

*3D simulation of a silicon quantum dot in a magnetic field based on current spin density functional theory*

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# 3D simulation of a silicon quantum dot in a magnetic field based on current spin density functional theory

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**Abstract** We have developed a code for the simulation of the electrical and magnetic properties of silicon quantum dots in the framework of the TCAD Package NANOTCAD-ViDES. We adopt current spin density functional theory with a local density approximation and with the effective mass approximation. We show that silicon quantum dots exhibit large variations of the total spin as the number of electrons in the dot and the applied magnetic field are varied. Such properties are mainly due to the silicon band structure, and make silicon quantum dots interesting systems for spintronic and quantum computing experiments.

**Keywords** Current spin density functional theory · Silicon quantum dot · Spintronics

## 1 Introduction

Silicon-based spintronics is the subject of intense research, mainly for two reasons. First, silicon technology is the most advanced semiconductor technology, thanks to decades of unparalleled investments. Compatibility with silicon increases by orders of magnitude the chances for a proposed solution to acquire industrial relevance. Second, spin in silicon has a large coherence time, which makes the material

interesting for applications in which conservation of coherence of the wavefunction is required, such as quantum computing. Therefore, a few all-silicon spintronic devices have been proposed in recent years [1–5].

The spin of semiconductor quantum dots is considered an interesting option for the implementation of qubits. The case of silicon quantum dots seems particularly promising [1, 3], because the multiple degeneracy of the conduction band can lead to a very high total spin. Some experiments have been performed, but are not conclusive on this aspect [6]. From the simulation point of view, there are a few papers in the literature in which the spin properties of III-V quantum dots in a magnetic field are computed, but none that focuses on silicon, probably because of the complexity of silicon conduction and valence bands, which makes simulation more cumbersome.

We have implemented a three dimensional simulator of semiconductor structures containing silicon quantum dots immersed in a magnetic field based on Current Spin Density Functional Theory (CSDFT) [7], in the framework of the NanoTCAD ViDES package. In this paper, we discuss the physical model and the numerical approach we adopt, and we present the simulation of sample quantum dot structures, in order to demonstrate what quantities can be simulated, and to compute the very high total spin that is achievable in silicon quantum dots.

## 2 Physical model and numerical aspects

The electrostatic potential is obtained by solving the three-dimensional Poisson equation in the whole simulation domain, including both “quantum” and “semiclassical” charge densities as source terms. The quantum charge density is obtained by solving the many body Schrödinger equation in

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the so-called “quantum” regions, identified as the regions in which quantum confinement is significant. The semiclassical charge density is only a function of the local potential and is the charge density in those regions of the simulation domain in which quantum confinement is considered to be negligible.

The many body Schrödinger equation is solved with CS-DFT, using the local density approximation and the effective mass approximation with parabolic bands. CS-DFT allows one to fully take into account the effect of magnetic field and spin, and is strictly applicable only to the calculation of ground states.

The single particle Schrödinger equation must be solved for each spin and for each pair of minima in the conduction band (or  $\Gamma$  degenerate or quasi-degenerate). It reads [7]:

$$\left[ \frac{\mathbf{p}^2}{2m^*} + \frac{e}{2m^*} (\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + V + V_{xc} \right] \Psi_{i,j,\sigma} = E_{i,j,\sigma} \Psi_{i,j,\sigma} \quad (1)$$

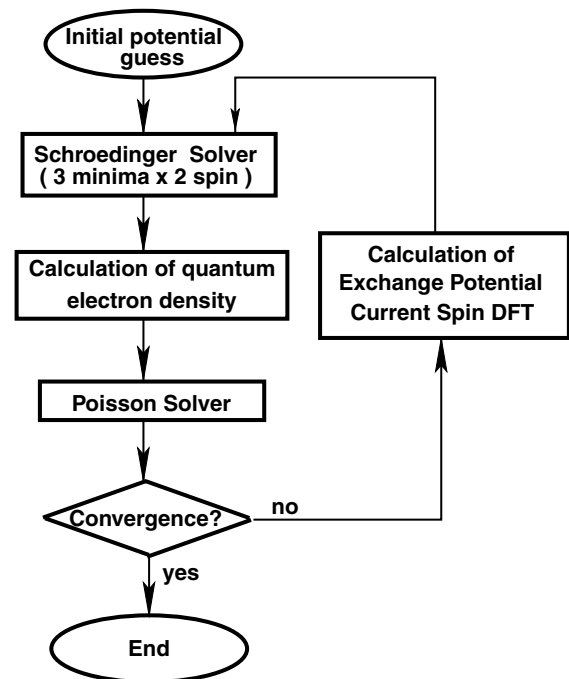
where  $\mathbf{p} = -i\hbar\nabla$  and  $\mathbf{A} = \mathbf{A}_0 + \mathbf{A}_{xc}$ .  $\mathbf{A}_0$  is the vector potential,  $V$  is the scalar potential, including Hartree and Zeeman terms.

$\mathbf{A}_{xc}$  and  $V_{xc}$  are the exchange-correlation vector and scalar potentials, respectively, computed as indicated in Ref. [8, 9] as a function of the local spin up and spin down electron densities, and of the local paramagnetic current density.  $\Psi_{i,j,\sigma}$  and  $E_{i,j,\sigma}$  are the  $i$ -th eigenfunctions and eigenvalues, respectively, of the  $j$ -th pair of minima ( $j = 1, 2, 3$ ), with spin  $\sigma$  ( $\sigma = +0.5, -0.5$ ). All single particle states are then cumulatively ordered and occupied in the order of increasing energy.

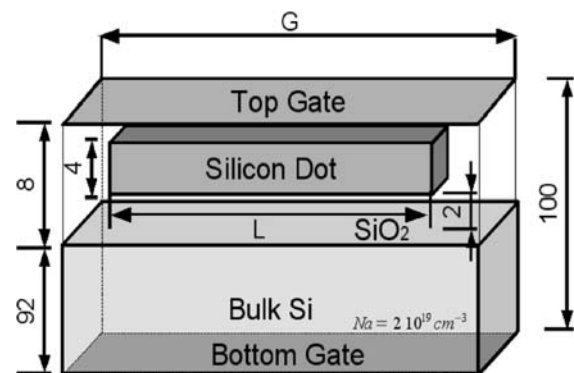
In Fig. 1 the flowchart illustrating the self-consistent solution of the Schrödinger and Poisson equations is shown. From a numerical point of view, the Schrödinger equation has been solved in momentum space [10], while the overall solution has been computed using the Newton/Raphson (NR) method with the Gummel interactive scheme. In particular, the Schrödinger equation is solved at the beginning of the each NR cycle of the Poisson equation, and the electron charge is kept constant until the NR cycle converges. The algorithm is then repeated periodically until the two-norm of the difference between the potential computed at the end of two subsequent NR cycles is smaller than 1 meV or the difference between two consecutive values of the electrochemical potential is smaller than 1  $\mu\text{eV}$ .

### 3 Numerical results

The structure considered in our simulation is shown in Fig. 2. It is an MOS structure with  $p$ -type silicon bulk



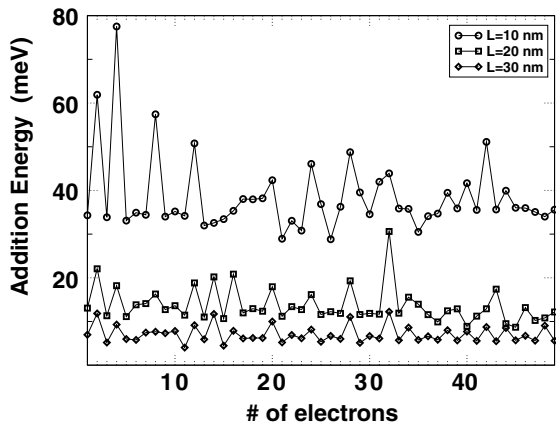
**Fig. 1** Flowchart illustrating the iteration for the self-consistent solution of Poisson and Schrödinger equations



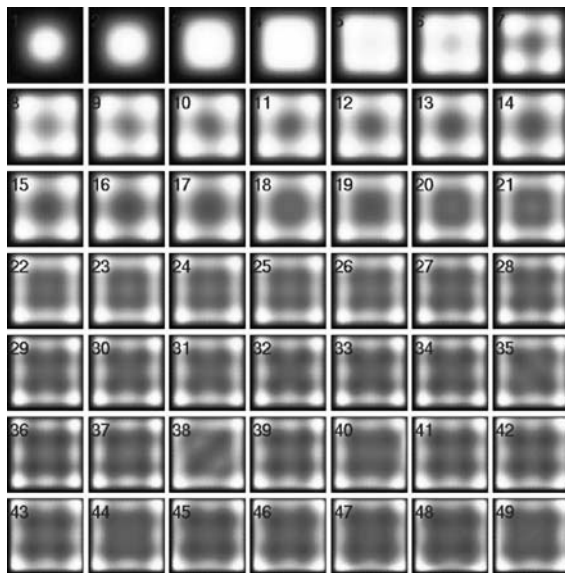
**Fig. 2** Simulated device structure. The base of the silicon quantum dot is a square  $L \times L$ , with  $L = 10, 20, 30$  nm

$N_A = 2 \times 10^{19} \text{ cm}^{-3}$ , 8 nm layer of silicon oxide and metal gate. An undoped silicon dot with height 4 nm and square base  $L \times L$  is embedded in the oxide layer. We consider three different dot sizes, corresponding to  $L = 10, 20$ , and 30 nm. The magnetic field is uniform along the vertical ( $z$ ) direction. We assume a silicon gyromagnetic factor of 2.6.

In Fig. 3 the addition energy of the three considered structures is shown for a number of electrons ranging from 1 to 49. It is particularly interesting the fact that convergence is obtained also for a very large number of electrons. Odd-even pairing is evident, as well as some features of the complicated shell structure. The electron density in the dot and the total spin for the case  $L = 20$  nm are shown in Fig. 4 and in Fig. 5, respectively.



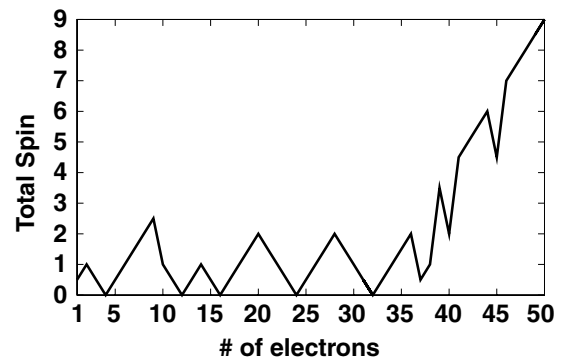
**Fig. 3** Addition energy for the three simulated structures at zero magnetic field for 1 to 50 electrons in the dot



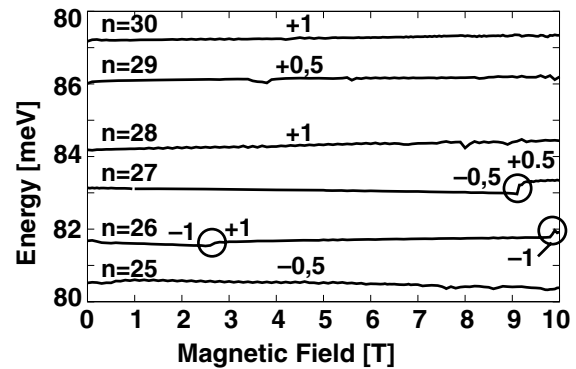
**Fig. 4** Electron density for 1 to 49 electrons in the dot for the 20 nm structure at zero magnetic field

One can observe that very large spins can be obtained, and that the addition of a single electron can substantially modify the total spin of the dot. This is due to the very important role played by the exchange potential and by the fact the three pairs of degenerate minima are present in silicon conduction band. Indeed, several single particle states are very close in energy, and their ordering and occupation is substantially modified by changes in the exchange potential due to the addition of a single electron.

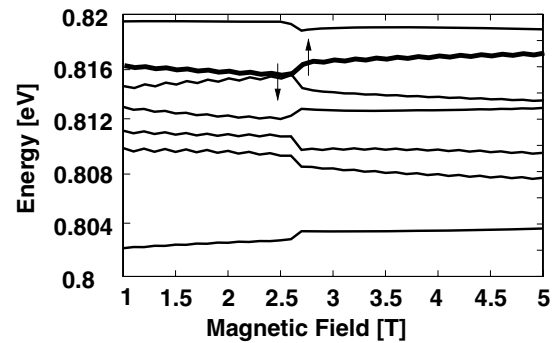
The electrochemical potential, given by Slater’s rule [11], is plotted as a function of the magnetic field in Fig. 6. As can be seen, evident changes of the total spin occur when the magnetic field modifies the ordering of single particle levels and in particular changes the spin of the highest occupied single particle level. The situation is shown in detail



**Fig. 5** Total spin for 1 to 50 electrons placed in the dot for the 20 nm structure at zero magnetic field



**Fig. 6** Electrochemical potential for the 20 nm structure from 25 to 30 electrons. Numbers placed on each curve indicate the total spin



**Fig. 7** Highest single particle energy level for the 20 nm structure when 26 electrons are in the dot as a function of magnetic field. Spin up and spin down single particle energies have opposite dependencies on the magnetic field, due to Zeeman effect. The bold line represents the electrochemical potential

in Fig. 7 for 25.5 electrons in the dot. In Fig. 7 the energies of the highest occupied single particle levels are plotted as a function of the magnetic field. The 26-th single particle level represents the electrochemical potential of the dot  $\mu(26)$ . As can be seen, for  $B = 2.6$  Tesla, the ordering changes and the total spin changes from  $-1$  to  $+1$ .

## 4 Conclusion

We have developed a code for the simulation of silicon quantum dots with current spin density functional theory, that allows us to simulate the electrical and spin properties of dots with up to 50 electrons in the presence of magnetic field. Silicon quantum dots exhibit a very rich spin behavior, due to the complex band structure, that is very intriguing and can be very interesting for spintronic applications.

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