The Materials Computation Center
Funded by NSF DMR 03-25939

Duane D. Johnson and Richard M. Martin (PIs)

New Monte Carlo Method for Interacting Electrons in Quantum Dot Devices

D. Das,[1] J. N. Kim,[3] R. M. Martin,[1] L. Zhang,[2] J. P. Leburton,[2] and M. Kalos[4]

[1]Dept. of Physics, [2]Dept. of Electrical and Computer Engineering, [3]Materials Computation Center, and [4]Lawrence Livermore National Lab

Statement of Problem

- **Quantum Dots:** systems in which electrons are confined on nanoscale dimensions so that quantum effects are essential in actual devices
- **Goal:** to create quantum alectronic – spintronic devices by control of electron number and spin as a function of device geometry and applied voltages
- **Challenges :**
  - Create novel structures for control of charge/spin
  - Accurate theoretical treatment of strongly interacting electrons
- **Research Objectives:** First-principles calculations of the charge and spin states in semiconductor quantum dots including all effects of material layers and patterned metal gates in real devices.

Methods for treating electrons in a nanoscale quantum device

Density Functional method (DFT)

Kohn-Sham equations for electrons

Approximate interactions between electrons by functional, e.g., local density approximation - LDA

Poisson equation for Coulomb Fields in Device

Finite Element method for solution of coupled differential equations:

Quantum Monte Carlo (QMC)

Treat quantum system of interacting electrons by stochastic sampling of positions of electrons

- **Variational Monte Carlo (VMC):** optimize a trial many-body wavefunction
- **Diffusion Monte Carlo (DMC):** improve over variational function by trial many-body wavefunction
  - The most accurate method known for many interacting electrons – but not exact for electrons because of the "sign problem"
  - Applicable to complex systems
  - Previous work – DMC assuming the usual 1/r interactions between electrons (not correct in a complex device) and a potential given by the solution of the approximate DFT equations

New Approach in this work

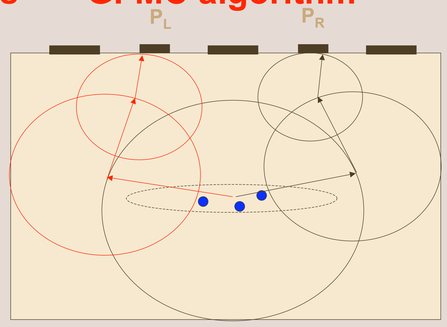
- **Solve full problem for interacting electrons in a complex device including all gate voltages and complex dielectrics**

Classical Green Function Monte Carlo GFMC

- Solve problem of interacting charges and applied voltages by sampling the Coulomb fields
- Exact simulation of interacting electrons in the real device with arbitrary metallic gates, dielectrics and boundary conditions

"Walk on Spheres" - GFMC algorithm

Example of two walks that sense the gate voltages: left (P_L) and right (P_R)



GFMC simulation of potential – Example at right

Agrees with standard grid methods for the external potential

Also treats exactly interactions between electrons in the dot – not done before

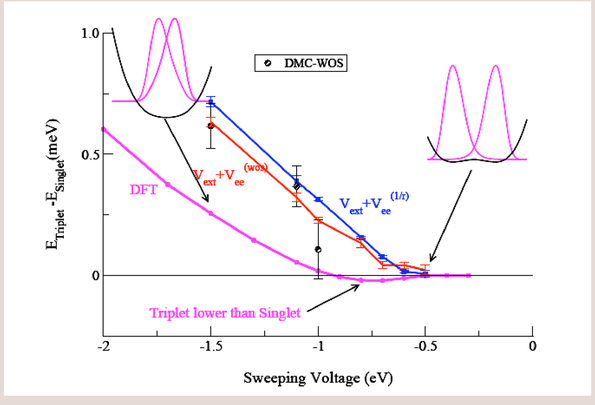
DMC simulation of quantum electrons in the dot simultaneously with the GFMC solution of the Poisson problem

Implemented in QMCtools codes

Allows future implementations with other QMC methods sich as reptation and path integerals that allow studies of energy differences and finite temperature

Example of Results

Comparison of DMC and DFT for the actual device



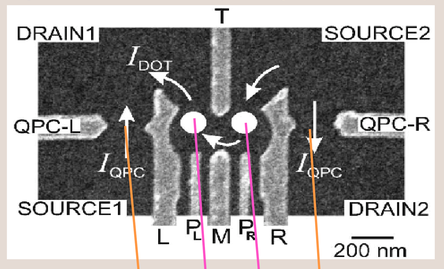
DFT has unphysical "broken symmetry" solution for weakly coupled dots

DMC gives correct result that singlet is always favored

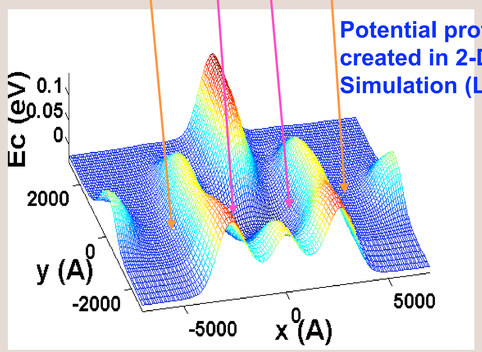
Example of quantum device

Double dot – occupations controlled by gates – detected by currents I_{QPC} that sense the potentials due to electrons in the dots

Experimental circuit lay-out (Kouwenhoven)



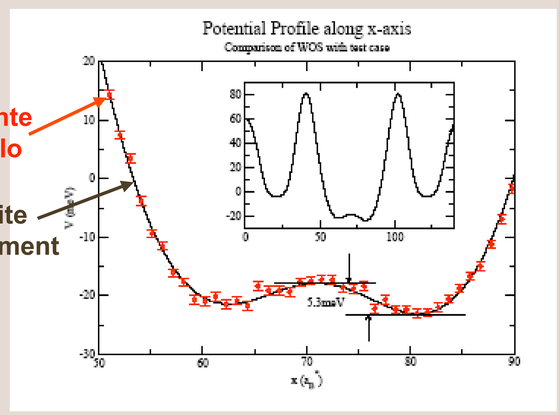
Potential profile in dot created in 2-DEG Simulation (Leburton)



Potential Profile in the dot

Monte Carlo

Finite Element



Summary

- First method to treat fully interacting electrons in the actual device geometry
- Feasibility demonstrated for two-electron problem – where the DMC is exact
- More advantageous for many electrons where many potentials can be calculated simultaneously
- Code implemented in QMCtools which allows extension to future QMC developments

References
Experiments by group of L. P. Kouwenhoven:
J. M. Elzerman, et al., Phys. Rev. B 67, 161308 (2003)
Finite Element Method:
P. Matagne and J.-P. Leburton, Phys. Rev. B 65, 235323 (2002).
Previous collaborations comparing LDA/QMC:
J. P. Leburton, S. Nagaraja , P. Matagne and R. M. Martin, Microelec J 34, 485-489 (2003).
Present Monte Carlo method:
D. Das, Thesis, Universit of Illinois, 2005
D. Das, R. M. Martin, and M. Kalos, submtted to Phys. Rev. B.