Quantum Information Science, KITP, Nov 2009

Recent Progress in Silicon-Based Quantum Computing

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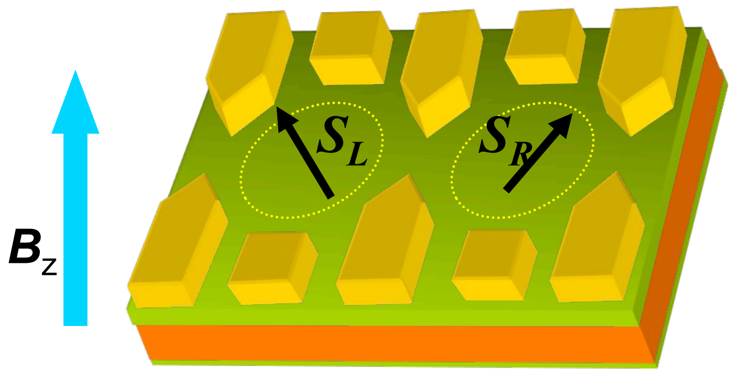
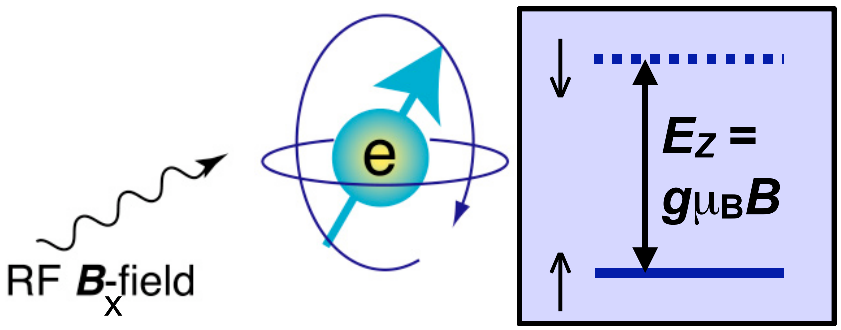
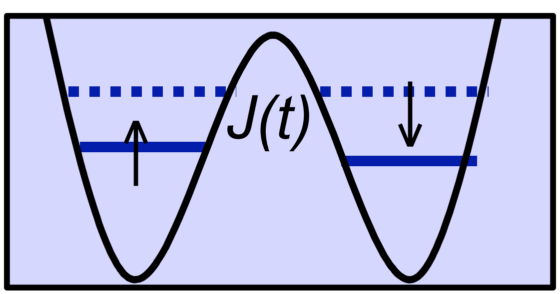
Experimental slides: **Andrea Morello, Mark Eriksson, Hongwu Liu**

Supported by NSA/LPS through ARO, Joint Quantum Institute, and DARPA QuEST

Quantum Dot Trapped Electron Spin Qubits







$$H_s(t) = J(t)\, S_L \cdot S_R$$

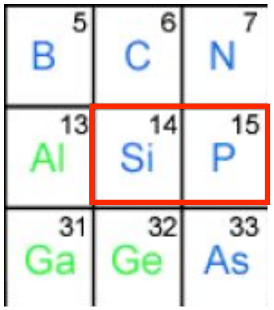
- Qubit defined by Zeeman-split levels of single electron in a quantum dot
- 1-qubit control:
  - magnetic (ESR-field)
  - electrical (EDSR)
- 2-qubit coupling: electrical (exchange interaction between dots)
- Read-out: convert spin to charge (spin filter) ⇒ measure charge

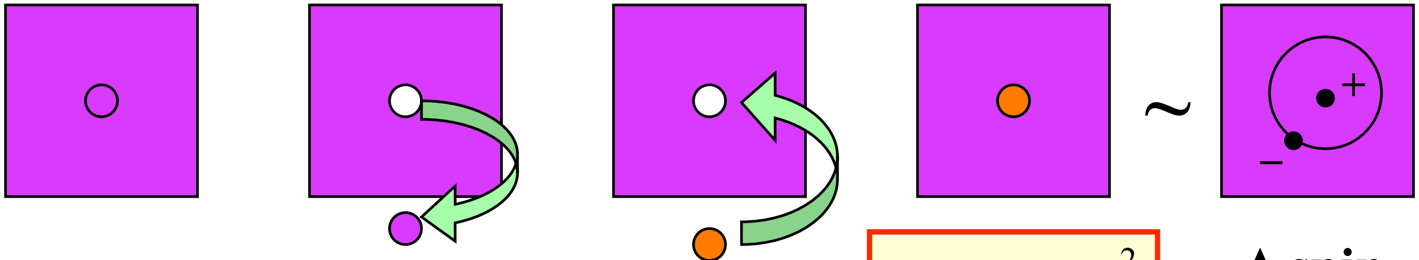
Advantages:

- Electron spin in semiconductors very stable: measured $T_1 \sim 1$ s, $T_2 \sim 100$ μs in GaAs;
- Scalable solid state technology?

Loss & DiVincenzo, PRA 57, 120 (1998).

A Hydrogenic Model for a P Donor in Si





$$U(r) = \frac{-e^2}{\varepsilon\, r}$$

A spin qubit?

$$[-\hbar^2\nabla^2/2m^* + U(r)]\psi(r) = -E_d^*\,\psi(r)$$

$$\psi(r) = (1/\sqrt{\pi a^{*3}})\exp(-r/a^*),\ \ a^* = a_0\varepsilon(m_0/m^*) \approx 30\,\mathring{A}$$

Ionization energy: 45 meV; ground-1st excited state gap > 10 meV

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

$$J(R) \sim E_0 \frac{e^2}{\varepsilon\, a^*}\left(\frac{R}{a^*}\right)^{\frac{5}{2}} \exp(-2R/a^*)$$

Identical qubits?!

Silicon-Based Quantum Computer Architecture: Kane's Proposal

articles

A silicon-based nuclear spin quantum computer

B. E. Kane

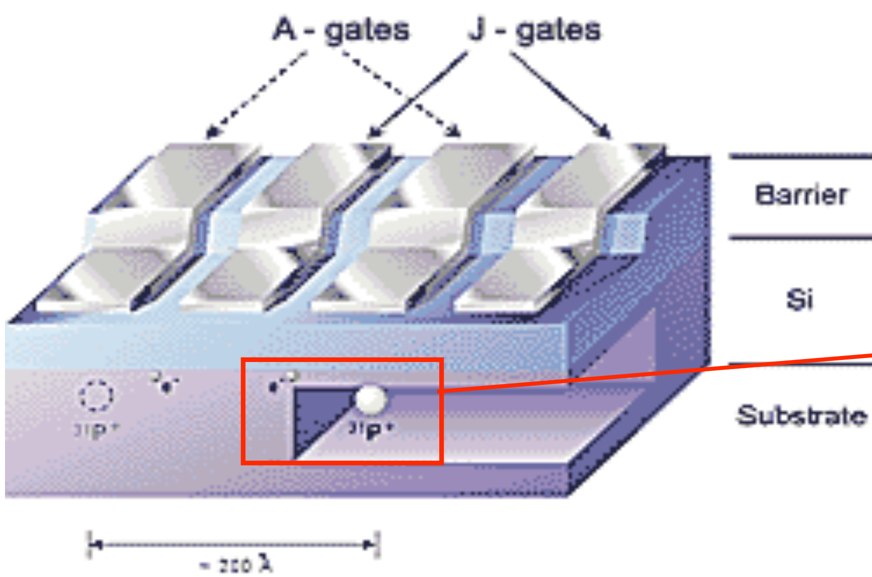
Semiconductor Nanofabrication Facility, School of Physics, University of New South Wales, Sydney 2052, Australia

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.

B.E.Kane, Nature (1998).

<u>Motivations</u>:

- ➢**Highly coherent donor spins** (G. Feher, PR, 1959, 1961, $T_{1e} \sim 10^3$ s; latest measured $T_{2e} \sim 0.3$ s);
- ➢**Identical QDs**;
- ➢Scalable Si technology;
- ➢Exchange coupling between donor confined electrons like in QDs;



P donors in Si

From the website of SNF at the University of New South Walws Sydney, Australia

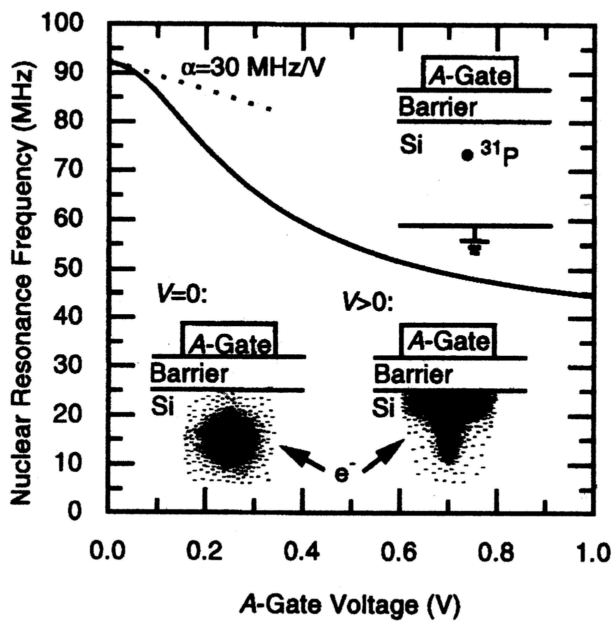
Quantum computation with a ^{31}P array in silicon

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[15]. Because the electron is sensitive to externally applied electric fields, the hyperfine inter-

Building Blocks of Kane's QC Proposal

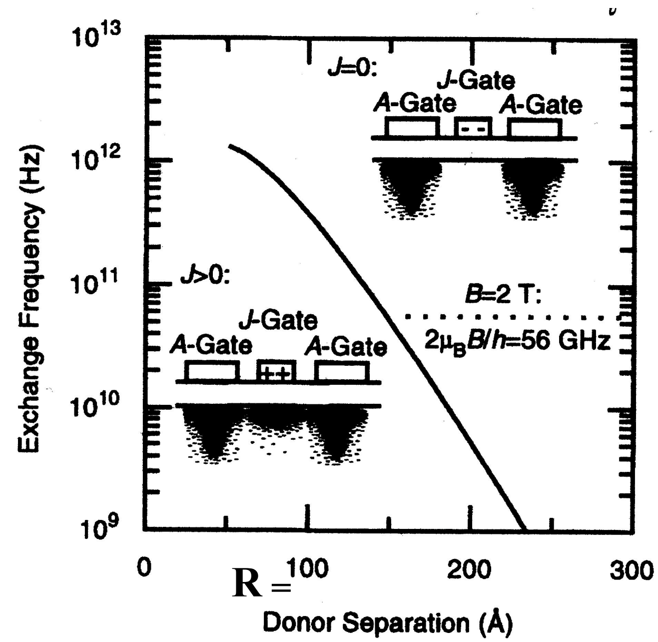
- Qubits are the ^{31}P nuclear spins (I = 1/2) in the Kane proposal
- Electron spin exchange interaction for two-qubit operations

1-qubit operations



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

2-qubit operations

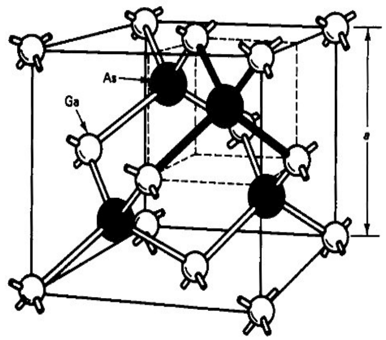


$$H(R) = H(B) + A_1\sigma_z^{1e}\cdot\sigma_z^{1n} + A_2\sigma_z^{2e}\cdot\sigma_z^{2n}$$
$$+ J(R)\,\sigma_z^{1e}\cdot\sigma_z^{2e}$$

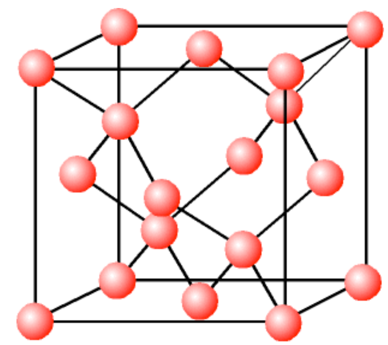
EXCHANGE

Energy Bandstructures of GaAs and Si

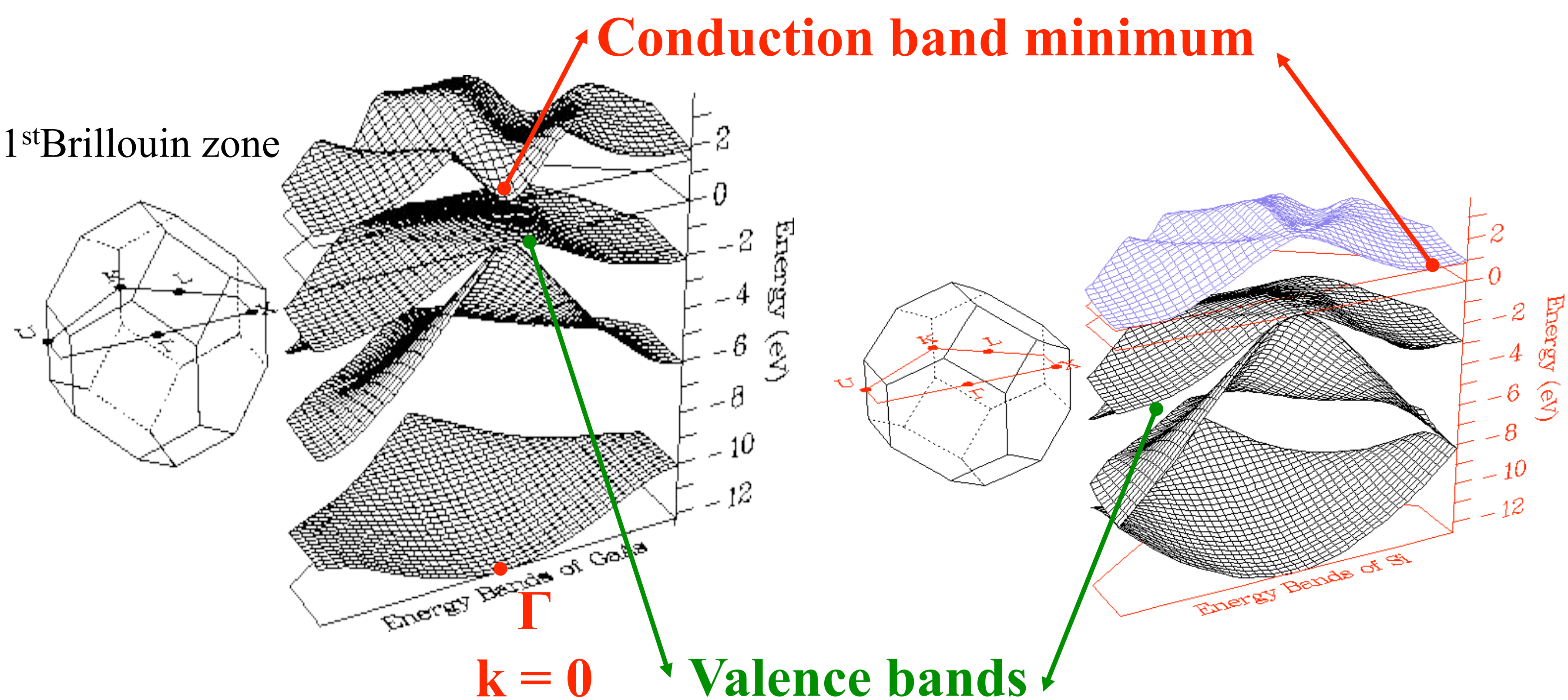
GaAs



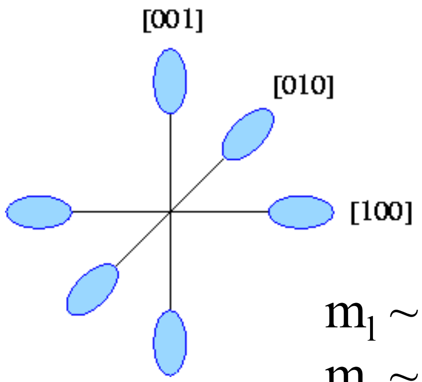
$$\varepsilon_n(\vec{k})$$



Si

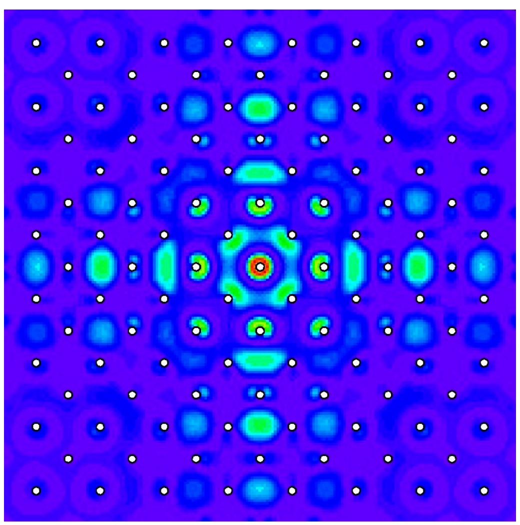


Effective of Valleys on Electron States



$m_l \sim 0.9\ m_0$
$m_t \sim 0.2\ m_0$

Conduction band Minimum:
Anisotropic and six-fold degenerate



Koiller et al, PRB (2004).

Single-electron wave function:

$$\psi(\mathrm{r}) = \sum_{\mu=1}^{6} \frac{1}{\sqrt{6}} F_\mu(\mathrm{r}) \phi_\mu(\mathrm{r})$$

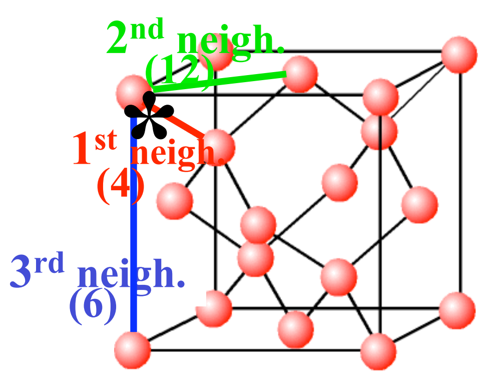
Bloch functions:

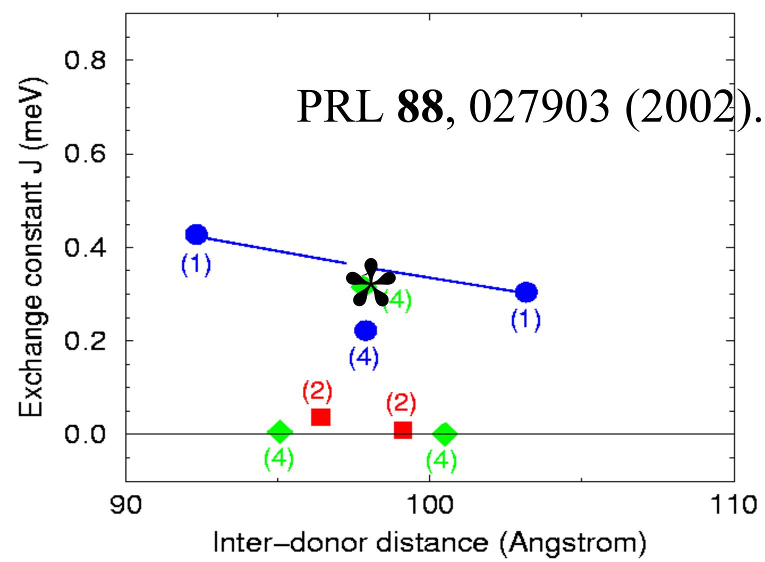
$$\phi_\mu = u_\mu(\mathbf{r}) e^{i\mathbf{k}_\mu \cdot \mathbf{r}},$$

$$u_\mu(\mathbf{r}) = \sum_{\mathbf{K}} c_\mu^{\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{r}}$$

Two-donor exchange:

$$J(\mathbf{R}) = \sum_{\mu,\nu} |\alpha_\mu|^2 |\alpha_\nu|^2 \mathbf{J}_{\mu\nu}(\mathbf{R}) \cos(\mathbf{k}_\mu - \mathbf{k}_\nu) \cdot \mathbf{R}$$

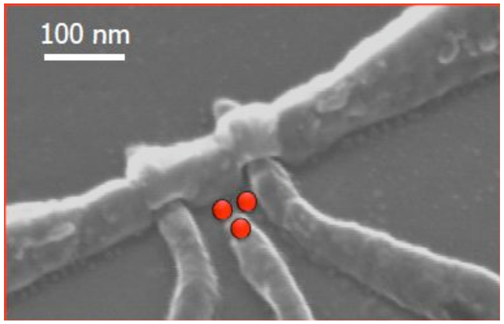


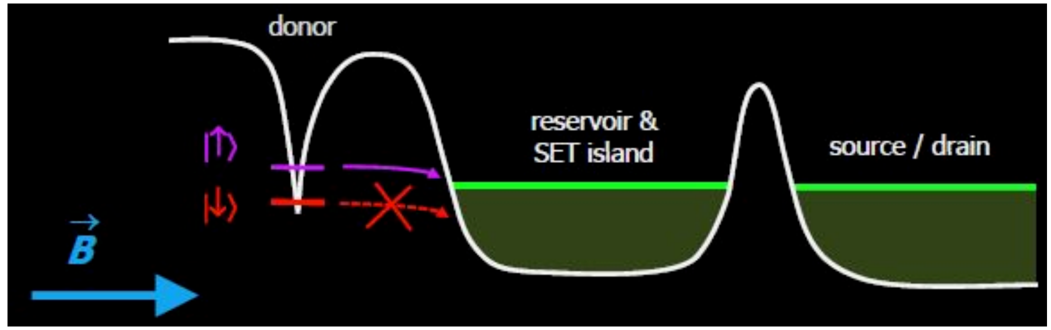


PRL **88**, 027903 (2002).

Detecting Donor Electron Spins with an SET

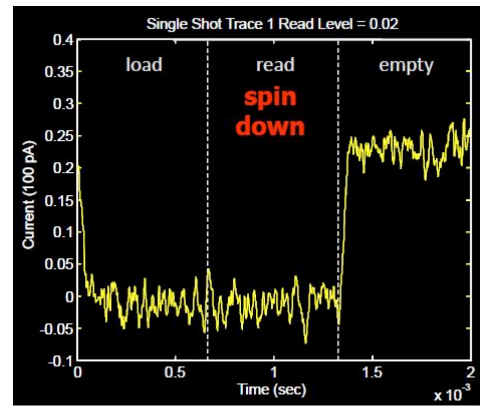
Andrea Morello, UNSW

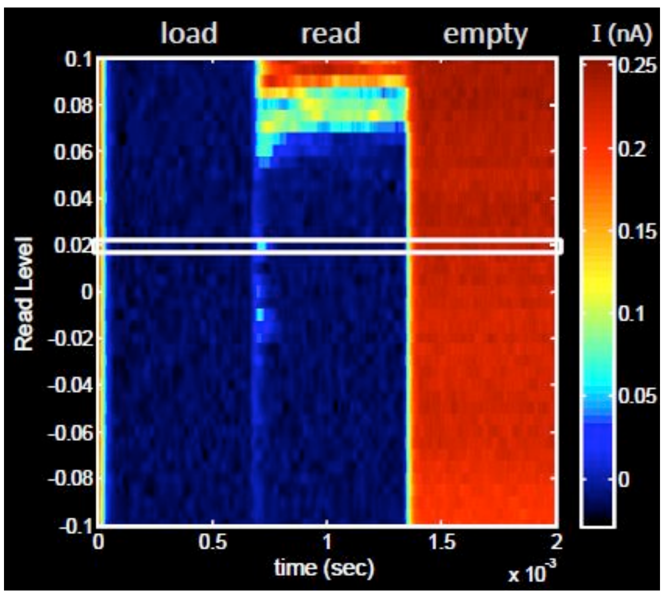


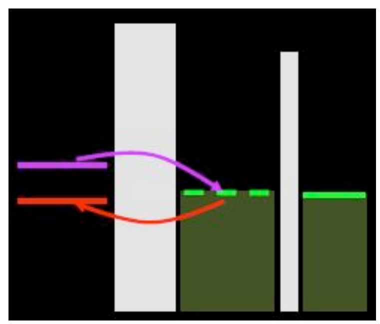


3 donors in a 30×30 nm^2 area.

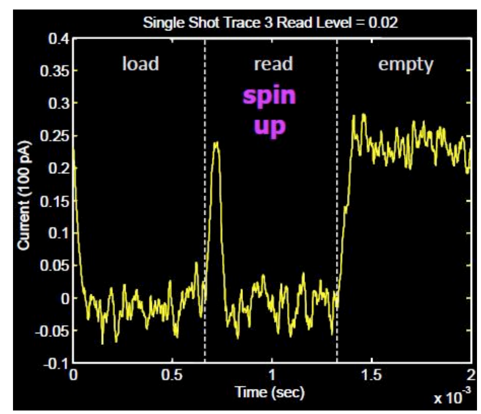
Spin down, cannot tunnel out







Spin up, tunnel out, then spin down comes in

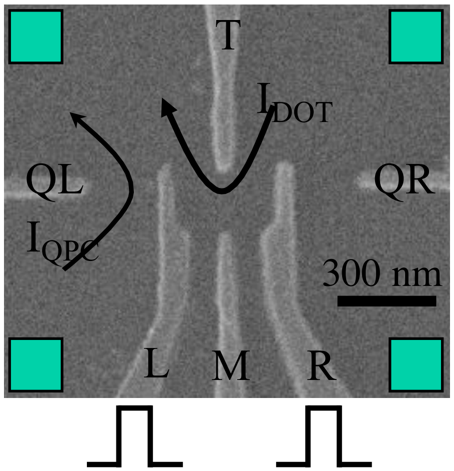


Similar to Elzerman et al, Nature (2004), in a GaAs dot.

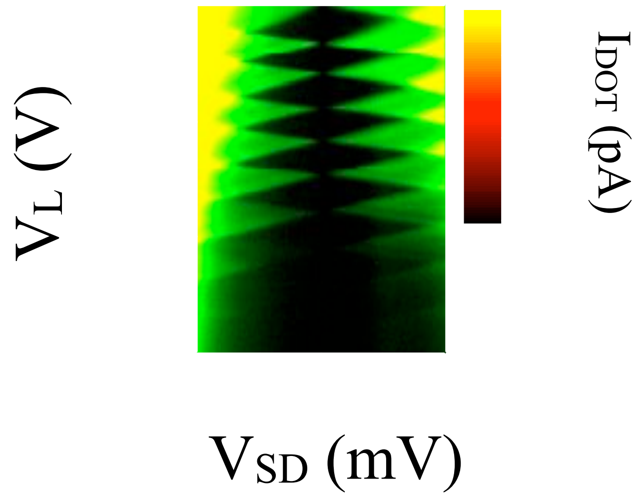
One-Electron Single & Double Quantum Dots in Si/SiGe

Mark Eriksson, Wisconsin

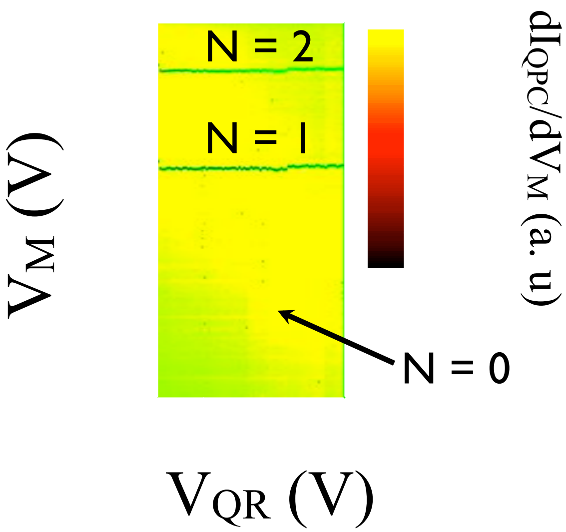
Gate layout



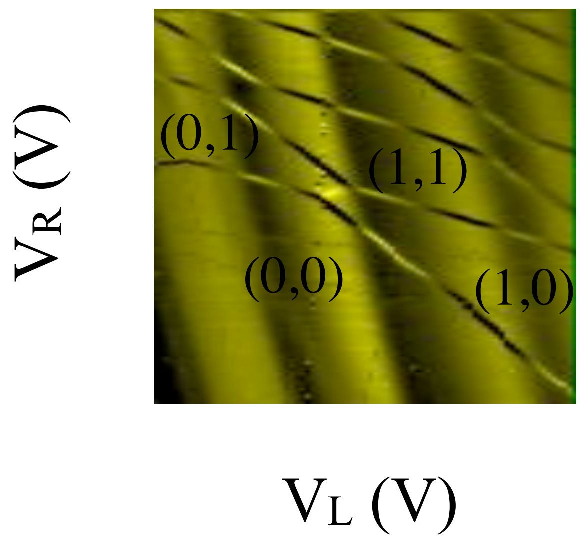
Coulomb diamonds



One-electron dot

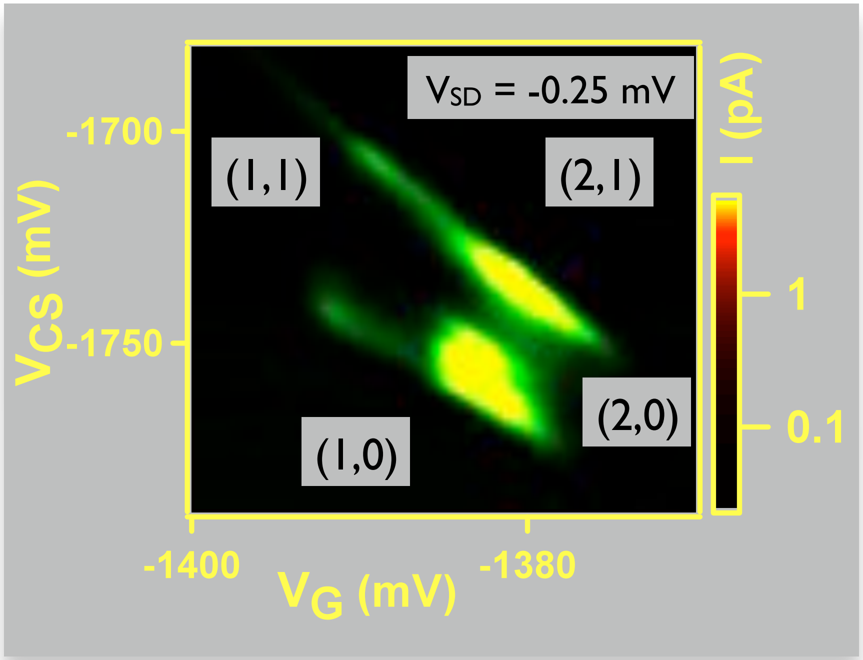


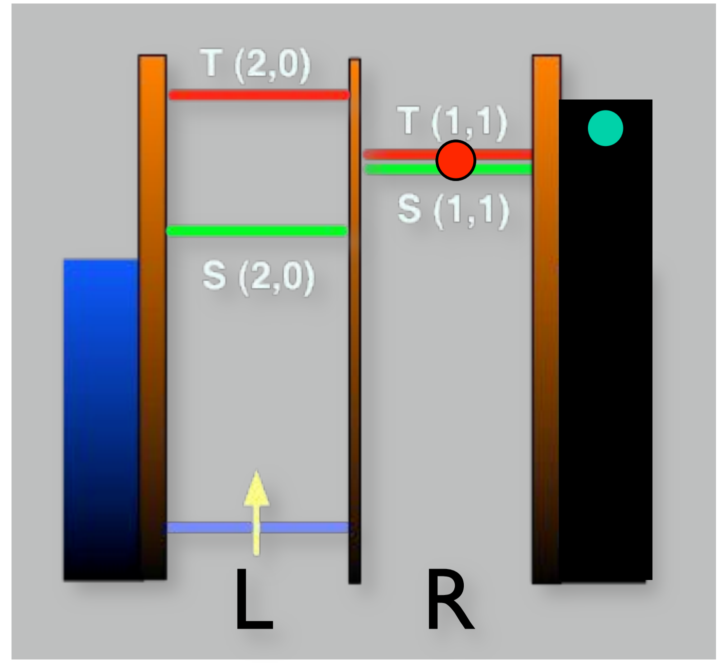
One-electron double dot



C.B. Simmons et al., Appl. Phys. Lett. **91**, 213103 (2007); M. Thalakulam et al., in preparation.

Spin Blockade in a Si/SiGe Double Quantum Dot

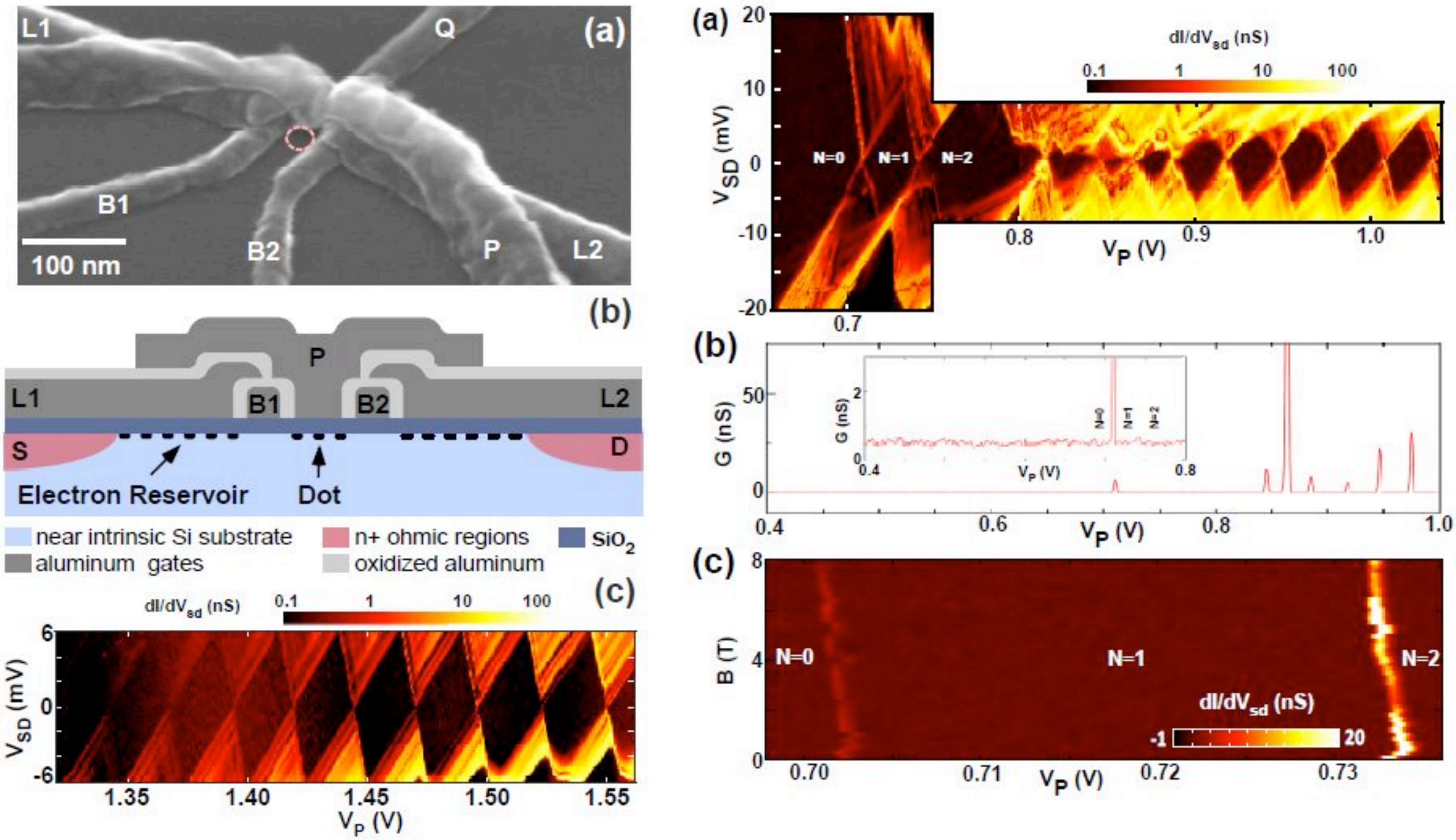




Mark Eriksson, Wisconsin

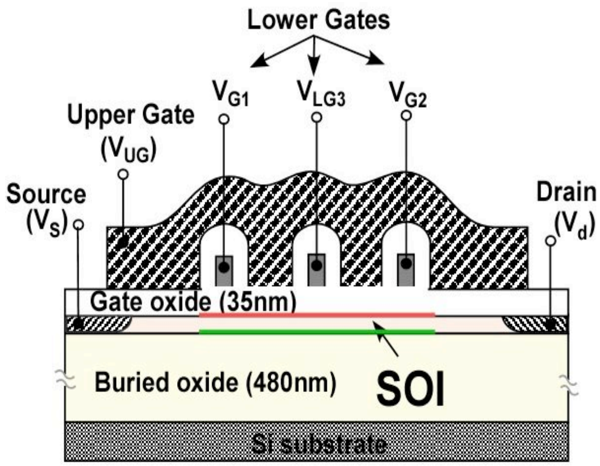
N. Shaji et al., Nature Physics 4, 540 (2008).

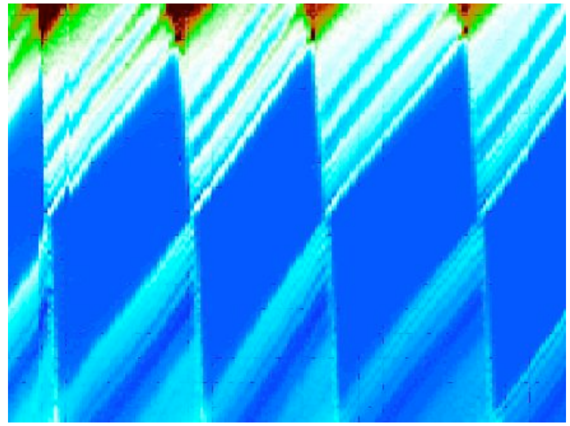
Getting to a Single Electron Quantum Dot At the Si/SiO$_2$ Interface



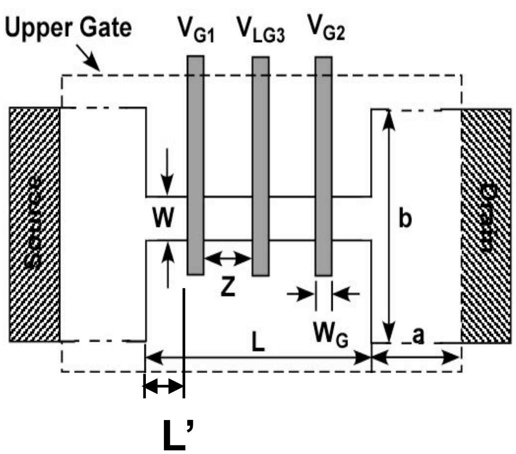
W.H. Lim et al. (UNSW group), aXiv:0910.5796

Si Quantum Dot in SOI

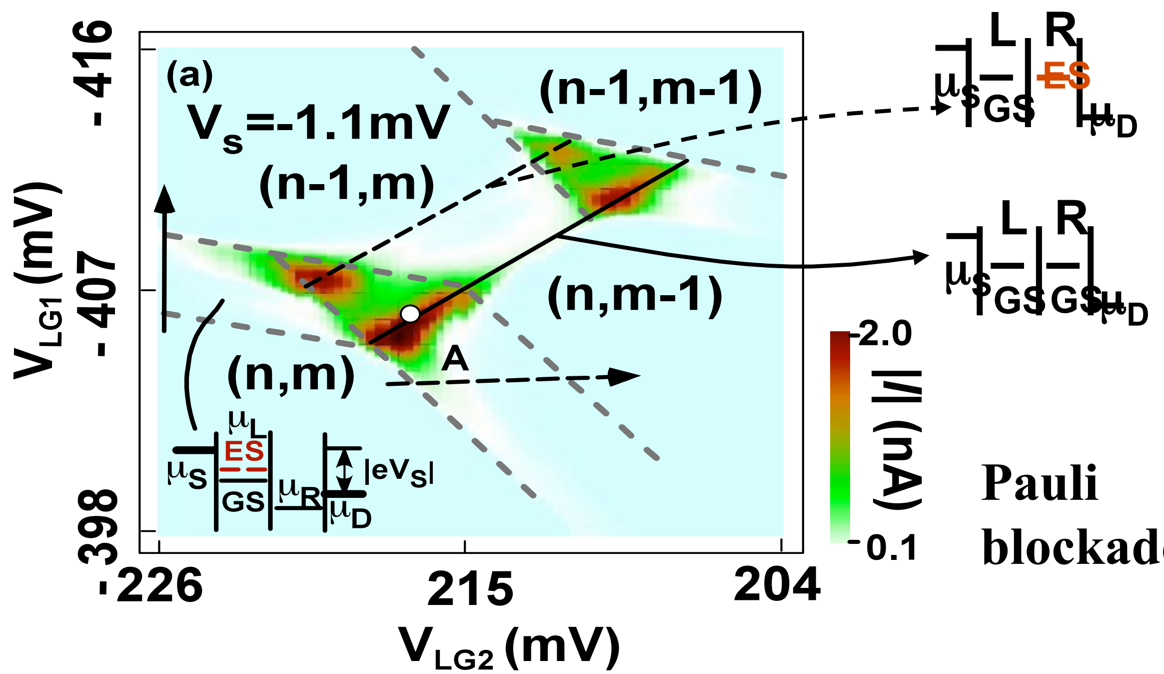




Tunneling spectroscopy of a single dot. Excited states observed. Minimum number of electrons: ~ 10



A structure with very smooth interfaces



Pauli blockade

H.W. Liu, Sendai H.W. Liu et al., PRB **77**, 073310 (2008); APL **92**, 222104 (2008).

Major Si-Based Spin QC Schemes: Experimental Status

Donors

- MBE growth of donor arrays;
- Implantations of a small number of P at a designated location;
- Single spin detection;

SiGe QD

- Single dot and double dot with controllable number of electrons;
- Spin-blockade;
- Charge sensing
- Tunable tunneling;
- Single-shot measurement?
- Finite valley splitting?

Si/SiO_2 QD

- Single-electron dot?
- Spin blockade;
- Excited states spectroscopy;

Major Theoretical Issues in Spin QC in Silicon

Quantum coherence:
- Single spin coherence;
- Multi-spin coherence;

Valley splitting in a Si heterostructure:
- What determines valley splitting;

Implications of valleys in a Si nanostructure:
- Single-spin manipulation;
- Two-spin manipulation;

Major Theoretical Issues in Spin QC in Silicon

Quantum coherence:

- **Single spin coherence**;
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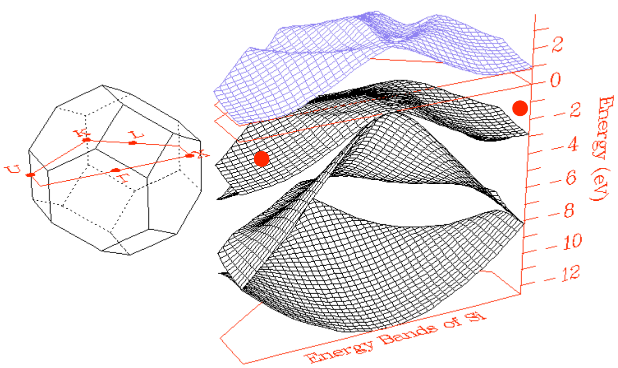
- Two-spin manipulation;

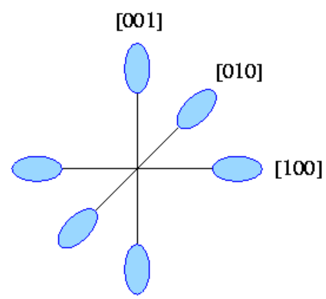
Hamiltonian for a Localized Electron Coupled to Nuclear Spins in Si

$$H = \boxed{H_{electron + SO}} + H_{Zeeman} + H_{hyperfine} + H_{nuclear\ dipole} + \boxed{H_{nuclear\ quadrupole}}$$

Weak in Si (under $H_{electron + SO}$) — **Absent in Si** (under $H_{nuclear\ quadrupole}$)

$$H_{hyperfine} = \sum_i \vec{S} \cdot \overleftrightarrow{A}_i \cdot \vec{I}_i = \sum_i A_i \vec{S} \cdot \vec{I}_i + \boxed{H_{anisotropic\ HF}}$$

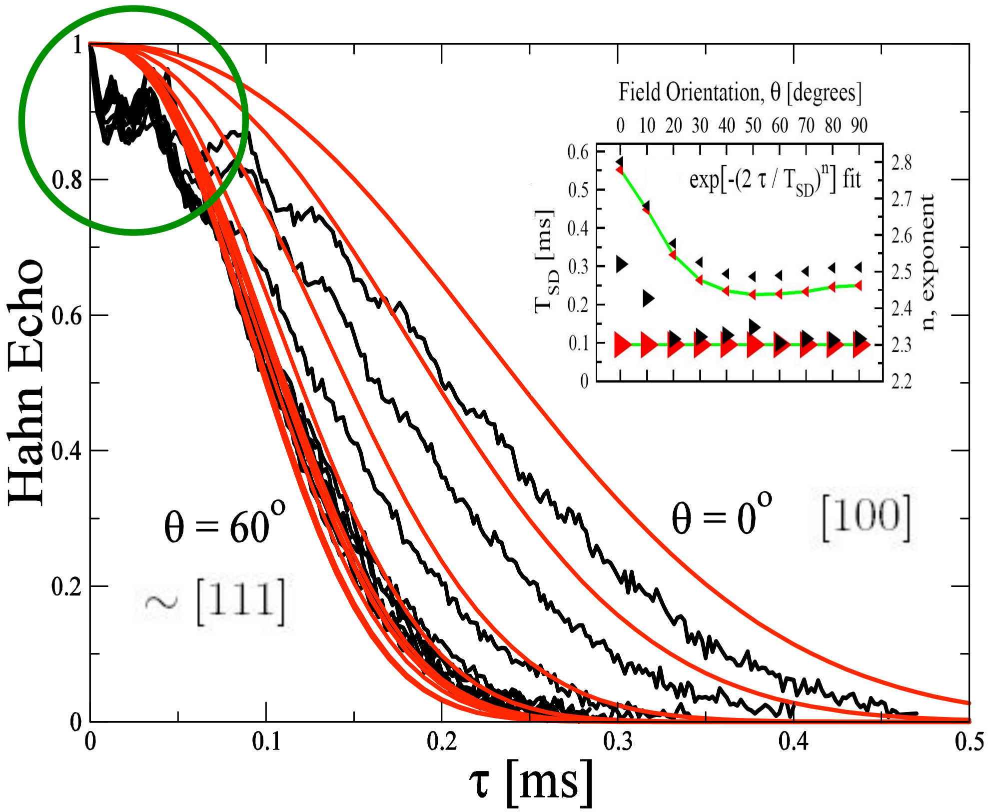




States at the bottom of Si conduction band have strong P and D atomic orbital components.

$$H_{nuclear\ dipole} = \sum_{i,j} \vec{I}_i \cdot \vec{B}_{ij} \cdot \vec{I}_j = \sum_{i,j} \frac{\mu_0}{4\pi\hbar} \frac{g_n^2 \mu_n^2}{r_{ij}^3} \left[\vec{I}_i \cdot \vec{I}_j - \frac{3}{r_{ij}^2} \left(\vec{I}_i \cdot \vec{r}_{ij}\right)\left(\vec{I}_j \cdot \vec{r}_{ij}\right) \right]$$

Decoherence from Spectral Diffusion in Si:P: Theory/Experiment Comparison



Electron spectral diffusion comes from nuclear dipolar interaction through Overhauser field:

$$H = \sum_{i}^{N} A\,|\psi(\mathbf{R}_i)|^2\ \hat{I}_i^z \hat{S}^z + \sum_{ij} B_{ij}\left(2I_i^z I_j^z - I_i^+ I_j^-\right)$$

Electron-mediated nuclear spin interaction induced dephasing can be corrected by spin spin echo.

W. Witzel and S. Das Sarma, Phys. Rev. B **72**, 161306(R) (2005); **74**, 035322 (2006).

What about the rapid drop initially and the oscillation thereafter?

General Form of Hyperfine Interaction

Hyperfine interaction is in essence dipolar coupling between electron and nuclear spins. As such it is in general anisotropic.

$$\mathcal{H}_{HF} = \boldsymbol{I} \cdot \boldsymbol{A} \cdot \boldsymbol{S}$$

$$\boldsymbol{A}_{ij} = \gamma_I \gamma_S \left(\frac{8\pi}{3} \left| \Psi(\mathbf{0}) \right|^2 \delta_{ij} + \boxed{\left\langle \Psi \left| \frac{3x_i x_j - \boldsymbol{r}^2 \delta_{ij}}{\boldsymbol{r}^5} \right| \Psi \right\rangle} \right)$$

Strong Applied Field (> 0.1 T):

$$\mathcal{H} = \mathcal{H}_0 + \sum_n \mathcal{H}_n$$

$$\mathcal{H}_0 = \omega_S S_z + A_P S_z I_z^P - \omega_P I_z^P,$$

$$\mathcal{H}_n = \boxed{A_n} S_z I_{nz} + \boxed{B_n} S_z I'_{nx} - \omega_I I_{nz}$$

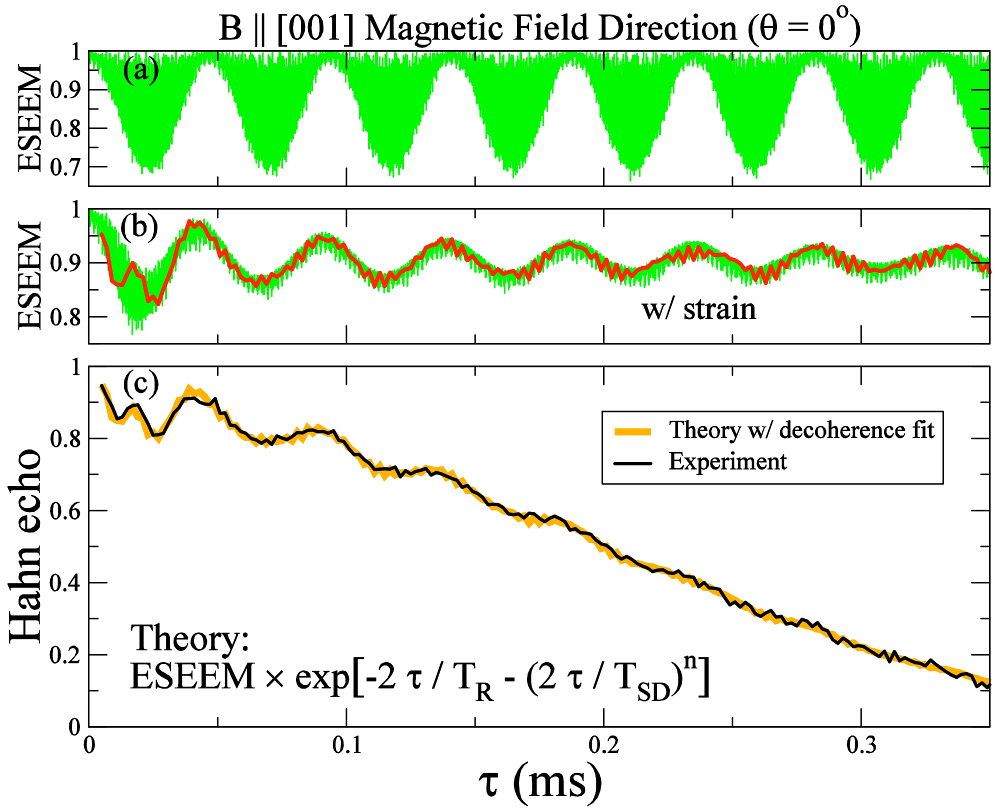
A_n ← A_{zz}

B_n ← $\sqrt{A_{xz}^2 + A_{yz}^2}$

Anisotropic hyperfine is important in Si:P, not so important in GaAs

S. Saikin and L. Fedichkin, PRB **67**, 161302 (2003).

Electron Spin Echo Envelope Modulation (ESEEM) in Si:P



ESEEM:

➢Mims, PRB **5**, 2409 (1972);

➢A. Schweiger and G. Jeschke, Principles of Pulse Electron Paramagnetic Resonance

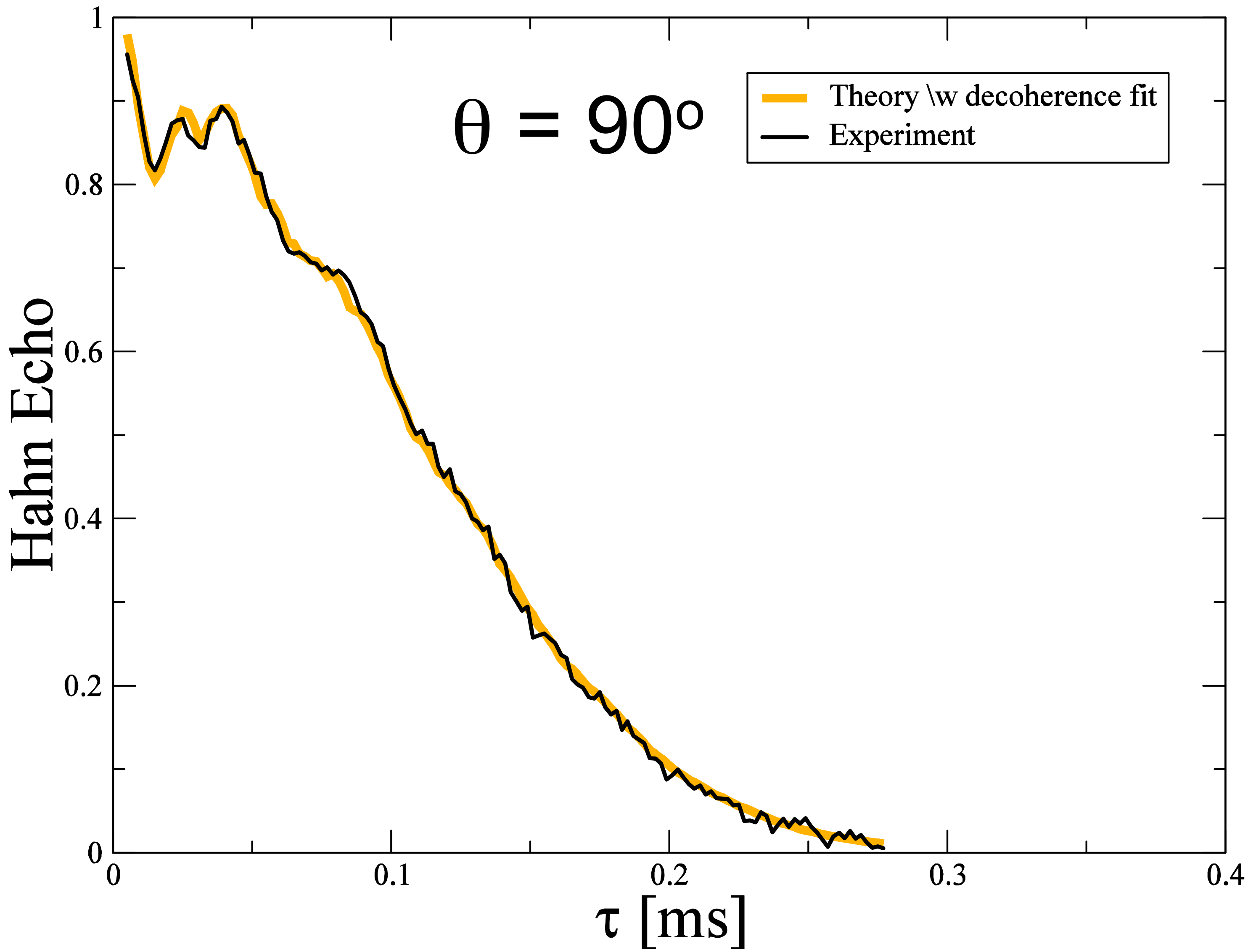
➢A 0.4% distribution of strain (which causes repopulation) is used to produce a distribution of ESEEM frequency.

➢Exponential decay from spin relaxation;

➢Super-exponential decay from spectrum diffusion;

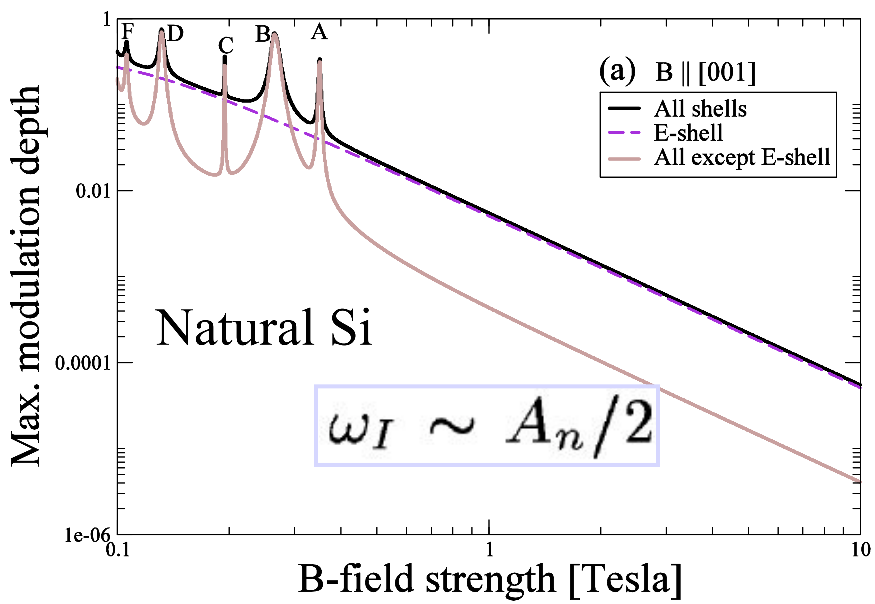
W. Witzel et al., cond-mat/0701341, PRB 76, 035212 (2007).

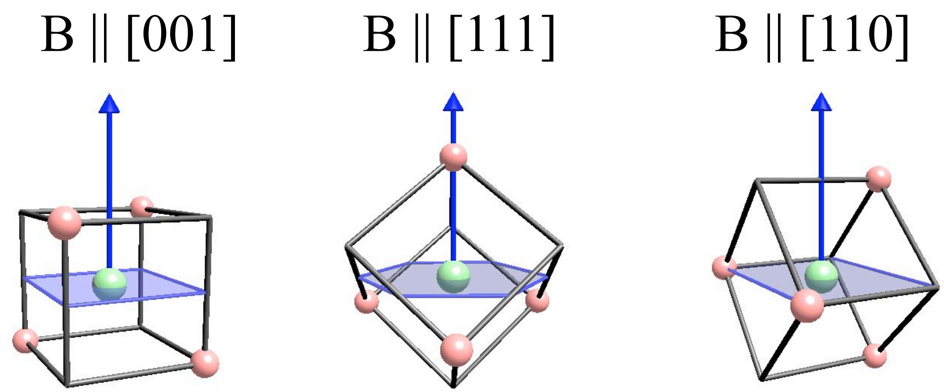
Si:P Fit with Experiment



Fit: $\exp[-(2\tau/T_R)-(2\tau/T_{SD})^n]$

Overcoming ESEEM





Under these fields the nearest neighbor sites all have the same echo modulation frequency, thus can be periodically removed.

➢Strong resonance behavior because ESEEM is the strongest when there is **cancellation of Zeeman and HF spitting**;

➢Anisotropic HF effects **dominated by the nearest neighbor sites** to the donors;

➢**Nearly complete understanding of Si:P donor electron decoherence!**

Major Decoherence Channels of A Quantum Dot Confined Electron Spin

Single Spin States:

- Low temperature to freeze out the orbital degrees of freedom;
- Spin environment from paramagnetic impurities (MOS QDs);
- Hyperfine coupling to nuclear spins + nuclear dynamics;
  - ✓Nuclear dynamics due to magnetic dipole interaction;
  - ✓Nuclear dynamics due to hyperfine interaction;
  - ✓…
- Spin-orbit interaction + electron-phonon interaction;

Need accurate knowledge of hyperfine interaction!

Hyperfine Interaction for a Conduction Electron in Si

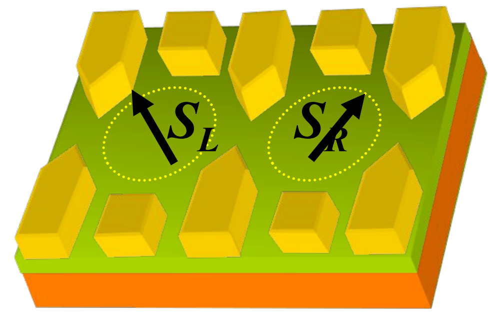
➢Important parameter for both electron spin decoherence and manipulation in Si quantum dots

✓Nuclear spin induced decoherence depends on the strength of hyperfine interaction;
✓Manipulation of two-spin states with inhomogeneous magnetic fields could use the Overhauser field, [for example, Petta et al (2005)].

➢Hyperfine interaction not well characterized theoretically. Not previous calculation exists for conduction electrons in Si.

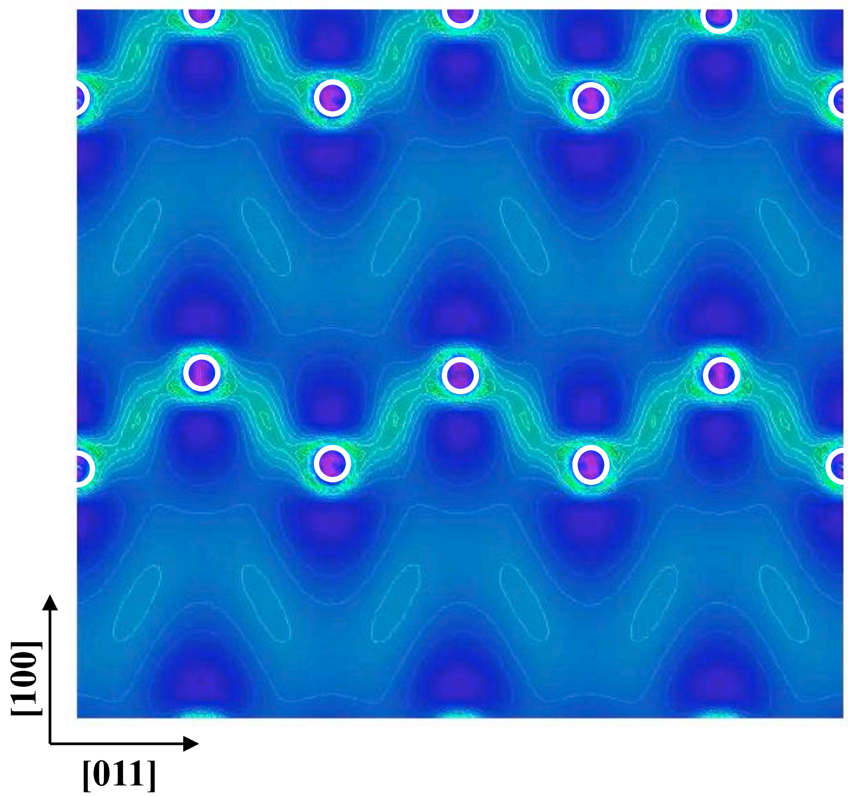
➢Pseudopotential method not reliable near the nuclei;

➢**All-electron approach (APW, WIEN2K package)**; Largest supercell size N = 64; Spin-orbit interaction included; Electron interaction described within the density functional framework.

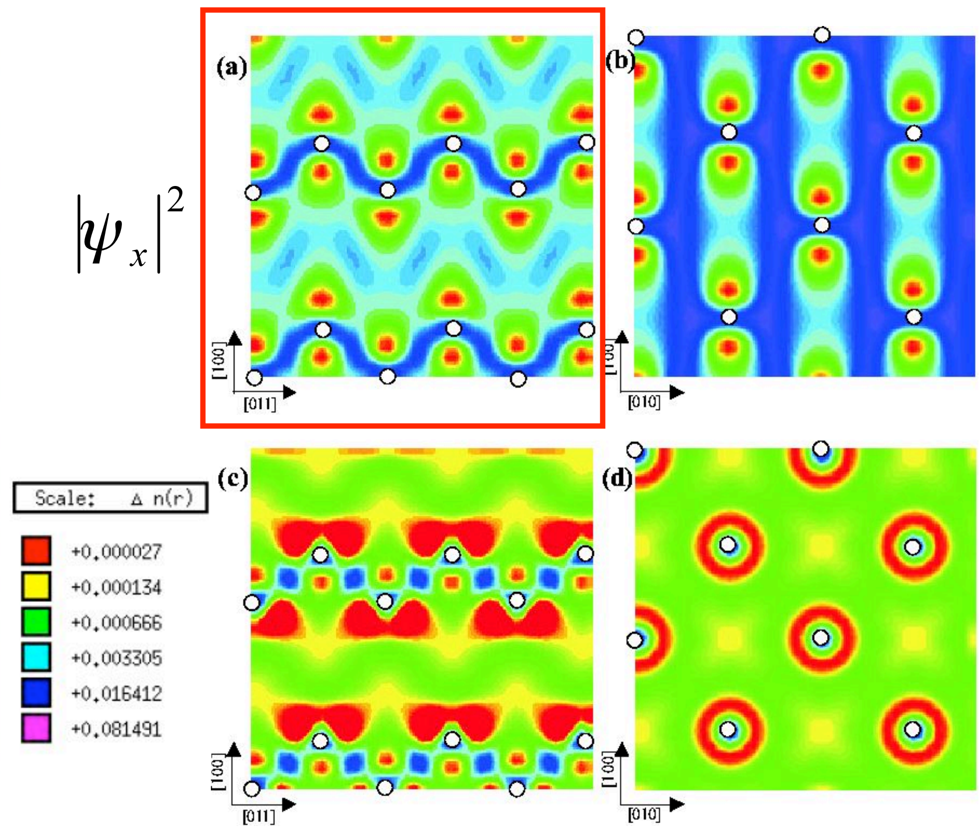


In SiGe heterostructures (Wisconsin, Purdue, Princeton, …) or SiMOSFET (Sandia, UCLA, NTT, UNSW, …)

Spin Density in Singly Negatively Charged Si



L.V.C. Asalli et al., in preparation.



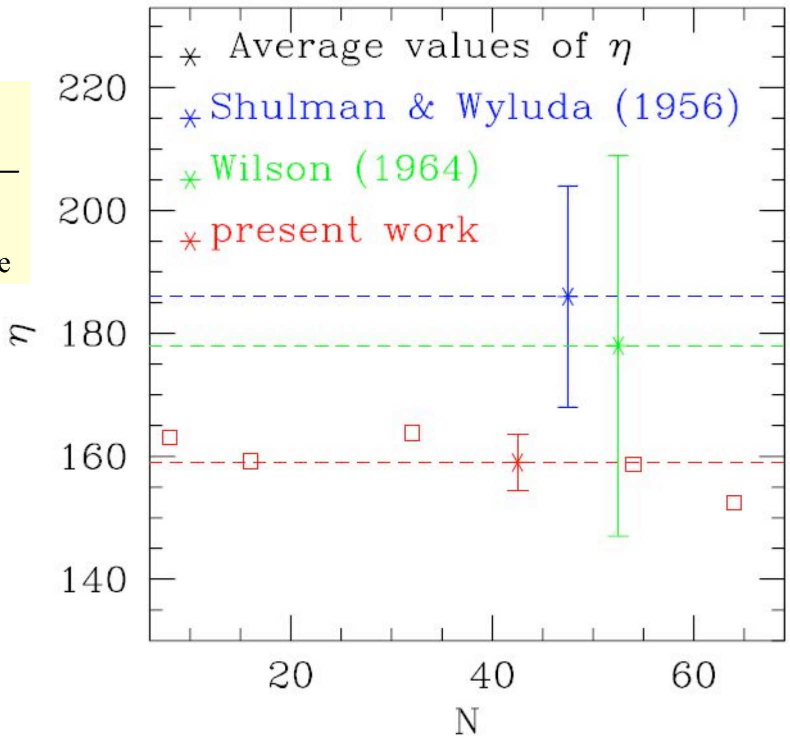
Koiller et al., PRB (2004).

Results in the interstitial region comparable to those obtained with pseudopotential method. On site the electron probability is much higher in the all-electron calculation.

Electronic Probability in the Core Region: Compared to Experimental Measurements

Definition:

$$\eta = \frac{|\psi(0)|^2}{\langle|\psi|^2\rangle_{ave}}$$



For comparison, in GaAs

$$\eta_{Ga} = 2700 \text{ and } \eta_{As} = 4500$$

With pseudopotential method

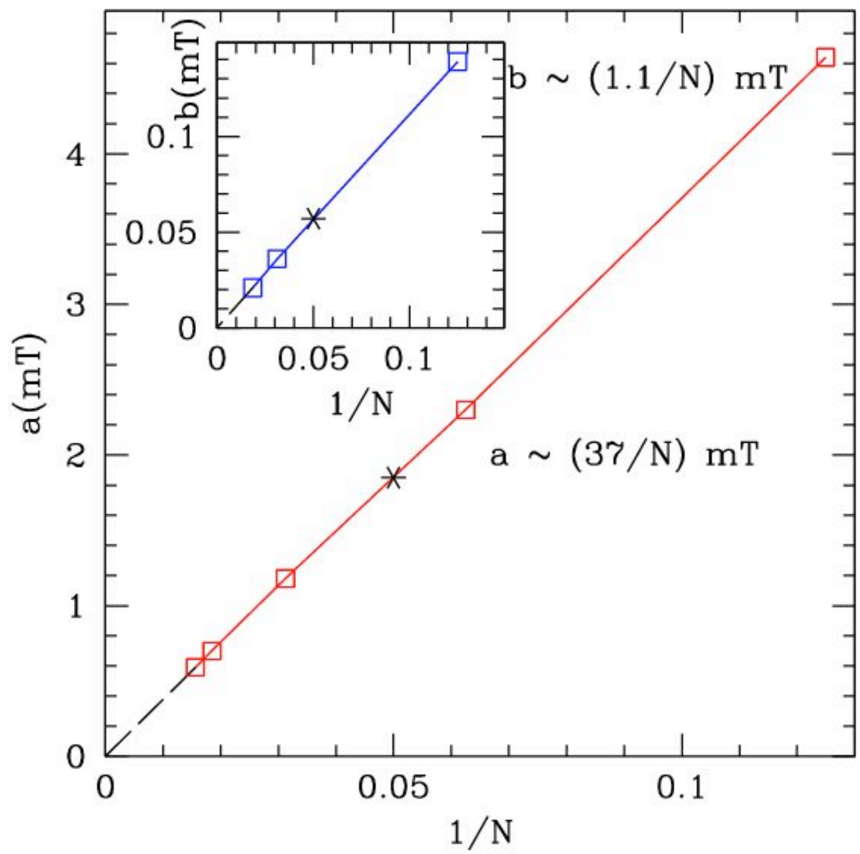
$$\eta_{Si}^{pp} \sim 3$$

Our calculation:

$$\eta_{Si} = 159.4 \pm 4.5$$

- Shulman and Wyluda, Phys. Rev. **103**, 1127 (1956), spin-lattice relaxation measurement $\eta = 186 \pm 18$
- I. Solomon, in D.K. Wilson, Phys. Rev. **134**, A265 (1964), spin-lattice relaxation measurement $\eta = 178$.
- Dyakonov and Denninger, Phys. Rev. B **46**, 5008 (1992), Overhauser field measurement, about twice as large as 180. η value not given.

Hyperfine Interaction Strengths in Si



- "N" size of the supercell. For natural Si, there is about 5% ^{29}Si;
- "a" contact hyperfine strength; a ~ 1.9 mT for N = 20.
- "b" anisotropic hyperfine strength when the electron is in a single valley, about 3% of "a".

Hyperfine Interaction in a Quantum Dot: GaAs and Natural Si

	QD size (# of atoms)	# of nuclei with finite spin	Maximum Overhauser field	Random Overhauser field	T_2^*
GaAs	10^6	10^6	100 μeV	0.1 μeV	10 ns
Natural Si	10^6	5×10^4	200 neV	1 neV	1 μs
Natural Si	10^5	5×10^3	200 neV	3 neV	300 ns
^{29}Si	10^5	10^5	4 μeV	10 neV	100 ns

The T_2^* time in Si QD will be 1~ 2 orders of magnitude longer than in GaAs!

Major Theoretical Issues in Spin QC in Silicon

Quantum coherence:

- Single spin coherence;
- Multi-spin coherence;

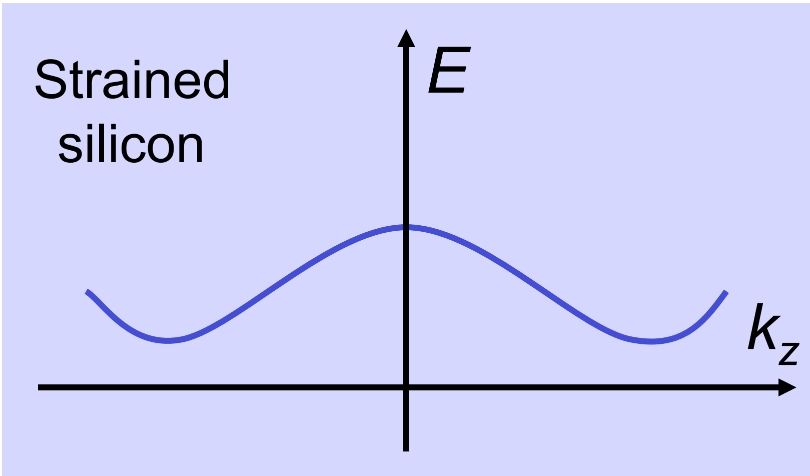
Valley splitting in a Si heterostructure:

- **What determines valley splitting**;

Implications of valleys in a Si nanostructure:

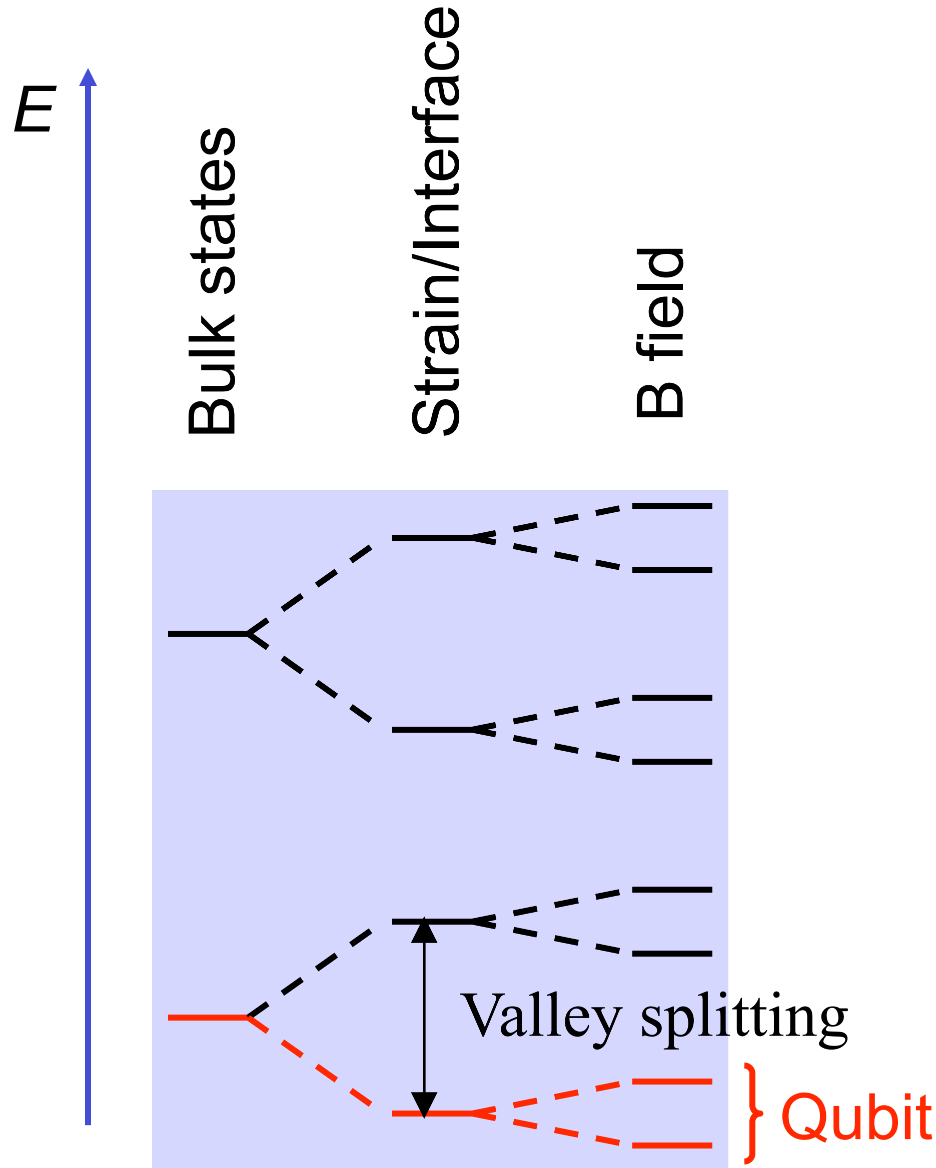
- Single-spin manipulation;
- Two-spin manipulation;

Why Do We Care about Valley Splitting in Si



Valley degeneracy is broken by strain, interface and confinement

Are the qubit states well separated from higher excited states?



qc.physics.wisc.edu

M. Friesen

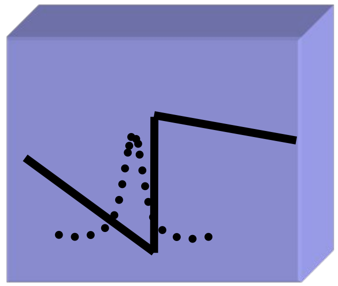
Works on valley splitting at an interface

- Ohkawa and Uemura, JPSJ **43**, 907 and 917 (1977);
- Sham and Nakayama, PRB **20**, 734 (1979).
- T. Ando et al., RMP **54**, 437 (1982).
- …
- T.B. Boykin et al., APL **84**, 115 (2004).
- T.B. Boykin et al., PRB **70**, 165325 (2004).
- N. Kharche et al., APL **90**, 092109 (2007).
- M. Friesen et al., PRB **75**, 115318 (2007).
- S. Chutia et al., PRB **77**, 193311 (2008).
- …
- A. Saraiva et al., PRB **80**, 081305 (2009).
- …

Effective Mass Theory: Single Step Model

$$H_0 ® 2 \varsigma_{q=x,y,z} \frac{\hbar^{22}}{2m_q} \frac{\Leftarrow}{\Leftarrow^2}$$

$$U(z)(z)(z) 2 \frac{F}{J} 2 \quad I$$

⇨ 

Effective Mass Approx. for a valley with anisotropic mass

$$U(z) = U_0 \Theta(z - z_I)$$

Finite Differences Method

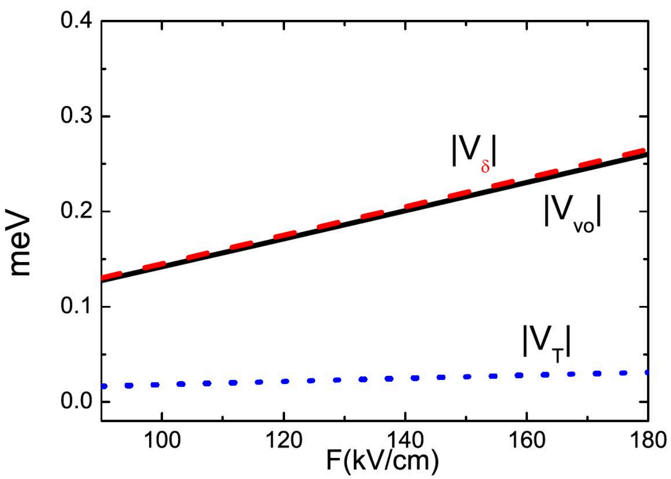
$$\left\{ \frac{-\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + U(z) - Fz \left[\Theta(-z + z_I) + \eta \Theta(z - z_I) \right] \right\} \Psi(z) = E \Psi(z)$$

$$\phi_{\pm} = \Psi(z) e^{\pm i k_0 z} \sum_{\mathbf{G}} c_{\pm}(\mathbf{G}) e^{i \mathbf{G} \cdot \mathbf{r}}$$

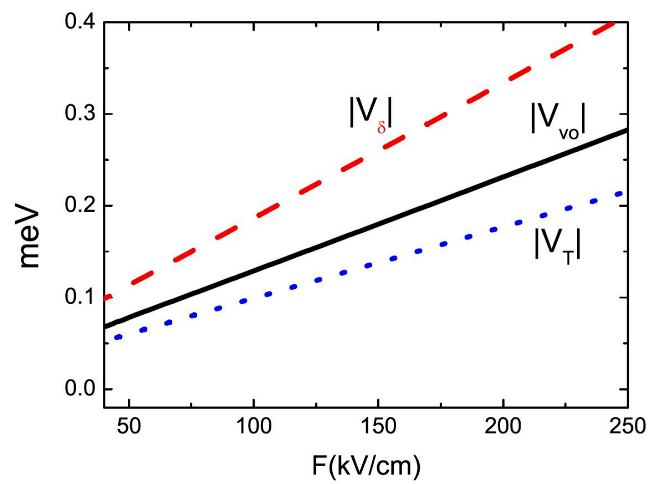
From psuedopotential calc.

Valley Splittings: Calculated Results

U_0 = 150 meV ~ SiGe



U_0 = 3 eV ~ SiO_2

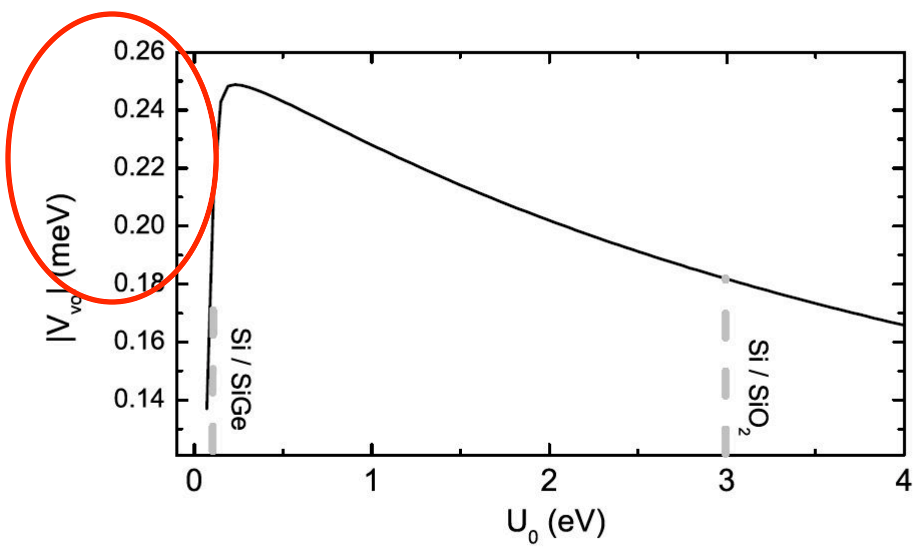


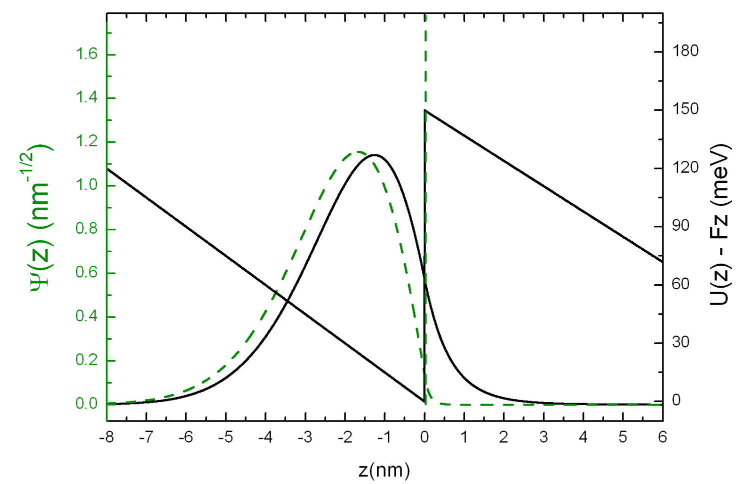
interface

$$V_{vo} = V_\delta + V_T + V_F$$

Evanescent wave

field





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- **Two-spin manipulation**;

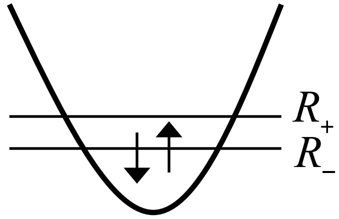
Two-Electron States in a Single Si Quantum Dot

Let us define the single-dot (right dot) ground orbital states in the two valleys as R_+ and R_-.

The two-electron states that can be constructed from these orbitals are thus:

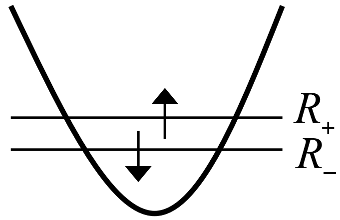
- Both electron in the lower valley: 1 singlet

$$S(02,--)=R_-R_-\times\frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle-\left|\downarrow\uparrow\right\rangle\right)$$



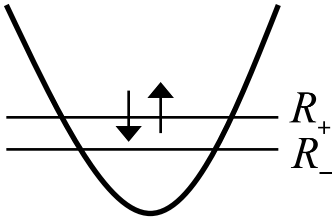
- One electron each in the two valleys: 1 singlet and 1 triplet

$$\begin{matrix}S\\T\end{matrix}(02,+-)=\frac{1}{\sqrt{2}}\left(R_+(1)R_-(2)\pm R_+(2)R_-(1)\right)\times\frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle\mp\left|\downarrow\uparrow\right\rangle\right)$$

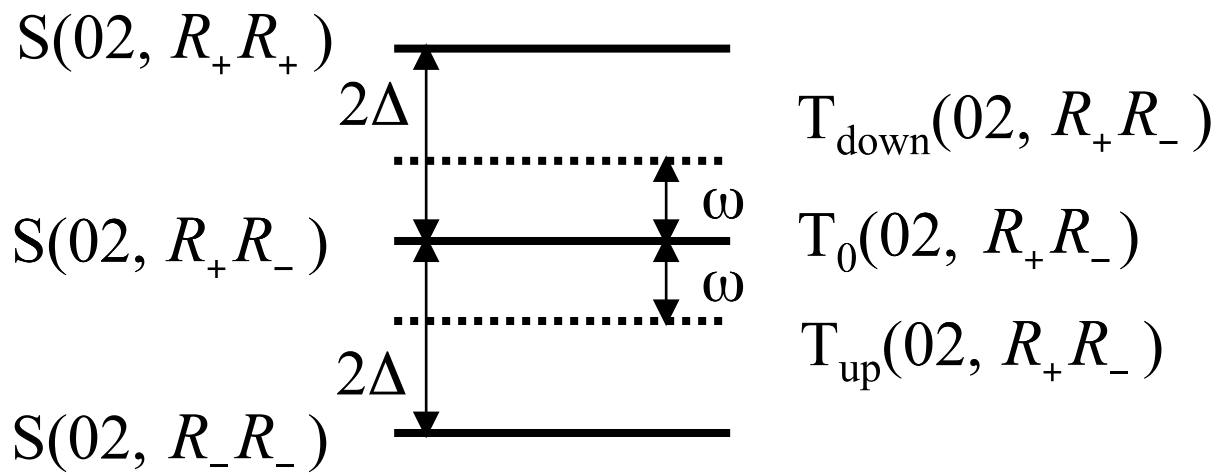


- Both electron in the higher valley: 1 singlet

$$S(02,++)=R_+R_+\times\frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle-\left|\downarrow\uparrow\right\rangle\right)$$



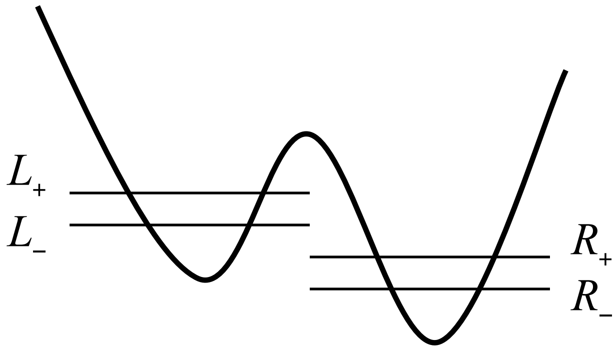
Two-Electron States in a Si Quantum Dot In a Finite Magnetic Field



- The two polarized triplet states are split from the unpolarized triplet by an energy ω. If $\omega > 2\Delta$, one of the triplet would be the ground state.
- The only non-exponentially-small inter-valley contribution by the Coulomb interaction is (very small, < 0.2 μeV):

$$\int d1\,d2\,\left[R_+^*(1)R_-(1)\right]\left[R_-^*(2)R_+(2)\right]V_{ee}(1,2)$$

Two-Electron States in a Si Double Dot: How Many HM States?



In each dot there are two ground orbital states, thus there are totally 4 orbital states for the double dot:

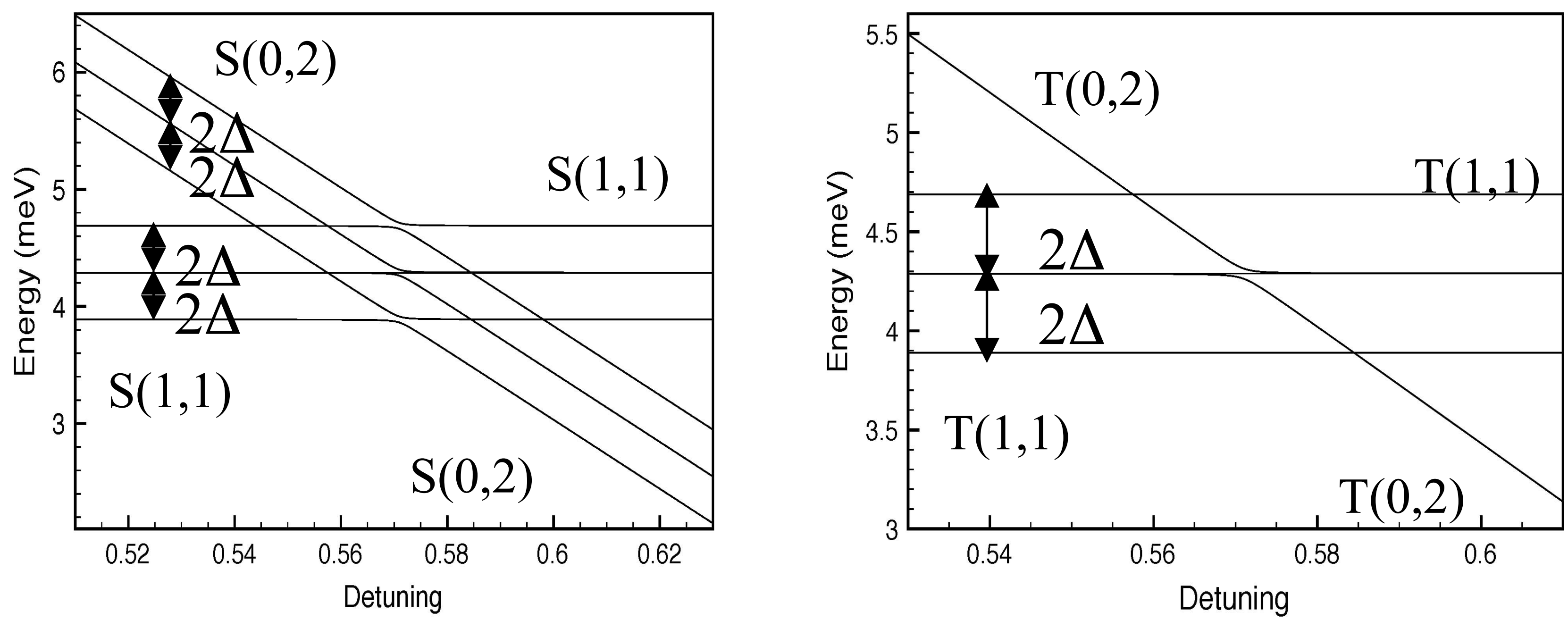
$$L_-, L_+, R_-, R_+$$

Possible (02) states: 3 singlet (--,+-,++), 1 triplet (+-). There are **6 states**.

Possible (11) states: 4 singlet (--,-+,+-,++), and 4 triplet (--,-+, +-,++). There are totally **16 states**.

We do not consider (20) states.

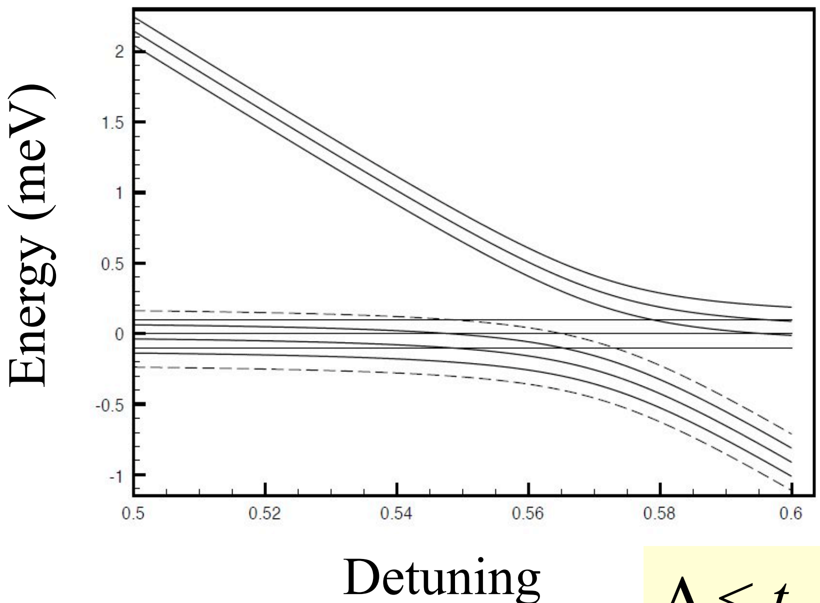
Two-Electron States in a Biased Si Double Dot: Large Valley Splitting Limit



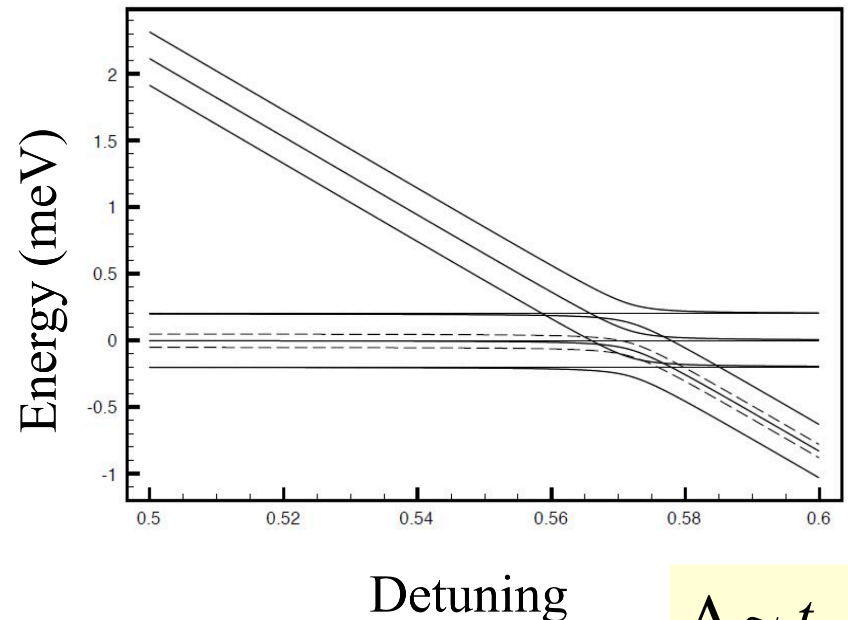
At the limit of **large valley splitting and small anti-crossing** (in this case 200 μeV vs. 6 μeV), and **zero applied field**.

Definition of detuning: interdot energy difference/$\hbar\omega d$, where d = interdot distance/Fock-Darwin radius.

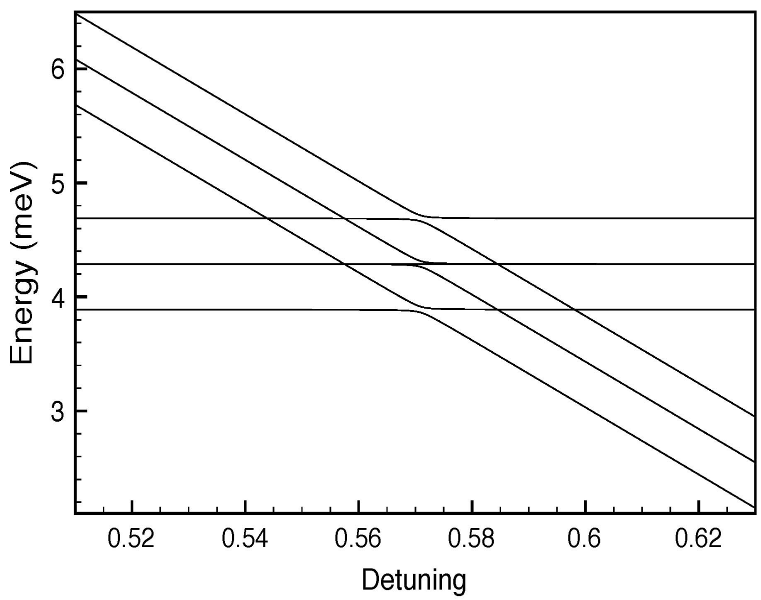
Two-Electron States in a Biased Si Double Dot



$\Delta < t$



$\Delta \sim t$

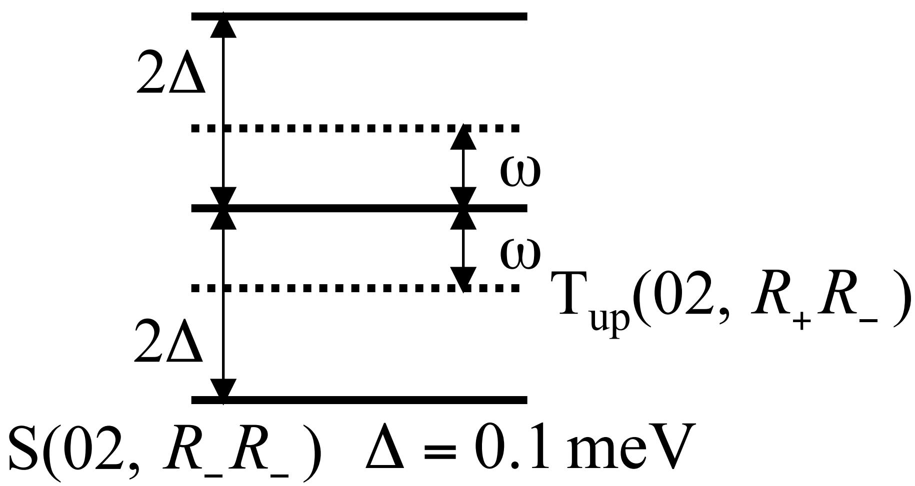


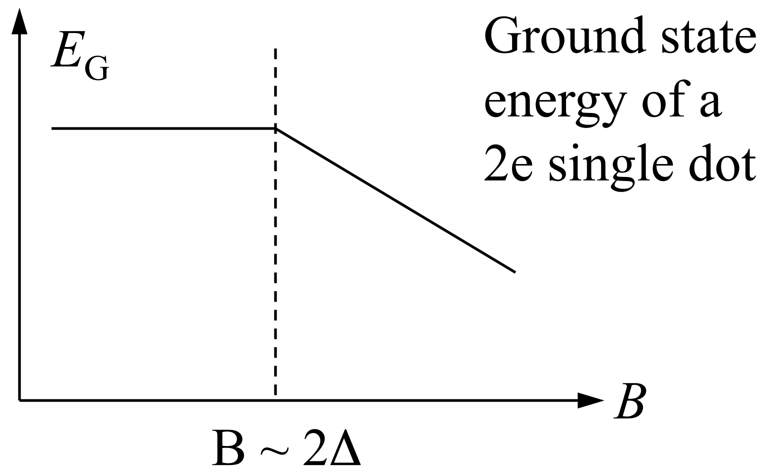
$\Delta > t$

- ➢Smooth confinement means no population transfer between valleys.
- ➢Coulomb interaction does not affect valley splitting.

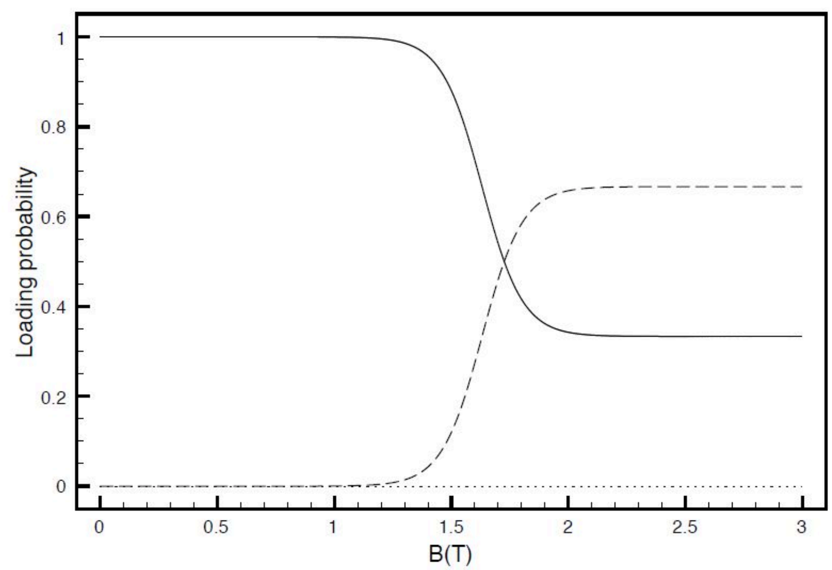
How do we know whether we have large valley splitting?

Loading a Single Si Quantum Dot: Large Valley Splitting



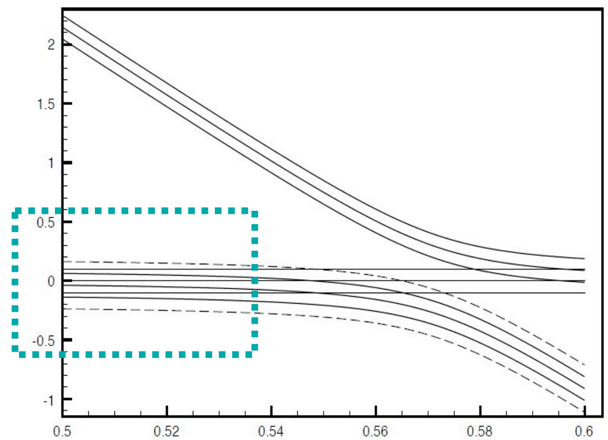


- Choose Fermi level on resonance with $S(02, R_-R_-)$; $k_BT << 2\Delta$.
- At low field only loading the singlet ground state.
- At higher fields probability of loading the triplet is twice as high as the singlet (2/3 vs 1/3).



Implication of Loading a Polarized Triplet State

The Petta experiments measure how much mixing happens when two-electron singlet and triplet states are brought to near degeneracy so that Overhauser field become the dominant energy scale.



S-T_0 mixing needs: ΔB_{Nz}

S-$T_{\uparrow\uparrow}, T_{\downarrow\downarrow}$ mixing needs: $\Delta B_{Nx}, \Delta B_{Ny}$

T_0- $T_{\uparrow\uparrow}, T_{\downarrow\downarrow}$ mixing needs: total B_{Nx}, B_{Ny}

- **In a finite field, S, T_0 - $T_{\uparrow\uparrow}, T_{\downarrow\downarrow}$ mixing would be suppressed because of the energy difference**;
- **The applied field at which S and T have similar loading probability gives an estimate of the valley splitting**;
- With an applied field one can engineer the different field components to differentiate the different mixing.

Summary

- **Good understanding of bulk Si:P donor electron spin coherence.**

- **Hyperfine interaction weak for conduction electron in Si.**

- **Charge noise and phonon effects need to be accounted for.**

- **Calculated valley splitting a fraction of an meV.**

- **For large enough valley splitting with small external field, Petta experiment can be done in Si** like in GaAs, but with an applied field.

- **Pulsed experiments in Si can be run to estimate the size of the valley splitting**, helped by an applied uniform field. The basic reason is the crossing of the low energy triplet state and singlet state.

Open Questions

- **Effects of interface defects such as P_b centers.**

- **Spin coherence (whether donor bound or QD bound) near an interface.**

- **Single- and two-spin ESR in Si:P and quantum dots.**

- **Alternative approaches to combat valley interference effects.**

- **Better understanding of how interface roughness affects valley splitting.**

- …