SWAP gate can be realized with donor-clusters
  » Individual manipulation of two coupled qubits with ESR
• Characterization of donor-cluster qubits with electron spin resonance (ESR) technique
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• Manipulation of two donor qubits with ESR
  » Two-qubits SWAP gate can be realized with donor-clusters
  » Individual manipulation of two coupled qubits with ESR
Configurations of the two qubits are unknown. Q1/Q2 could have various configurations.

Images from B. Weber et al., unpublished.
Importance of a donor-cluster configuration

A characterization technique is needed to identify configuration.

Q1 and Q2 are exchange coupled.


A characterization technique is needed to identify configuration.
Drawback of existing method

Binding energy (BE) of donor-clusters

![Graph showing binding energy vs electron number]

**Binding energy (meV)**

Electron number

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**Experiment:**
- $V_{G1} = V_{G2}$
- $V_{G1} = 1.3 V_{G2}$

**Donor-cluster configuration**

Quantum confinement

Binding energy

 Compare measurement and theory

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Drawback of existing method

Binding energy (BE) of donor-clusters

BE is measurable.

Is there a more general metrology that can characterize the donor-cluster configuration?
A metrology based on ESR to characterize clusters

Donor-cluster configuration

Quantum confinement

Hyperfine interaction $A$

Electron spin resonance (ESR) spectrum

A metrology based on ESR is proposed to characterize a donor-cluster qubit.
Spin manipulation with ESR technique

• ESR: electron spin resonance

Free electron in vacuum:

Apply a static external B-field

\[ \Delta E = E_1 - E_0 = h\nu \]

Bound electron in a donor-cluster in Si:

More complicated for donor-clusters in Si
• Electronic structure
• Spin interaction with background nuclei

Example: Single P in silicon

J. J. Pla et al., Nature 489, 541-545 (2013)
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The effective spin Hamiltonian is

\[ H_{\downarrow \text{spin}} = H_{\downarrow \text{Zeeman}} + H_{\downarrow \text{hyperfine}} \]

Involved spins in a P donor in Si

\[(\uparrow/\downarrow)\]

\[(\uparrow/\downarrow)\]

External B-field polarizes the spins.

Only with \( H_{\downarrow \text{Zeeman}} \) (without hyperfine interaction):

\[ \gamma_{\downarrow \text{ESR}1} = \gamma_{\downarrow \text{ESR}2} \] (a.c. B-field frequency)

Can only detect 1 frequency. Why 2 in experiment?
The effective spin Hamiltonian is

\[ H_{\downarrow\text{spin}} = H_{\downarrow\text{Zeeman}} + H_{\downarrow\text{hyperfine}} \]

Involved spins in a P donor in Si

\[ \gamma_{\downarrow\text{ESR}2} = \gamma_{\downarrow\text{ESR}1} \gamma_{\downarrow\text{ESR}2} \neq \gamma_{\downarrow\text{ESR}1} \]

\[ H_{\downarrow\text{hyperfine}} \] couples electron and nuclear spin, \n\[ H_{\downarrow\text{hyperfine}} \] depends on electron wavefunction \( \propto |\psi(r_0)|^2 \).

Different donor-clusters have different \( H_{\downarrow\text{hyperfine}} \).

We need to calculate \( H_{\downarrow\text{hyperfine}} \) accurately.
• To obtain $H_{\downarrow \text{hyperfine}} (\propto |\psi(\downarrow 0)| \uparrow 2)$ accurately, a good solution to wavefunctions of P donors in silicon is needed.

Impurity model in atomistic TB

• Capture Fermi-contact hyperfine interaction (A)\(^1\), anisotropic hyperfine interaction (D)\(^2\) of P donors in silicon to construct $H_{\downarrow \text{hyperfine}}$

2. Park et al., PRL 103, 106802 (2009)

Atomistic TB provides good solutions to A and D of P donors in silicon to construct hyperfine Hamiltonian.

$H_{\downarrow \text{spin}} = H_{\downarrow \text{Zeeman}} + H_{\downarrow \text{hyperfine}}$
General effective spin Hamiltonian

A donor-cluster configuration (input)

Spin Hamiltonian constructor (this work)

Spin Hamiltonian and γ
(output)

\[ H_{\downarrow{spin}} = H_{\downarrow{Zeeman}} + H_{\downarrow{hyperfine}} \]

- Generalized for few-spin system (m nuclei, n electrons)
- Analyze the ESR frequencies of donor-clusters

What are the ESR frequencies of different donor-clusters solved from \( H_{\downarrow{spin}} \)?
**Outline**

- Characterization of donor-cluster qubits with electron spin resonance (ESR) technique
  - ESR of a donor-cluster in silicon
  - Determine the configuration of a donor cluster using ESR
    1. Donor number
    2. Donor locations
    3. Electron number

![Diagram showing different configurations of donor clusters with electron spin resonance (ESR).](image)
1. Detection of the donor number in a cluster

The number of ESR frequencies goes up with the number of donor nuclei.
2. Detection of donor locations in 2P clusters

Different two-donor configurations

Si atoms

Hyperfine interaction and the separation between ESR frequencies decrease with the distance between two donors.
3. Detection of electron number in a cluster

- Multi-electron occupation: self-consistent field method (which captures the D-binding energy, 2\textsuperscript{nd} e in 1P*) \cite{Rahman2011}

- Hyperfine interaction decreases from 101.8 MHz (1e) to 10.5 MHz (3e). \( A \propto |\psi(\mathbf{r}_0)|^2 \)

Hyperfine interaction and the separation between ESR frequencies decrease with the number of electrons.
The objectives of this work

A STM-patterned two-qubit device from our collaborator

- **Characterization**
  - ✔ Number of donors
  - ✔ Donor locations
  - ✔ Number of electrons

- **Feasibility**
  Show that two-qubit operations can be realized

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• Manipulation of two donor qubits with ESR
  » Two-qubits SWAP gate can be realized with donor-clusters
  » Individual manipulation of two coupled qubits with ESR
Two-qubit operations with exchange

One qubit
Single spin rotation driven by ac B-field

Two qubits
Couple two qubits with exchange (J)

Multiple qubits

Experiment highlights:
• coherence time: 0.5 s
• control fidelity: 99.6%
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J. Muhonen et al., Nature Nanotechnology 9, 986 (2014)

Kane, Nature 393, 133(1998)

Two qubits are coupled by exchange which can be controlled.
Two-qubit logic: Yes
Central 2 qubits: 2 e-spins in DQD
Exchange-coupled?: Yes
Exchange control: With G1 & G2
ESR: Yes

Two-qubit gates can be realized by controlling exchange and ESR.

What if we have ESR?
Operation details: J off, ESR off

Exchange-coupled

<table>
<thead>
<tr>
<th>Gate bias $\rightarrow$ exchange (J)</th>
<th>ESR $\rightarrow$ individual qubit</th>
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<tbody>
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<td>No bias, J is off</td>
<td>No ESR</td>
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Wavefunctions:
- e1
- e2

Small overlap $\rightarrow$ small exchange $\rightarrow$ slow evolution
Operation details: J on, ESR off

**Gate bias $\rightarrow$ exchange (J)**
- with bias, J is on

**ESR $\rightarrow$ individual qubit**
- No ESR

Wavefunctions:
- $e_1$
- $e_2$

Large overlap $\rightarrow$ large exchange $\rightarrow$ fast evolution
Qubit 2 shouldn’t be affected.
Operation details: J off, ESR on $\gamma/2$

Qubit 1 shouldn’t be affected.

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Two-qubit gates can be realized by controlling J: on/off and ESR: on/off by timing and switching J and ESR accordingly, various two-qubit gates can be realized.

Summary:

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<td>No bias, J is off</td>
<td>$\gamma_{J1}$</td>
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<td>No bias, J is off</td>
<td>$\gamma_{J2}$</td>
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By timing and switching J and ESR accordingly, various two-qubit gates can be realized.
Challenges of MOSDQD qubits and opportunities of STM donor devices

- ESR source implemented, ESR frequencies tunable with gates
- Actual metal gate size hard to control
  -- hard to control separation
- Confined at interface
  -- sensitive to interface traps, charge in oxide, gate noise …

- ESR source not yet implemented
- ESR frequencies not tunable
- With atomic precision
  -- accurate qubit placement

- Confined deep away from interface/surfaces
  -- can work in low noise regime

Donor qubit devices with STM lithography technique is more promising to scale up.
Proposed two-qubit device schematics with donors

Images from B. Weber et al., unpublished.

B. Weber et al., Science 335, 64 (2012);

- Coupled through e-e exchange: turned on and off by G1, G2
- Individual qubit manipulation with ESR
By timing and switching J and ESR accordingly, various two-qubit gates can be realized.

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What kind of system provides good J-controllability?
2P-1P provides large exchange tunability.

Exchange coupling can be switched on and off in asymmetric 2P-1P systems.

\[ E \]

Symmetric: small J-tunability

Asymmetric: large J-tunability

Wang et al., unpublished.
• Effective spin Hamiltonian:

\[ H_{\text{spin}} = H_{\text{Zeeman}} + H_{\text{hyperfine}} + H_{\text{exchange}} \]

Truth table of a logical SWAP gate

<table>
<thead>
<tr>
<th>IN</th>
<th>OUT</th>
<th>Input</th>
<th>Output</th>
</tr>
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<tbody>
<tr>
<td>a</td>
<td>b</td>
<td>0 0</td>
<td>0 0</td>
</tr>
<tr>
<td>b</td>
<td>a</td>
<td>0 1</td>
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Basis:  
\[
\begin{align*}
\uparrow\uparrow & \quad \uparrow\downarrow & \quad \downarrow\uparrow & \quad \downarrow\downarrow \\
& \quad & \quad \quad & \\
H_{\text{spin}} &= (\begin{array}{cccc}
E & 0 & 0 & 0 \\
0 & E & 0 & 0 \\
0 & 0 & -J/2 & 0 \\
0 & 0 & 0 & -J/2
\end{array})
\end{align*}
\]

J: exchange coupling

Two-qubit SWAP gate can be realized with electron-electron exchange interaction.
Two-qubit SWAP gate can be realized in a 2P-1P system.

- **Time evolution**

\[ |\Psi(t)\rangle = e^{\frac{-iH_{\text{spin}}t}{\hbar}} |\Psi(0)\rangle \]

\( (H_{\text{spin}} \text{ is projected on a given nuclear spin configuration}) \)

<table>
<thead>
<tr>
<th>J (MHz)</th>
<th>1.6 (off)</th>
<th>2623.1 (on)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( G_1(-), G_2(+) )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( G_1(+), G_2(-) )</td>
<td></td>
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- **Table**

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<th>J (on/off)</th>
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<th>output</th>
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<tr>
<td>Off(&lt;3ns)</td>
<td>ab</td>
<td>ab</td>
</tr>
<tr>
<td>On(&gt;3ns)</td>
<td>ab</td>
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\( a,b: \uparrow(0)/\downarrow(1) \)
By timing and switching J and ESR accordingly, various two-qubit gates can be realized.

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<tr>
<td>$\gamma\downarrow 1$</td>
<td>$\gamma\downarrow 2$</td>
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$|\gamma\downarrow 1 - \gamma\downarrow 2|$ should be large enough to be resolved.

Is it true for 2P-1P?
Individual qubit manipulation with ESR

- Individual qubit manipulation can be realized in the 2P-1P system.

Qubit1 (2P)  Qubit2 (1P)

Initial state (input): ↓↓

\[ |↓↓\rangle - |↑↓\rangle \text{ transition} \]

\[ \gamma_{↓1} = 39.1 \text{ GHz} \]

\[ |↓↓\rangle - |↑↓\rangle \text{ transition} \]

\[ \gamma_{↓2} = 39.3 \text{ GHz} \]

Benefit from using donor cluster (asymmetric system): manipulating one won’t affect another.
The objectives of this work

A STM-patterned two-qubit device from our collaborator

- Characterization
  - Number of donors
  - Donor locations
  - Number of electrons

✔ Feasibility
- two-qubit operations can be realized by controlling exchange + ESR
- Asymmetric systems are favorable

• Characterization of donor-cluster qubits with ESR
  » The configuration of a donor-cluster can be distinguished by its ESR spectrum:
    ✓ Donor number
    ✓ Donor locations
    ✓ Electron number

• Manipulation of two donor-qubits with ESR
  exchange + individual qubit operations: two-qubit gates
  » Two qubits with donor-cluster (asymmetric systems): better exchange tunability and distinct driven frequencies
  » Individual qubit of two coupled qubits can be manipulated with ESR
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