# Exchange Coupling in Si-Quantum-Dot-Based Quantum Computer

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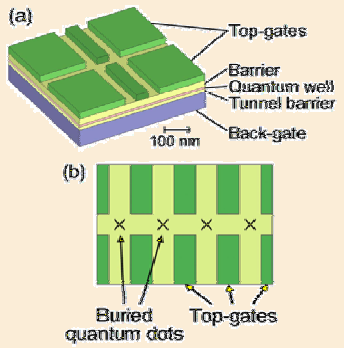
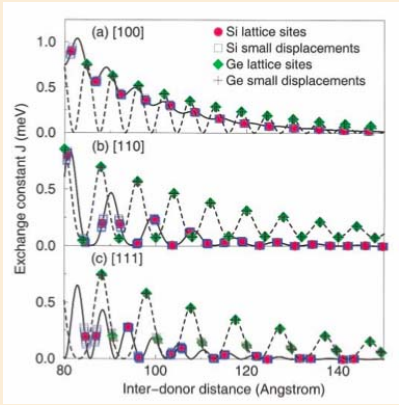
# Overview

- **Motivation:** Electronically confined quantum dots in a Si/SiGe quantum well are proposed to be used for quantum computers. The exchange coupling is used for two-qubit gates. [PRB, 67, 121301R (2003)]
- **Question:** Would the exchange coupling in the Si-QD architecture oscillate rapidly with change of gate positions as predicted in Si:P architecture? [PRL, 88, 27903 (2002)]
- **Result:** Tight-binding simulation shows that the exchange coupling varies smoothly with the change of gate positions. No atomic-level oscillatory behavior is observed.
- **Conclusion:** Si-QD-based quantum computer architecture do not require gate positioning in atomic level precision.




Si-QD-Based Quantum Computer
PRB, **67**, 121301 (2003)

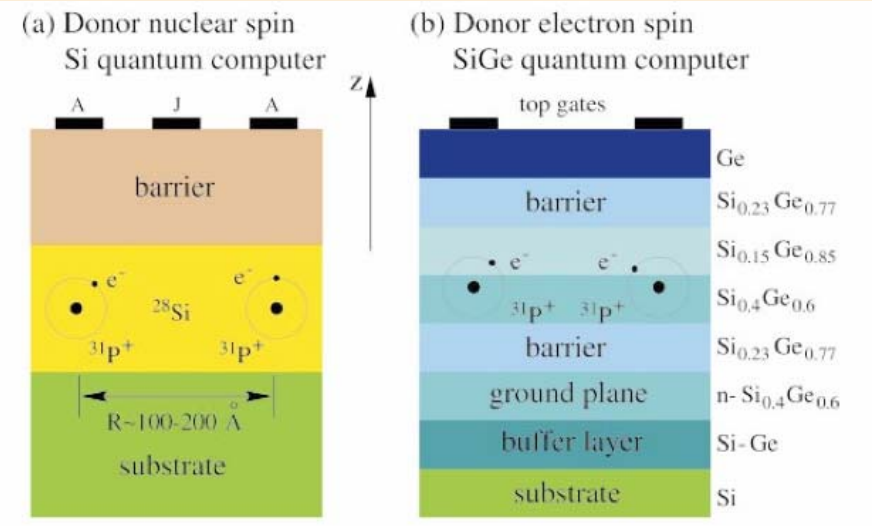



Exchange Coupling in Si:P Architecture
PRL, **88**, 27903 (2002)

# Exchange Coupling in Si:P quantum computer

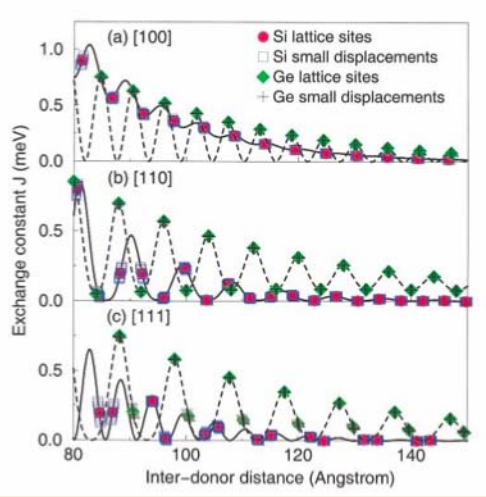
## Facts

- Si:P architecture uses a donor electron or nuclear spin state as a qubit, and uses exchange coupling for two-qubit gates.
- Si has the six conduction band minima (valleys) located along the <100> directions, leading to the fast oscillations in the donor electron wave functions.
- It was predicted that the interference between these valleys causes fast oscillations in the exchange coupling with respect to inter-donor distance.




B.E. Kane,
Nature **393**, 133 (1998)

R. Vrijen et al.,
PRA, **62**, 012306 (2000)

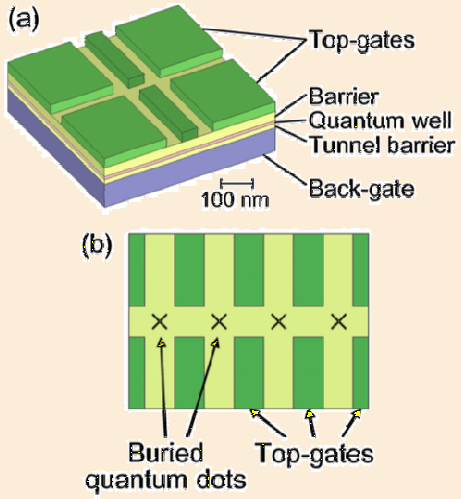



B. Koiller et al., PRL, **88**, 27903 (2002)
B. Koiller et al. PRB, **66**, 115201 (2002)

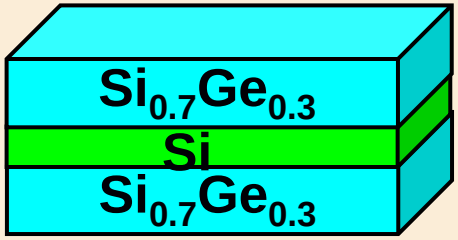
# Exchange Coupling in Si QD quantum computer

## Theoretical Arguments

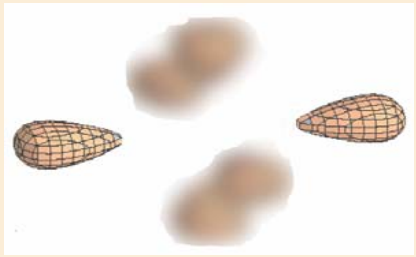
- **Strain** reduces the six-fold valley degeneracy to two-fold, eliminating the fast oscillations of electron wave functions in the quantum well plane.
- **Confinement potential** aligns the oscillation of the electron density along out-of-plane direction.
- Therefore, the source of the fast oscillation of the exchange coupling, **the intervalley electronic interference**, is eliminated in Si/SiGe quantum-dot architecture.




PRB, **67**, 121301 (2003)



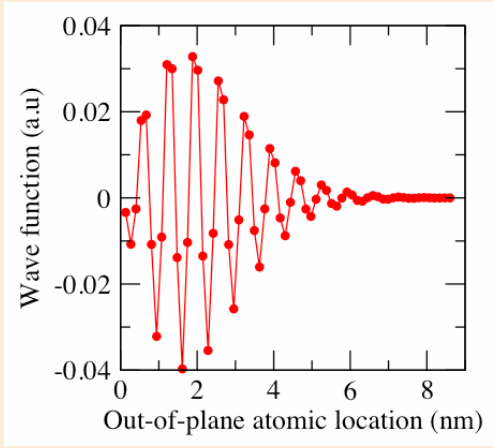

In-plane Strain: 1.27%
Out-of-plane Strain: -0.98%



The two-fold valleys split due to translational symmetry breaking.

In-plane wave function

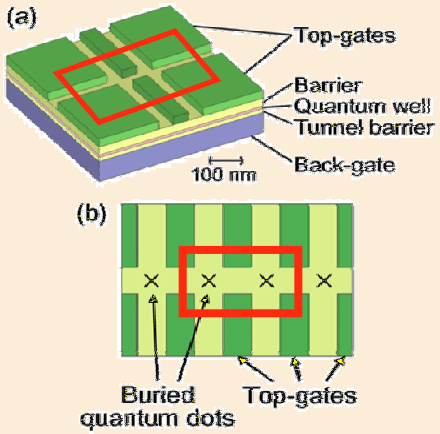
Out-of-plane wave function



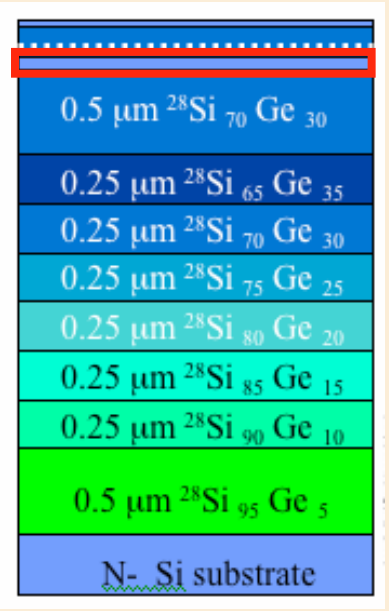
# Si Double Quantum Dot

## Experimental Setup

1. Gate




2. Quantum Well




## Theoretical Setup

1. Gate Potential

$$V_g(r) = A\{1-\exp[-(x^2+y^2)/a^2]\} + A\{1-\exp[-((x-d)^2+y^2)/a^2]\} + Ez$$

where $A = 0.02$ eV, $a = 5.5$ nm, $E = 0.02$ eV/nm, d = 25 - 30 nm

2. Quantum Well

8.5 nm thick, strained Si well with hard wall

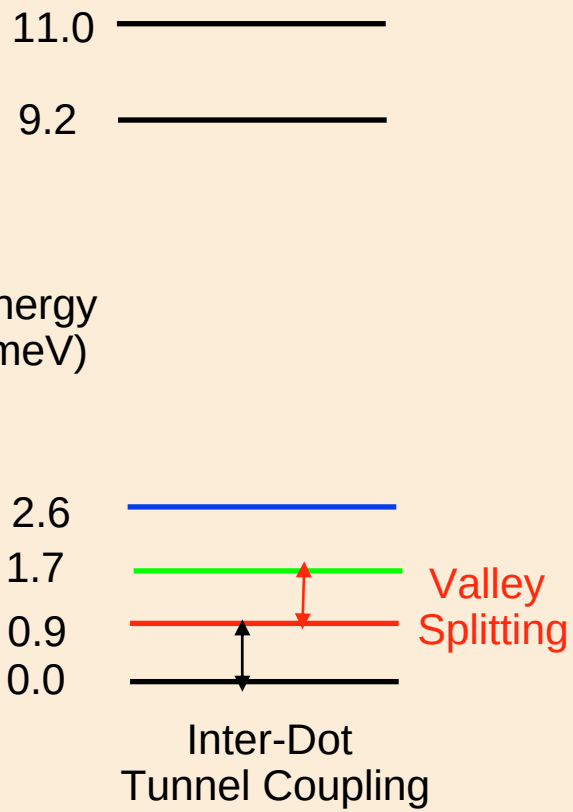
3. Model

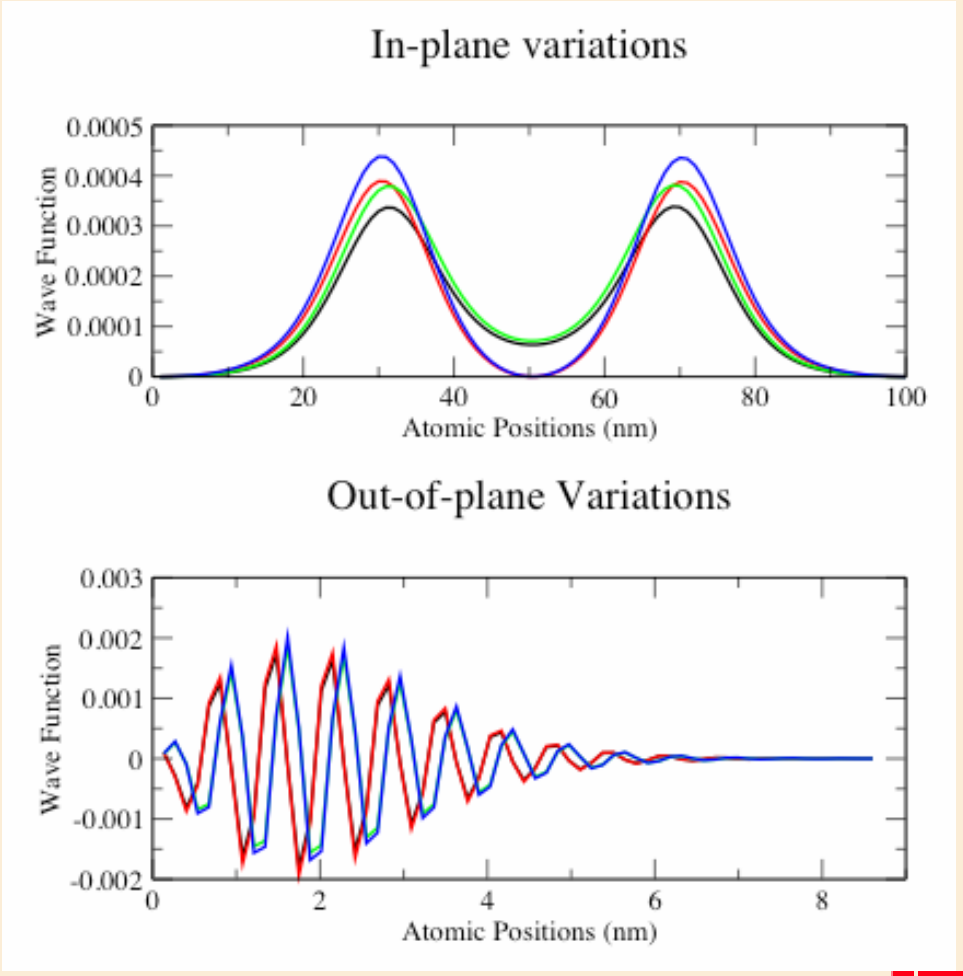
* Tight-binding model for single-electron
  - nearest neighbor interaction
  - $sp^3d^5s^*$ orbitals
  - strain-dependent TB parameters [PRB, **69**, 115201 (2004)]
* Configuration interaction for two-electron
* Simulation performed with NEMO3D

# Single-Electron States in Si Double QD

**Empirical Tight Binding Model**
**TB Hamiltonian includes 640,000 atoms (6,400,000 basis states).**

Single-Electron Energy Levels



# Two-Electron States in Si Double QD

**Configuration Interaction**
**Two-electron Hamiltonian includes 28 basis states.**

Single-Electron States

$$H_1(p,r)|\psi_i\rangle = E_i|\psi_i\rangle$$

Four Single-Electron States

Two-Electron Basis States

$$\Psi_s^{(i,j)}(r_1,r_2) = \frac{1}{\sqrt{2}}\left[\psi_i(r_1)\psi_j(r_2)+\psi_i(r_2)\psi_j(r_1)\right]\chi_s, \quad \text{if } i \neq j$$

$$= \frac{1}{\sqrt{2}}\left[\psi_i(r_1)\psi_j(r_2)+\psi_i(r_2)\psi_j(r_1)\right]\chi_s, \quad \text{if } i = j$$

singlet

$$\Psi_t^{(i,j)}(r_1,r_2) = \frac{1}{\sqrt{2}}\left[\psi_i(r_1)\psi_j(r_2)-\psi_i(r_2)\psi_j(r_1)\right]\chi_t, \quad i \neq j$$

triplet

28 Two-Electron Basis States

Two-Electron Hamiltonian within Configuration Interaction

Hamiltonian Size: 28 x 28

$$H_2(r_1,p_1,r_2,p_2) = H_1(r_1,p_1) + H_1(r_2,p_2) + \frac{e^2}{\varepsilon|r_1-r_2|}$$

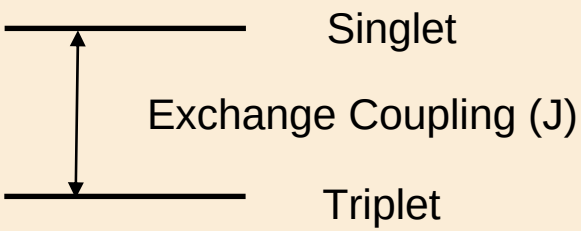
$$\left\langle \Psi_\alpha^{(i,j)} \middle| H_2 \middle| \Psi_\beta^{(m,n)} \right\rangle = (E_i + E_j)\delta_{i,m}\delta_{j,n}\delta_{\alpha,\beta}$$

$$+\delta_{\alpha,\beta}\int dr_1 dr_2 \Psi_\alpha^{(i,j)}(r_1,r_2)\frac{e^2}{\varepsilon|r_1-r_2|}\Psi_\alpha^{(m,n)}(r_1,r_2)$$

Coulomb Interaction

# Exchange Coupling vs Inter-Dot Distance

Two-electron Levels

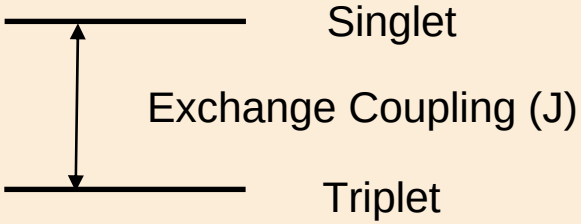



Two-qubit Operations

$$J\vec{S}_1 \cdot \vec{S}_2$$

# Exchange Coupling vs Inter-Dot Distance

Two-electron Levels

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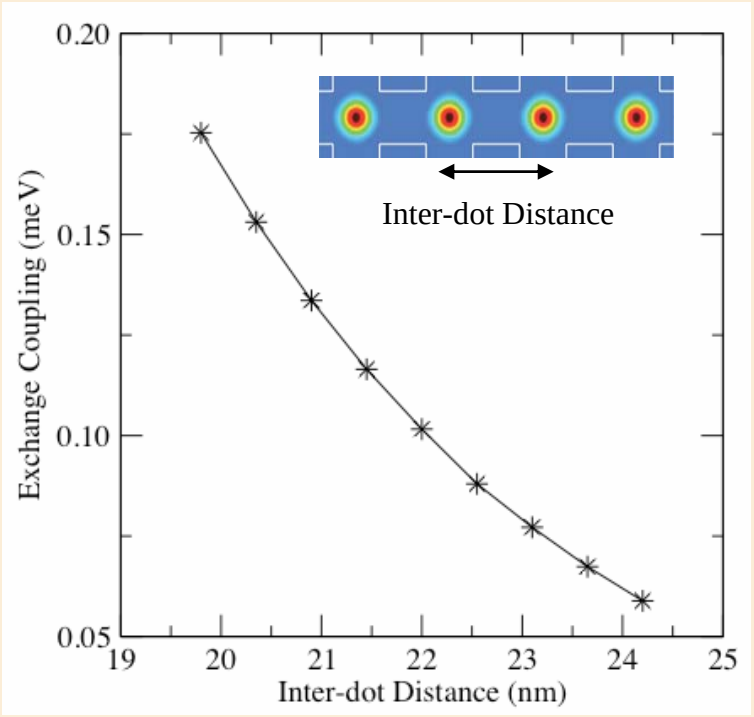
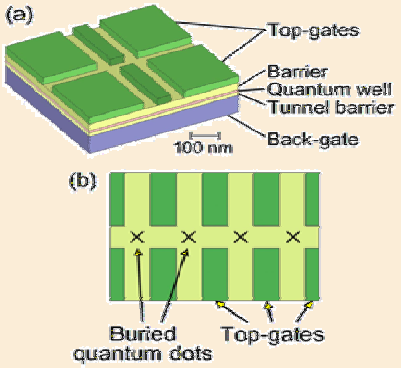



1. As the inter-dot distance increases, the exchange coupling decays smoothly without atomic-level oscillations.

2. Quantum-computer architectures based on Si/SiGe quantum dots do not require gate positioning with atomic-level precision.

# Summary

- We address the stability of exchange coupling with respect to gate positioning in Si-QD-based quantum computer architecture.
- We expect that strong in-plane strain and confinement potential would eliminate the intervalley interference, the source of oscillatory exchange coupling.
- We find with tight-binding simulation that the exchange coupling varies smoothly with the change of gate positions.
- Si/SiGe QD based quantum computer architecture do not require gate positioning with atomic level precision.




PRB, **67**, 121301 (2003)