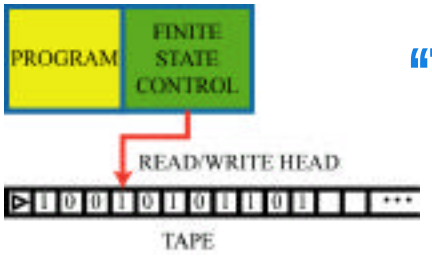
Control of Exchange Interaction in a Double Dot System

M. Stopa

Tarucha Mesoscopic Correlation Project, ERATO-JST

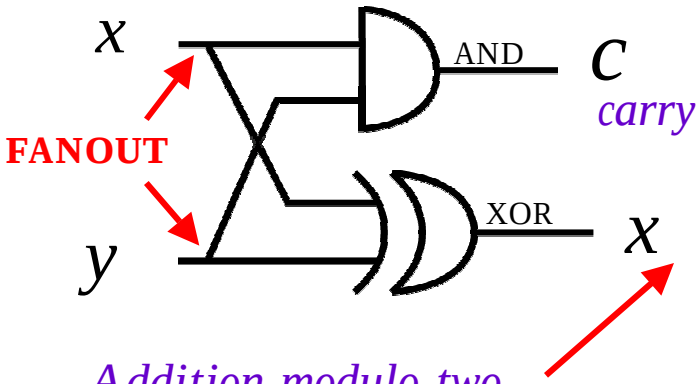
1. *Information is physical*
2. *Genesis of quantum computing*
3. *QC in a double dot*
4. *Exchange interaction and 2 qubit operations*
5. *Density functional theory and exact diagonalization*

Alan M. Turing, Proc. Lond. Math. Soc. **2**, 42:230, 1936.



"Turing machine"

Addition circuit



"bits" of information

$x, y, c, x \quad y \quad \{0,1\}$

physics

"qubit"

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

$$|\alpha|^2 + |\beta|^2 = 1$$

Quantum NOT gate

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix}\beta\\ \alpha\end{pmatrix}$$

Multiple qubits

$$|\psi\rangle = (\alpha_1|0\rangle + \beta_1|1\rangle)\ (\alpha_2|0\rangle + \beta_2|1\rangle)$$
$$= \alpha_{01}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Controlled NOT gate

$$\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}\begin{pmatrix}\alpha_{00}\\ \alpha_{01}\\ \alpha_{10}\\ \alpha_{11}\end{pmatrix} = \begin{pmatrix}\alpha_{00}\\ \alpha_{01}\\ \alpha_{11}\\ \alpha_{10}\end{pmatrix}$$

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Quantum computation

1. Assemble N qubits, prepare initial state, e.g. $|0\rangle|0\rangle,\ldots,|0\rangle$.
2. Apply unitary transformation U to the N qubits (often transforming only a few qubits at a time).
3. Measure qubits by projecting each onto $\{|0\rangle,|1\rangle\}$ basis; this is the result of the computation and the information is now classical.
4. Publish output.

Advantages of quantum computing

Deutsch's algorithm – see Preskill's notes at http://www.theory.caltech.edu/people/preskill/ph229/

State of the art for classical computers is "number field sieve" (see J. Derbyshire, *Prime Obsession*, **(Joseph Henry Press, 2003))**

$$T \approx \exp\left(c(\ln n)^{1/3}(\ln[\ln n])^{2/3}\right)$$

130 digit number → two 65 digit factors, few hundred workstations, one month
400 digit number in 10^{10} years.

Shor's algorithm (P.W. Shor, SIAM J. Comp., 26(5):1484-1509, 1997)

$$T \sim (\ln(n))^3$$

IF we had a quantum computer that factors 130 digit number in one month
400 digit number in 3 years.

Physical Implementations

REQUIREMENTS

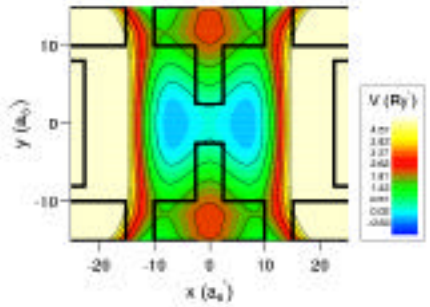
1. **Define a qubit**
2. **State preparation**
3. **Long coherence time**
4. **Gates (Hamiltonian)**
5. **Scalability**
6. **Readout**

EXAMPLES

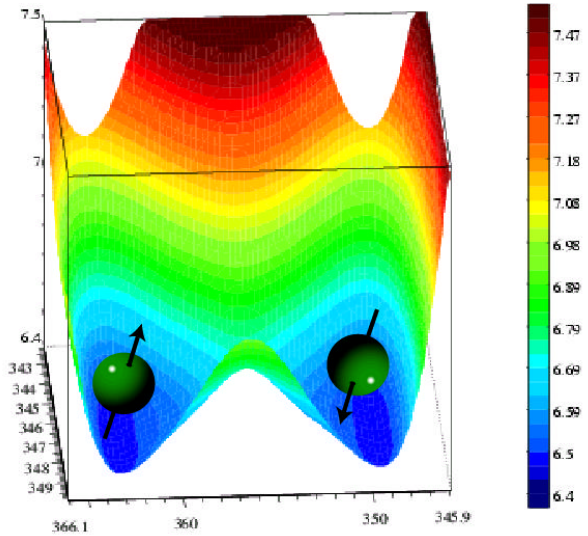
1. **Ion traps**, J. I. Cirac and P. Zoller, Phys. Rev. Lett. 74, 4091 (1995).
2. **Cavity QED**, Pellizzari *et al.*, Phys. Rev. Lett. **75**, 3788 (1995).
3. **NMR**, L. Vandersypen *et al.*, Phys. Rev. Lett. **85,** 5452 (2000).
4. **Cooper Pair Box** (superconducting charge qubit), Y. Nakamura, Y.A. Pashkin and J.S. Tsai, Nature **398**, 786 (1999).
5. **Superconducting flux qubit**, T. Orlando *et al.*, Phys. Rev. B **60**, 15398 (1999).
6. **Semiconductor quantum dots**, D. Loss and D. DiVincenzo, Phys. Rev. A **57**, 120 (1998).

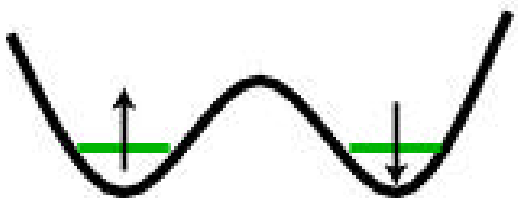
Quantum dots for quantum computing

Daniel Loss and David DiVincenzo, Phys. Rev. A **57**, 120 (1998).



potential





Define a qubit: single spin in a quantum dot

Evolution operator:

$$U_S(t) \equiv T\exp\left[-i\int_0^t dt' H_S(t')\right]$$

$$|\Psi(t)\rangle = U_S|\Psi(0)\rangle$$

Single qubit evolution $H_S = g\mu_B B S_z$

Two qubit operation

USE EXCHANGE COUPLING $H_S = -J(t)\vec{S}_1\ \vec{S}_2$

J(t) is proportional to the tunnel coupling between the dots which can be modulated in time

$$|\psi\rangle = \alpha_{\downarrow\downarrow}|\downarrow\downarrow\rangle + \alpha_{\downarrow\uparrow}|\downarrow\uparrow\rangle + \alpha_{\uparrow\downarrow}|\uparrow\downarrow\rangle + \alpha_{\uparrow\uparrow}|\uparrow\uparrow\rangle$$

$$\langle H_S\rangle = \frac{J}{4}\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Exchange coupling

$$2\vec{S}_1 \cdot \vec{S}_2 = S^2 - S_1^2 - S_2^2 = S^2 - \frac{3}{2} = \begin{cases} -\frac{3}{2} & \text{singlet} \\ \frac{1}{2} & \text{triplet} \end{cases}$$

$$H_S = -J\vec{S}_1 \cdot \vec{S}_2$$

singlet-triplet splitting

$$E_S = \varepsilon_L + \varepsilon_R + V_{dir} + V_{ex}$$

$$(\psi_L(\mathbf{r}_1)\psi_R(\mathbf{r}_2) + \psi_R(\mathbf{r}_1)\psi_L(\mathbf{r}_2))\chi_S$$

singlet

$$E_T = \varepsilon_L + \varepsilon_R + V_{dir} - V_{ex}$$

$$(\psi_L(\mathbf{r}_1)\psi_R(\mathbf{r}_2) - \psi_R(\mathbf{r}_1)\psi_L(\mathbf{r}_2))\chi_T$$

triplet

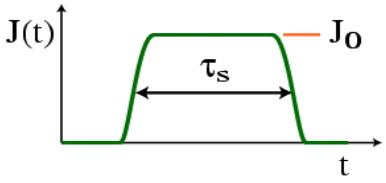
$$V_{dir} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \psi_L^*(\mathbf{r}_1)\psi_R^*(\mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2)\psi_L(\mathbf{r}_1)\psi_R(\mathbf{r}_2)$$

$$V_{ex} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \psi_L^*(\mathbf{r}_1)\psi_R^*(\mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2)\psi_R(\mathbf{r}_1)\psi_L(\mathbf{r}_2)$$

Overview

1. *Single qubit operations via local magnetic fields which act only on a single spin (very difficult).*
2. *Interaction between pair of qubits via tunable exchange coupling.*
3. *Tuning accomplished by varying the barrier between electrons.*

$$\int dt J(t) = J_0 \tau_S = \pi \qquad U_S \rightarrow U_{swap} = \exp\left\{-i\pi \vec{S}_1 \ \vec{S}_2\right\}$$



$$U_{swap}\left|\sigma_1 = \uparrow, \sigma_2 = \downarrow\right\rangle = \left|\sigma_1 = \downarrow, \sigma_2 = \uparrow\right\rangle$$

More generally, it can be shown that

$$U_{XOR} = e^{i(\pi/2)S_{1z}} e^{-i(\pi/2)S_{2z}} U_{swap}^{1/2} e^{i\pi S_{1z}} U_{swap}^{1/2}$$

performs the exclusive OR operation; i.e. it flips the spin of 2 if and only if the spin of 1 is up.

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Time scales and bottlenecks

1. Spin coherence time ~100 μs
2. Number of operations to do typical factoring algorithm ~10,000 (??)
3. Switching time for inter-dot gates ~ps (i.e. plenty fast).
4. Electron spin resonance spin rotation time: NOT even accomplished yet, but ~ μs (?)

   much too slow.

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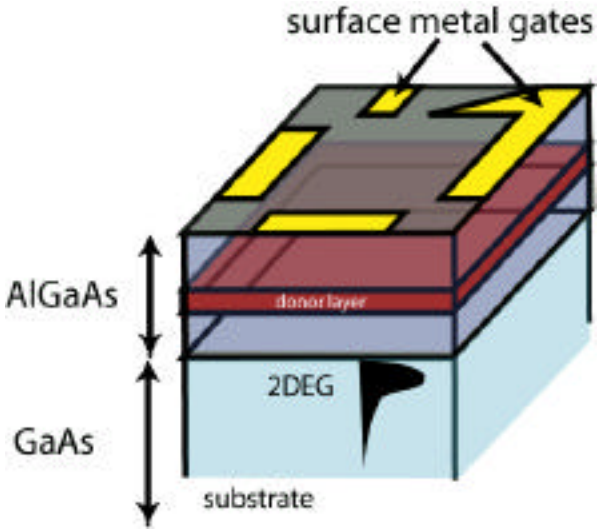
Electronic structure of lateral semiconductor heterostructures

Inputs:

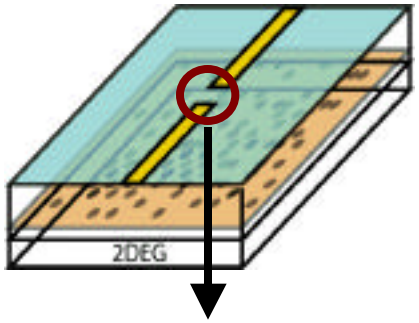
1. **Wafer profile** → **band offset**, **effective mass**, **dielectric constant**, **g factor**, **spin-orbit coupling**
2. **Donor profile / concentration**
3. **Gate pattern / voltages**
4. **Temperature**
5. **Magnetic field**



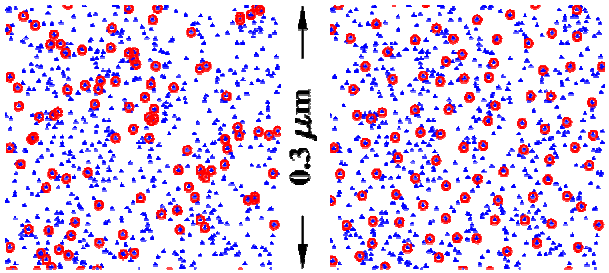
Outputs:

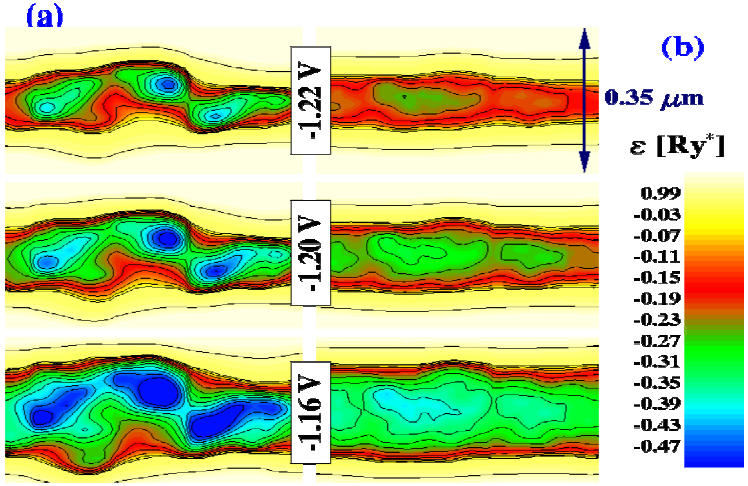
1. **electrostatic potential $\varphi(r)$**
2. **charge density $\rho(r)$**
3. **for a confined region (i.e. a dot)**
   1. **eigenvalues E_i**
   2. **eigenfunctions ψ_i**
   3. **tunneling coefficients γ_i**
4. **total free energy $F(N,V_g,T,B)$**

donor layer disorder/order



Blue dots are donors, red circles are ions

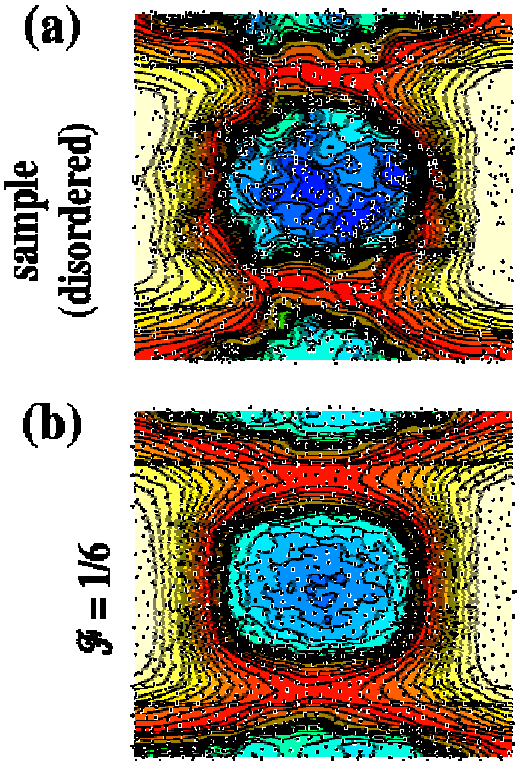


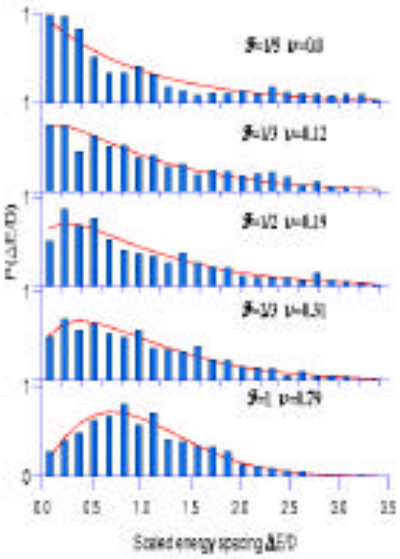


M. Stopa, Phys. Rev. B, **53**, 9595 (1996)

Statistics of quantum dot level spacings

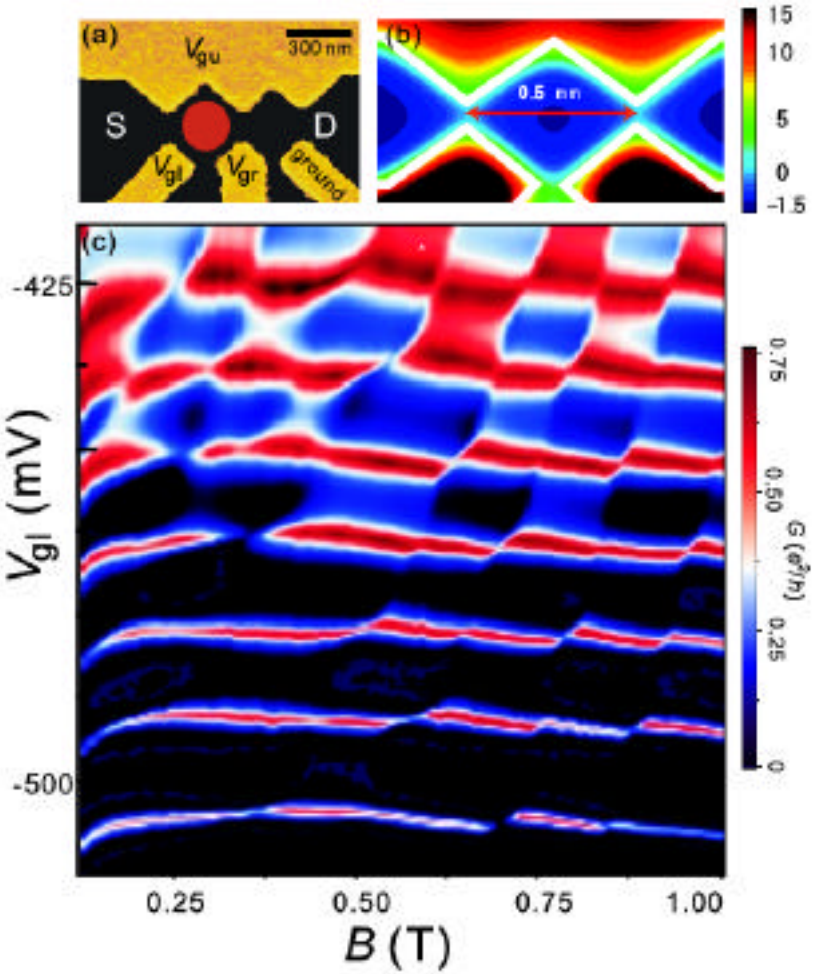
Transition from Poisson statistics to Wigner statistics as disorder increases





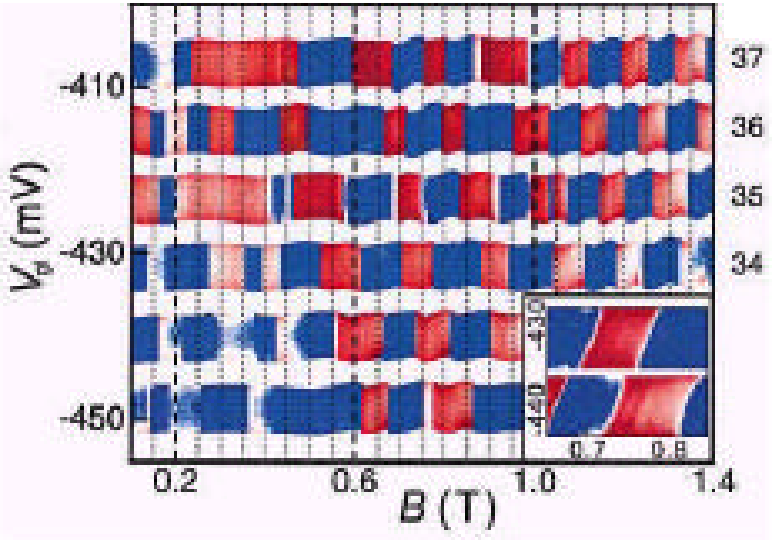
M. Stopa, Superlattices and Microstructures, **21**, 493 (1997)

Kondo chessboard pattern



Definition of Kondo co-tunneling amplitude, computed from ground state electronic structure calculation results.

$$K \equiv \sum_{p,\sigma} n_{p,\sigma}(1-n_{p,\bar{\sigma}})\sqrt{\gamma_{p\rho}\gamma_{p,\bar{\sigma}}}$$
$$[\frac{1}{F(N+1,V_{gl}B)-F(N,V_{gl},B)}+$$
$$\frac{1}{F(N-1,V_{gl},B)-F(N,V_{gl},B)}]$$



M. Stopa, W. van der Wiel, S. DeFranceschi, L. P. Kouwenhoven and S. Tarucha, PRL **94**, 046601 (2003).

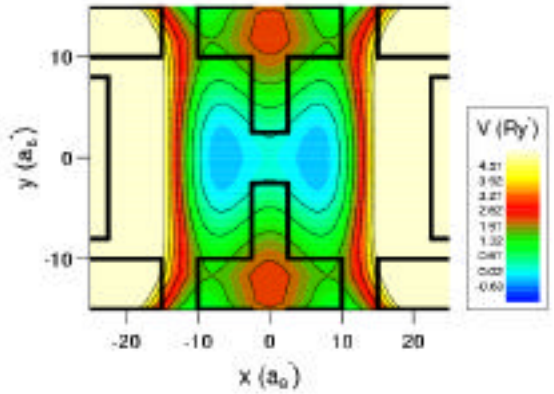
Double dot case

DFT: effective single particle theory, including exchange and correlation via a local potential. Allows full incorporation of wafer profile, geometry, gate voltages, etc.

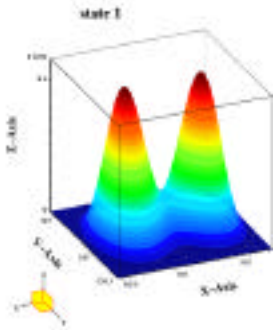
$$\left[\frac{1}{2}\left(-i\nabla + \frac{e}{c}\mathbf{A}\right)^2 + e\varphi(\mathbf{r}) + V_{xc}(\mathbf{r})\right]\psi_n(\mathbf{r}) = \varepsilon_n\psi_n(\mathbf{r})$$

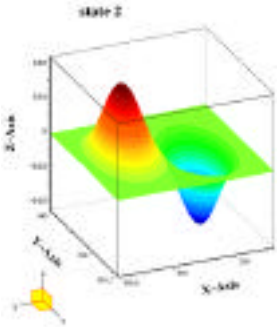
$$-\nabla^2\varphi(\mathbf{r}) = \frac{4\pi e}{\kappa}\rho(\mathbf{r}) \qquad \rho(\mathbf{r}) = \sum_{n=1}^{N}|\psi(\mathbf{r})|^2 + \rho_{leads}(\mathbf{r}) + \rho_{donors}(\mathbf{r})$$

Self-consistent potential at 2DEG level



Lowest two eigenstates





Drawback: contains uncompensated self-interaction and therefore inadequately describes many-body correlation

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Using DFT as a basis for exact diagonalization

Q. What is the best direct product basis for representing the correlated many electron state (for a double dot or in general) ?

A. Not immediately obvious. Try the following.

1. **Solve DFT problem for spinless electrons with full device fidelity.**
2. **Remove Coulomb interaction of dot electrons with themselves, also remove exchange-correlation potential.**
3. **Truncate basis to something manageable (L basis states) and form all symmetric and anit-symmetric combinations of two-electron states.**
4. **Compute Coulomb matrix elements using Poisson's equation.**
5. **Diagonalize Hamiltonian.**

Exact diagonalization for N=2

$$H = \sum_{i=1}^{2} h(\mathbf{r}_i) + V$$

$$h(\mathbf{r}) = \left[-i\nabla + \frac{e}{c}\mathbf{A} \right]^2 + e\varphi_{ext}(\mathbf{r}) \qquad -\nabla^2 \varphi_{ext} = \frac{4\pi e}{\kappa}\left(\rho_{leads} + \rho_{donors}\right)$$

Single particle energies must not contain Coulomb interaction with dot electrons.

$$\tilde{\varepsilon}_n = \varepsilon_n - \langle n | e\varphi_{dot} + V_{xc} | n \rangle \qquad -\nabla^2 (\varphi_{dot}(\mathbf{r}) - \varphi_0(\mathbf{r})) = \frac{4\pi}{\kappa} \sum_{n=1}^{2} |\psi_n(\mathbf{r})|^2$$

$$-\nabla^2 \varphi_0(\mathbf{r}) = 0$$ ⇐ Potential due to charge on surface metal gates

Form all symmetric and anti-symmetric combinations of basis states for singlet and triplet two electron states, resp.

Symmetric states

$$\begin{cases} |S\rangle \equiv O_S |nm\rangle = \frac{1}{\sqrt{2}}\left[|nm\rangle + |mn\rangle \right] & n \neq m \\ = |nm\rangle & n = m \end{cases}$$

Anti-symmetric states

$$|A\rangle \equiv O_A |nm\rangle = \frac{1}{\sqrt{2}}\left[|nm\rangle - |mn\rangle \right]$$

Coulomb matrix elements from Poisson equation

$$\langle nm|V|pq\rangle = \int d\mathbf{r}_1\, d\mathbf{r}_2 \psi_n^*(\mathbf{r}_1)\psi_m^*(\mathbf{r}_2)v(\mathbf{r}_1,\mathbf{r}_2)\psi_p(\mathbf{r}_1)\psi_q(\mathbf{r}_2)$$

Compute matrix elements by solving for Poisson equation using product of two wavefunctions as source and correcting for gate potential.

$$-\ {}^2\varphi_{mq}(\mathbf{r}) = \frac{4\pi}{\kappa}\psi_m^*(\mathbf{r})\psi_q(\mathbf{r})$$

$$\tilde{\varphi}_{mq}(\mathbf{r}_1) = \varphi_{mq}(\mathbf{r}_1) - \varphi_0(\mathbf{r}_1) = \int d\mathbf{r}_2 \psi_m^*(\mathbf{r}_2)\psi_q(\mathbf{r}_2)v(\mathbf{r}_1,\mathbf{r}_2)$$

gate charge potential

$$\Rightarrow \quad \langle nm|V|pq\rangle = \int d\mathbf{r}_1 \left[\psi_n^*(\mathbf{r}_1)\psi_p(\mathbf{r}_1)\right] e\tilde{\varphi}(\mathbf{r}_1)$$

Advantages:

Highly efficient. No double integrals. Full 3D wave function taken into account.
One solution of Poisson's equation gives L^2 integrals by single quadrature.

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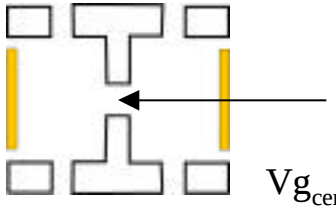
Main points of calculation

1. Basis is complete except for cutoff. No artificial introduction of tunnel coupling “t” between left and right dots.
2. Coulomb matrix elements use basis of states of realistic potential determined by gate voltages. Basis evolves self-consistently with gate voltages and magnetic field.
3. Screening by gates in Coulomb interaction is automatically included.
4. Background dielectric constant of GaAs is included.

DFT (single electron) properties

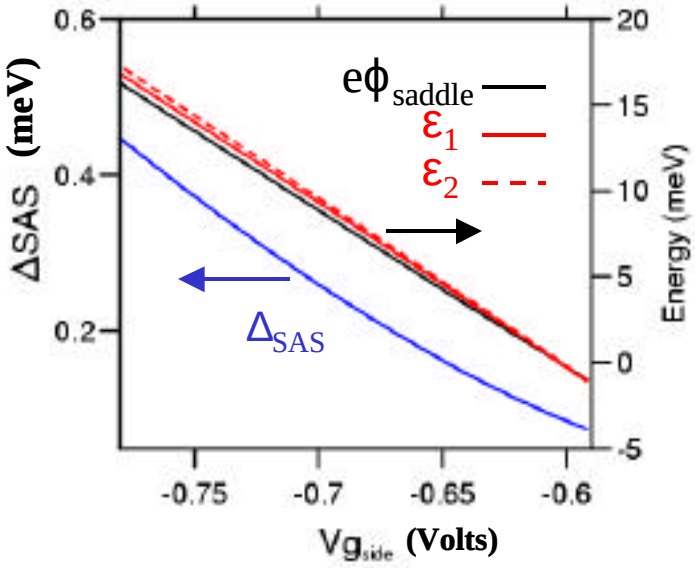
Side and center gate voltage dependence of saddle point potential $e\phi_{saddle}$, symmetric level energy ε_1, anti-symmetric level energy ε_2, and symmetric/anti-symmetric splitting $\varepsilon_2 - \varepsilon_1$.

Side gates sweep

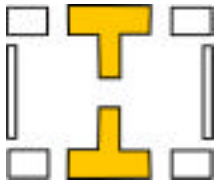


saddle point

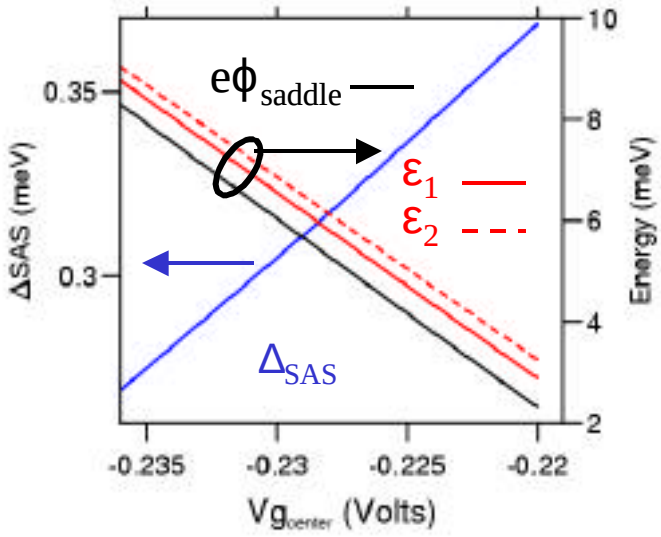
Vg_{center}=-0.235 V



Center gates sweep



Vg_{side}=-0.7 V



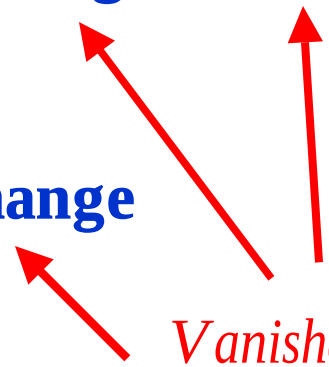
Strong cross-capacitance.

Side gates influence saddle point strongly; push dots together.

What do we expect for behavior of singlet-triplet splitting as we vary the barrier between the two dots ?

Singlet energy = single ptcls. + exchange - delocalization

Triplet energy = single ptcls. - exchange



Vanishes as dots move apart ("tunneling" t decreases)

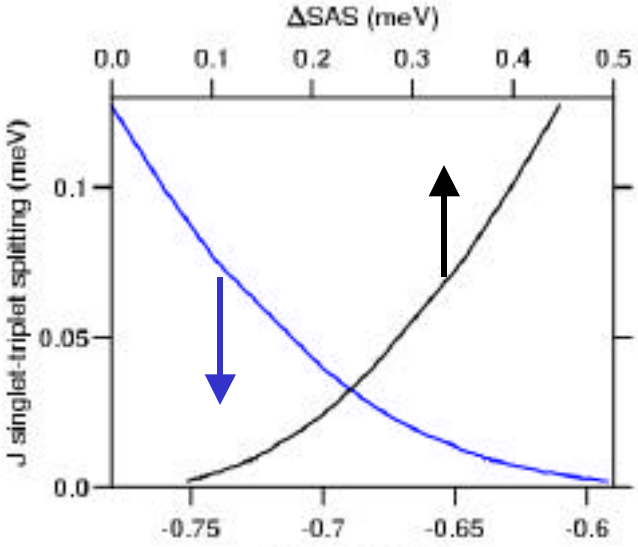
Singlet-triplet splitting J versus Δ_{SAS}

$J = E_T - E_S$ Difference of ground state triplet and singlet energies

Singlet-triplet splitting decreases as dots move further apart (less negative side gate voltage)

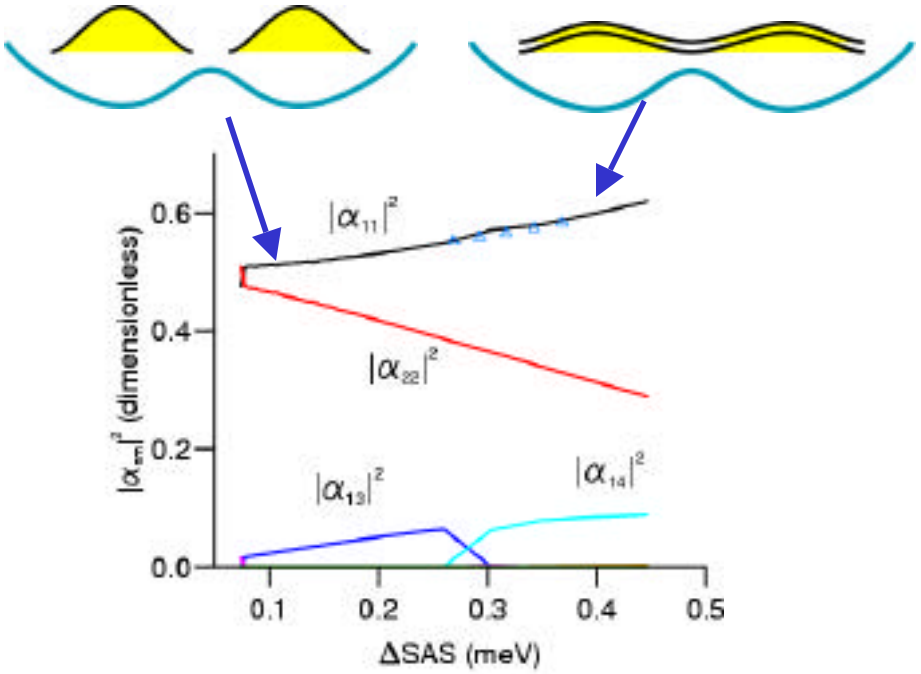
Heitler-London-like Single-particle-like

dot coupling stronger



Vg_{center}=-0.235 V

dot coupling weaker



What about magnetic field dependence ?

B causes wave functions to contract and localize on respective dots, so variation should be the same as with central barrier height, which isolates dots.

Singlet energy = single ptcls. + exchange - delocalization

Triplet energy = single ptcls. - exchange

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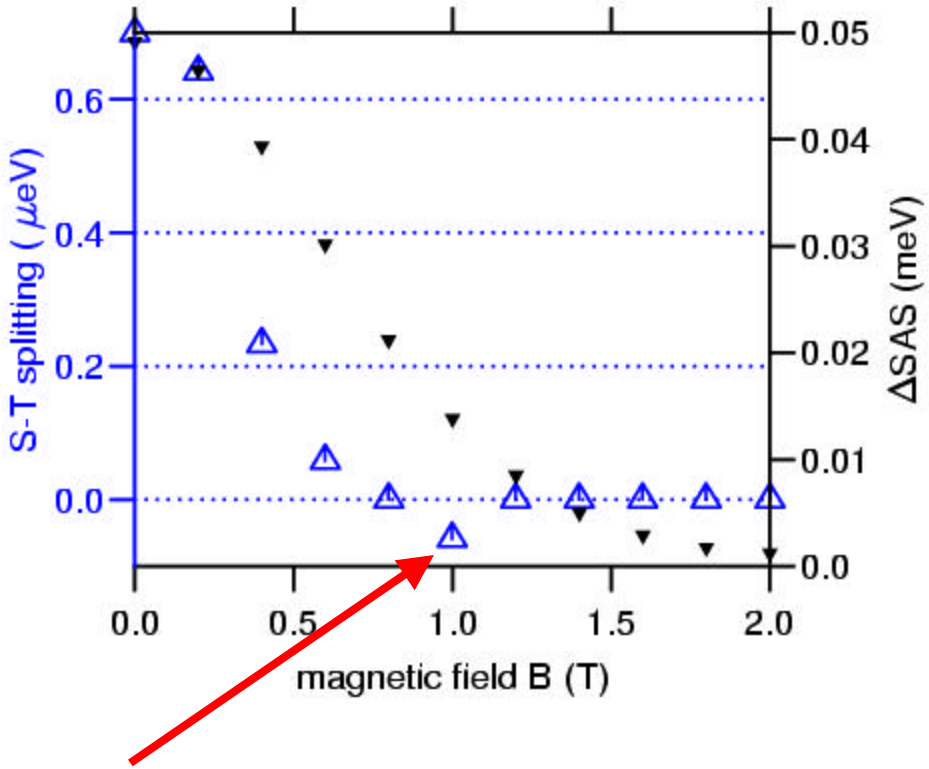
J becomes negative for relatively well-isolated dots

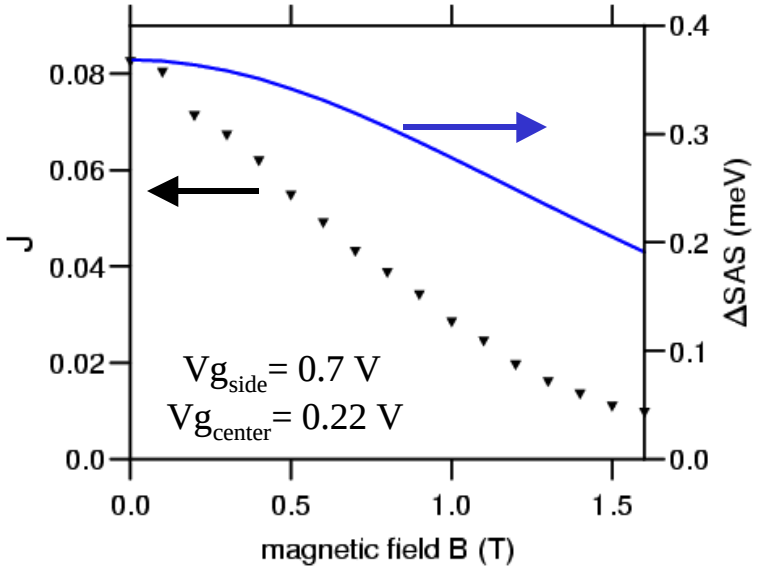
N.B. →

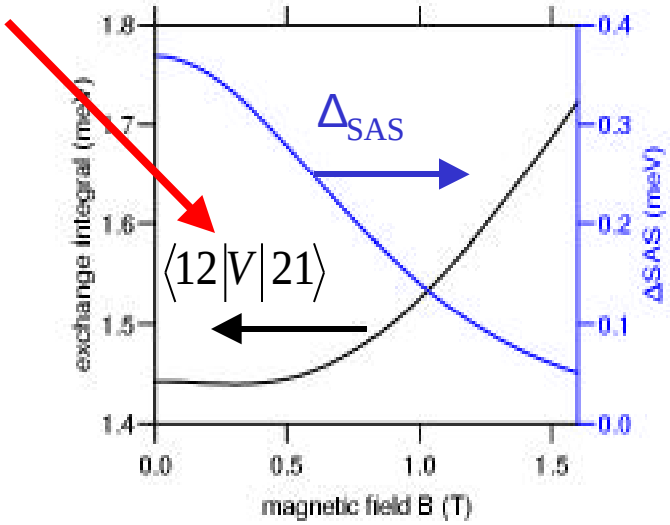


Very slightly negative (big deal to some people).

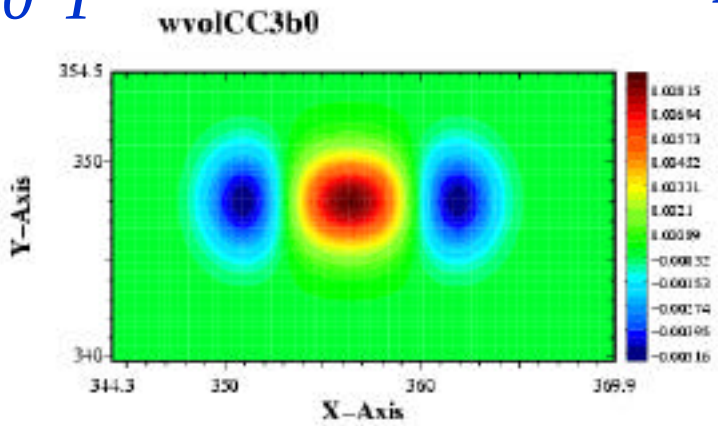
Magnetic field dependence

$$V_{ex} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \psi_L^*(\mathbf{r}_1)\psi_R^*(\mathbf{r}_2) V(\mathbf{r}_1,\mathbf{r}_2)\psi_R(\mathbf{r}_1)\psi_L(\mathbf{r}_2)$$





B=0 T



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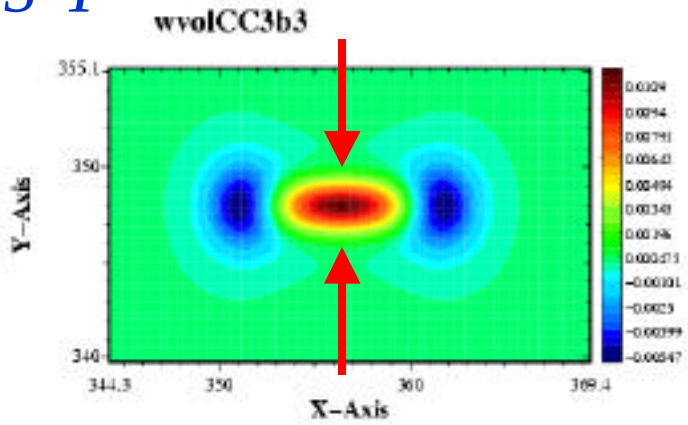
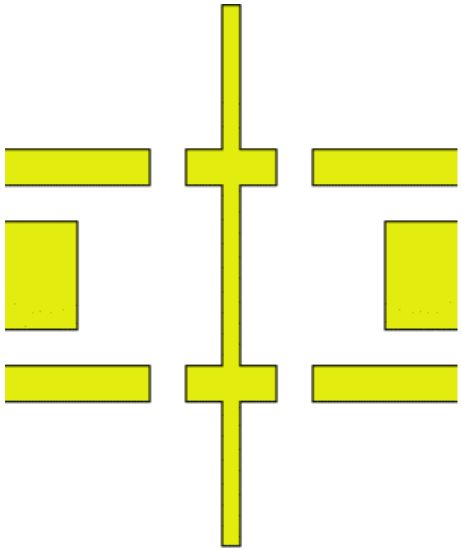
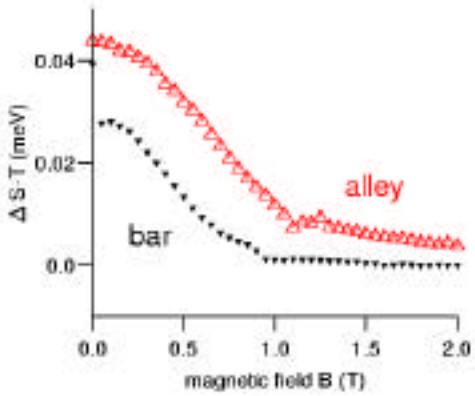


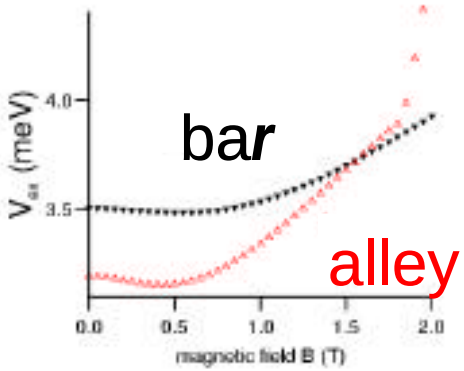
Increase in exchange integral due to LATERAL contraction of wave function

Varying gate pattern

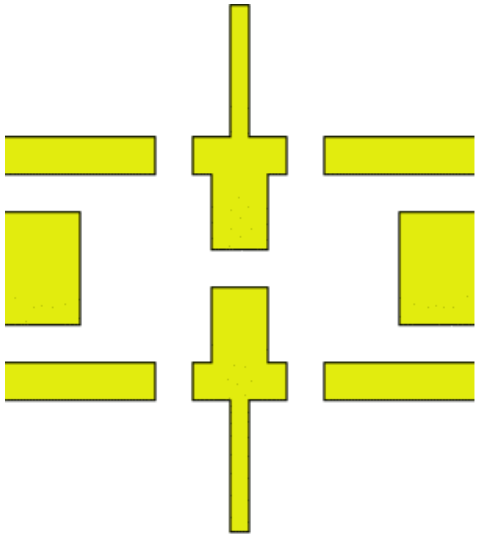
Bar

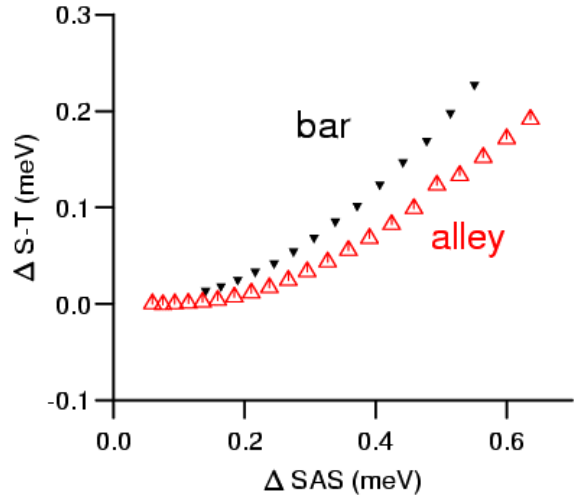






Alley





Conclusions

- Double dot electronic structure calculated for N=2 employing geometrically realistic basis of states determined from DFT.
- Basis of states evolves self-consistently with applied gate voltages and magnetic field.
- Can adjust surface gate pattern to vary relationship between exchange integral and tunnel coupling (ΔSAS).
- Magnetic field influences saddle point potential self-consistently and therefore leads to a weaker variation of J. Specifically, J does not become negative for most parameters.