11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

3D Simulation of a Silicon Quantum Dot in a Magnetic Field Based on Current Spin Density Functional Theory

M. Lisieri, G. Fiori, and G. Iannaccone
Dipartimento di Ingegneria dell'Informazione, Università di Pisa,
Via Caruso 16, I-56100 Pisa, Italy
e-mail: michele.lisieri@iet.unipi.it

Recent research considers silicon a promising material for spintronic applications, because of its high spin coherence time and its mature technology [1], [2]. A detailed investigation of the spin properties of a quantum dot would require a suitable simulation tool, of which there are no examples in literature.

In this work, we present a numerical simulation of a silicon quantum dot in a magnetic field based on the solution of the many body Schrödinger equation, on the basis of Current Spin Density Functional Theory (CSDFT) [3], in the Local Density and Approximation (LDA), based on the formulation proposed by Koskinen et al. [4]. The effective mass approximation is used; mass anisotropy and degeneracy of conduction band minima are taken into account.

In Fig. 1, we show the flow chart of the simulation. Starting from an initial guess, the single particle Kohn-Sham equation is solved 6 times in the dot region, for each spin in each conduction band minimum (3 for silicon). Each single particle level is filled in the order of increasing energy, and the electrochemical potential μ is calculated with Slater's rule.

Once spin up and spin down electron densities are computed, the nonlinear Poisson equation is solved in the three dimensional domain by means of the Newton-Raphson method. The algorithm is then repeated cyclically till convergence is achieved.

In Fig. 2 we show the 3D structure of the simulated device, which has a square transverse cross section. The dot is a $4 \times 30 \times 30$ nm^3 silicon box embedded in SiO_2. In Fig. 3, we show a cross section of the electron density for 3 electrons in the dot for $B = 0$ T and $B = 4.75$ T.
In Fig. 4 we show the addition energy $\Delta_2(N) = \mu(N+1) - \mu(N)$ of the dot, where N is the total number of electrons in the dot. The maxima are for multiples of four electrons in the dot, due to the double degeneracy of each conduction band minimum. In Fig. 5 we show the first seven eigenvalues as a function of the magnetic field for three electrons in the dot. As can be seen, for $B = 2$ T there is a change of spin polarization.

In the final version of the paper, we discuss all the convergence issues and the behavior of spin polarization of the quantum dot as a function of the magnetic field, of the number of electrons, and of the dot geometry.

Authors gratefully acknowledge support from EU through the network of Excellence SINANO (EC contract n. 506844).

REFERENCES

[1] S. Das Sarma, R. de Sousa, X. Hu, B. Koiller, *Spin quantum computation in silicon nanostructures* Solid State Communications **133**, 737-746, (2005).

[2] L. P. Rokhinson, L. J. Guo, S. Y. Chou, and D. C. Tsui, *Spin transitions in a small Si quantum dot*, Physical Review B **63**, 035321 (2001).

[3] S. M. Reimann and M. Manninen *Electronic structure of quantum dots*, Review of Modern Physics, **74**, 1283-1342, (2002).

[4] M. Koskinen, J. Kolehmainen, S. M. Reimann, J. Toivanen, and M. Manninen,*Quantum dots in magnetic fileds: Unrestricted symmetries in the current spin-density functional formalism*, Eur. Phys. J. D, **9**, 487-490, (1999)

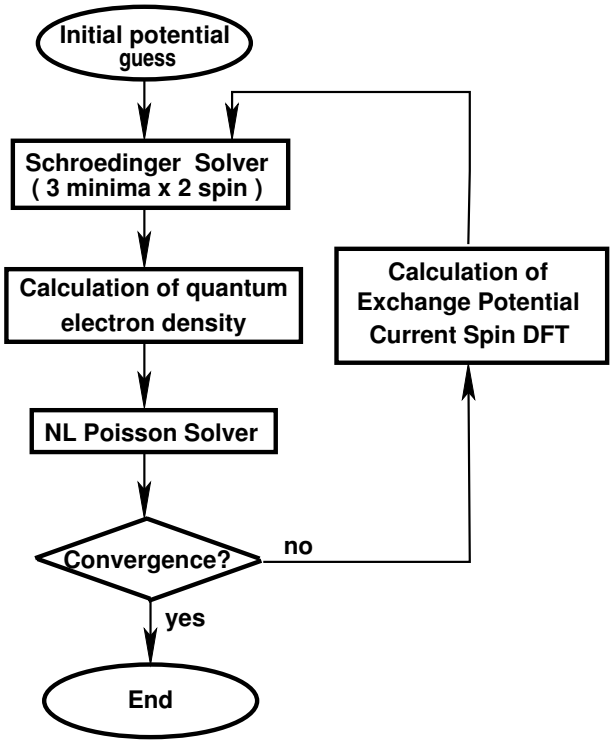

Fig. 1. Flow chart of the implemented 3D Poisson/Schrödinger solver.

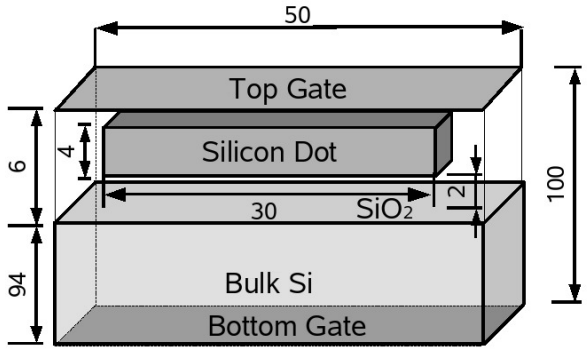

Fig. 2. Three dimensional simulated quantum dot structure: the silicon dot ($4 \times 30 \times 30$ nm^3) is embedded in SiO_2. The bulk is *p*-doped with N_A=10^{18} cm^{-3}. Dimensions in the figure are in nanometers.

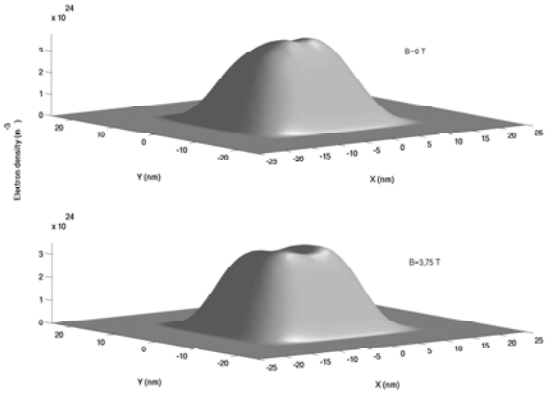

Fig. 3. Electron density for three electrons in the quantum dot for $B = 0$ T (top) and $B = 4.75$ T (bottom).

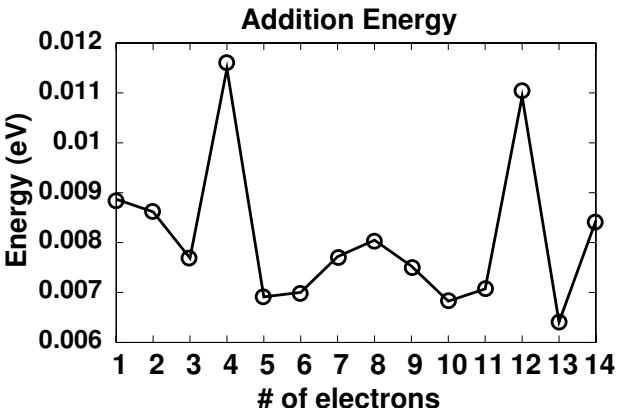

Fig. 4. Addition Energy as a function of the number of electrons in the dot.

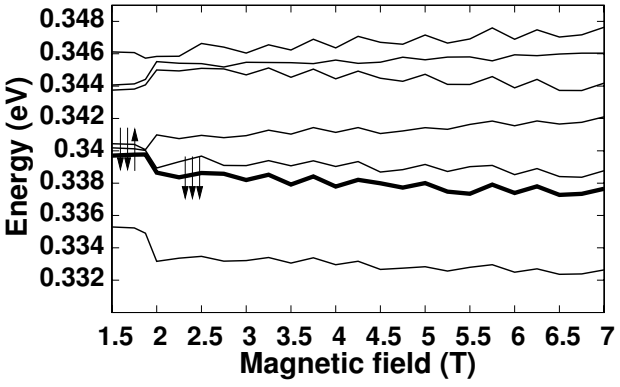

Fig. 5. First seven eigenvalues calculated when three electrons are in the dot as a function of the magnetic field. The bold line is the electrochemical potential, and the arrows indicate spin polarization.