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Exchange Gate Design in two Donor Qubits

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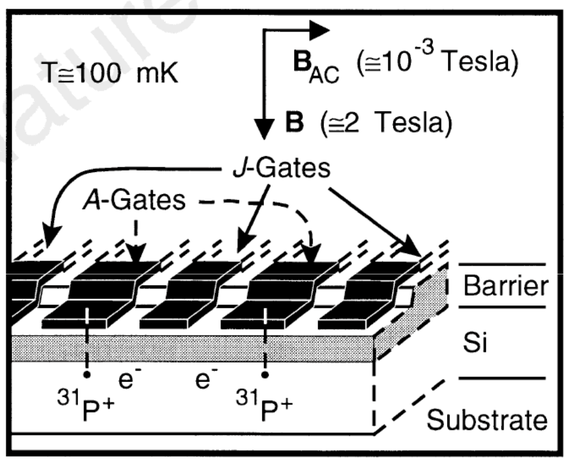
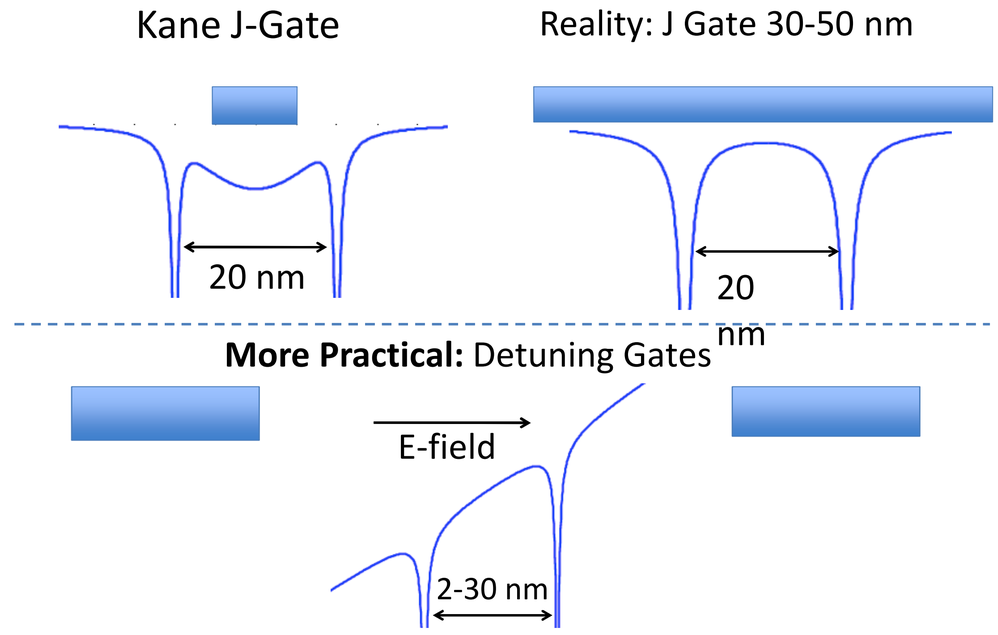
Kane Quantum Computer architecture [1]



- **Two-qubit operations:** Exchange energy between donor electrons. Modify wave function overlap by J-Gate bias => change exchange energy (J)
- **Problem:** Donor separation 20 nm, Gate length needs to be about 10 nm, too small for current technology.
- **Idea:** Use a detuning gate to generate a (1,1) to (0,2) charge transition.
- Access high and low J values, analogous to the double quantum dot qubit [2].



Method of Computation

Atomistic tight-binding (NEMO 3D)

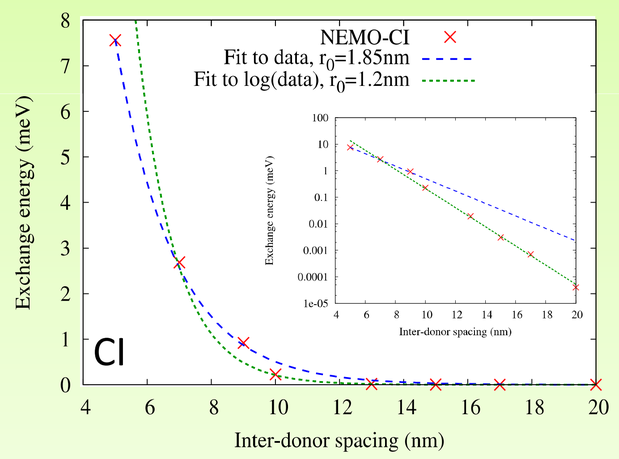
- LCAO, full band structure method (no extra parameter for valley-splitting)
- Donor & acceptor states
- miscut, crystal orientation,
- surface roughness, alloy disorder
- strain, hetero-structures, geometries
- E-fields, B-fields
- multi-million atom systems

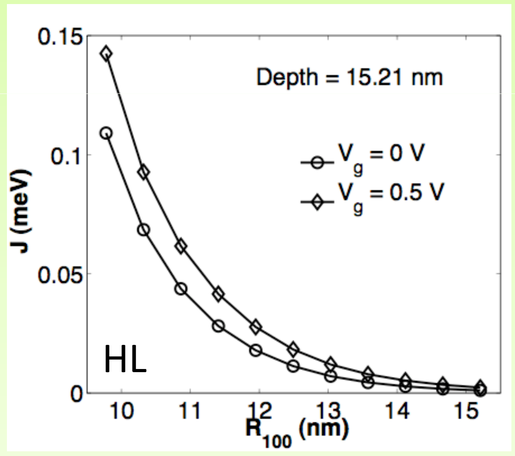
+

Full Configuration Interaction (FCI)

- e-e interaction: Coulomb, exchange, correlation effects
- Need a good 1 particle basis: atomistic tight-binding
- Diagonalize the 2e Hamiltonian in the basis of Slater Determinants
- Applied to the DQD system [3]

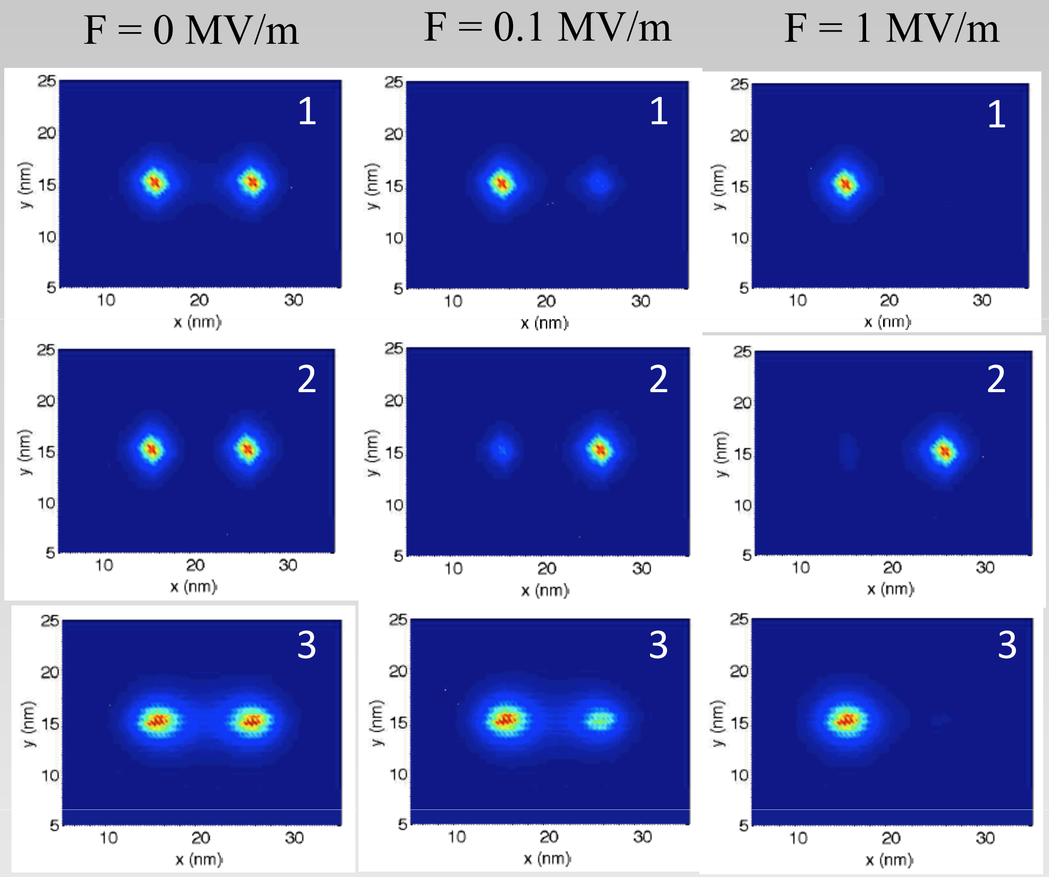
Comparison of methods: CI vs HL



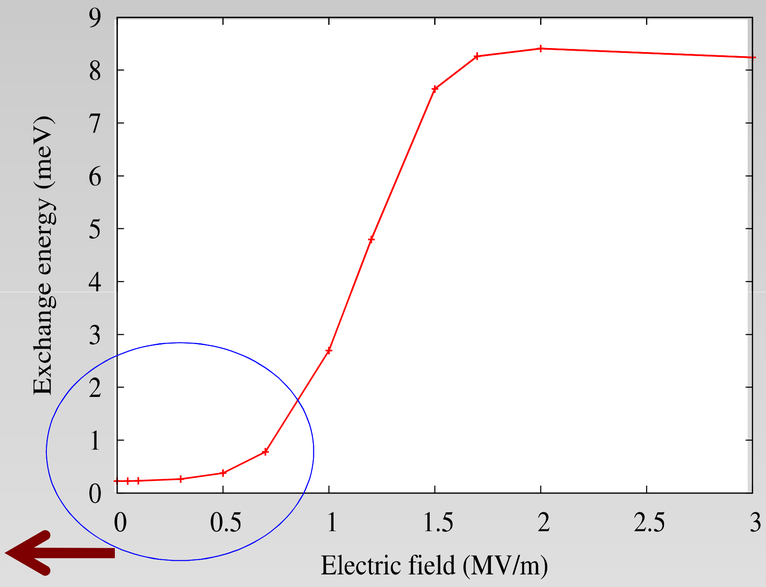


- Heitler-London (HL) approach valid for large donor separations (>=10 nm).
- CI agrees with HL for R>10 nm.

1e States: Charge Transitions



J curve with detuning



- States show charge transition between 2 donors with detuning field.
- Full CI calculation shows a similar exchange curve as a DQD
- A detuning gate seems more feasible as various donor separations are tolerant in the design.

Future Work:

High overlap case

- CI method with 1e basis fails to reproduce the 2e (D-) binding energy of the donor.
- Self-consistent Field (SCF) method yields the correct binding energy with 4% error.
- Combine CI with SCF method to improve the J calculations of the high-overlap 2e system.

References:
[1] B. E. Kane, Nature 393, 133 (1998).
[2] J. Petta, et. al., Science 309, 5744 (2005).
[3] R. Rahman, E. Nielsen, et. al. PRB 85, 125423 (2012).

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