Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

**QMC with a Stochastic Poisson Solver: An application to realistic models of quantum dots** DYUTIMAN DAS, JEONGNIM KIM, RICHARD MARTIN, L. ZHANG COLLABORATION, JP LEBURTON COLLABORATION, D. MELNIKOV COLLABORATION — Quantum Monte Carlo can be used to study interacting electrons in semiconductor quantum structures. We introduce a new approach in which the potential acting on each electron is found by sampling using a classical Monte Carlo "Walk On Spheres"(WOS) algorithm within the QMC calculation. This allows cheap and coarse estimates of the potential to be used, since the QMC averages the noise in the potential. The averaging is accomplished simply in VMC, and in DMC we use the penalty method [1] to modify the non-linear branching factor according to the noise in our potential estimate. The WOS algorithm is general enough to be applied to devices with arbitrary geometries, dielectric constants and gate biases. We employ this QMC-WOS hybrid approach to a real heterostructure as described in Ref.[2]. Specifically we calculate the singlet triplet splitting for a two electron double dot and compare with DFT calculations.
[1.] Ceperley D. M. and Dewing M. J. Chem. Phys. 110,9812 1999
[2.] Elzerman et. al. PRB 67, 161308(R) 2003

Dyutiman Das
University of Illinois at Urbana Champaign

Date submitted: 30 Nov 2004 Electronic form version 1.4