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VIEWPOINT

Effects of the magnetic field in quantum computing with silicon

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Abstract
The effects of magnetic fields on the wavefunctions of electrons bound to donor nuclei in semiconductors will alter the properties of qubits and qubit–qubit interactions that are intended to be used for quantum computing in silicon.

The seminal proposal of Kane (1998) inspired several other descriptions of quantum computers that use electrons or spin 1/2 nuclei of donor atoms in silicon or germanium in a magnetic field as qubits (Vrijen *et al* 2000, Shlimak *et al* 2001, Koiller *et al* 2002, Abe 2003, Skinner 2003, Stoneham *et al* 2003). The nuclear spins interact with one another and can be influenced by a high-frequency electromagnetic field through their contact with the wavefunctions of electrons that are bound to the positively charged nuclei.

However, the preparation of devices in silicon leaves behind imperfections that modify the electronic states and affect their use in quantum computing elements (Keyes 2003, 2005). The lack of perfect control of all process parameters causes differences between nominally identical devices. The juxtaposition of materials of differing thermal expansion coefficients stresses the semiconductor during the heating and cooling cycles that accompany device fabrication and leaves strains (Noyan *et al* 1999, Shen *et al* 1996) that shift the energies of the valleys in multivalley semiconductors. These effects and their undesirable consequences are well-known in silicon integrated circuit technology (Orshansky *et al* 2002).

Static electric (Ahn 2005) and magnetic fields can also influence silicon devices. In particular, the moderate magnetic fields that are needed to create two spin states of different energy in proposals that use magnetic resonance have striking effects on the hydrogen-like wavefunctions of bound electrons in semiconductors with small effective masses and large dielectric constants. The alteration of the wavefunctions by the magnetic fields changes the density of the electronic wavefunction at the donor nucleus and the interactions between neighbouring donors through overlap of their wavefunctions. Here the magnitude of these effects and their significance for proposals that depend on donor electron wavefunctions in a magnetic field are discussed.

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Table 1. Parameters of semiconductors in a 2 T magnetic field.

Semiconductor	Ge	Si	InSb
Dielectric constant	16	12	16
Transverse effective mass	0.082	0.19	0.014
ρ_c (nm)	44	64	24
Bohr radius (nm)	6.4	3	60

Considering a magnetic field in the z direction, the field adds a term in $(x^2 + y^2)$ to the Hamiltonian for an electron trapped at a positively charged donor nucleus (Yafet *et al* 1956):

$$H = \frac{p^2}{2m} + \frac{m\omega^2\rho^2}{8} - \frac{e^2}{4\pi\epsilon r}. \tag{1}$$

Here r is distance from the nucleus and ω is the cyclotron frequency $\omega = eB/m$, B is the magnetic field, and $\rho^2 = (x^2 + y^2)$. Mass m is an effective mass in a semiconductor with permittivity ϵ. The increase of the positive magnetic term in the energy with distance from the nucleus, ρ in equation (1), confines the electrons closer to the nucleus, increasing the energy binding the electron to the donor (Yafet *et al* 1956). Large effects on the electronic wavefunction must be expected at distances from the nucleus where the magnetic energy in equation (1) exceeds the attractive potential energy of the donor nucleus. This happens in the plane normal to the magnetic field when $\rho > \rho_c$, where the critical radius ρ_c is $(2m/\pi\epsilon B^2)^{1/3}$ (Sladek and Keyes 1961). At larger values of ρ the repulsive magnetic term in the energy dominates and tends to concentrate the wavefunction in the region of negative potential energy.

The reality of these effects on electronic wavefunctions has been well established by experiment. Indium antimonide is the most striking example of the effects because of its very small effective mass and its large dielectric constant ($m/m_0 = 0.014$ and $\epsilon = 16\epsilon_0$). The large donor states (Bohr radius ~600 Å) ordinarily overlap enough to cause electrons in InSb to form a metal-like statistically degenerate electron gas (Stern and Talley 1955). Shrinkage of the donor wavefunctions in a high magnetic field reduces the overlap and produces a metal–insulator transition (Keyes and Sladek 1956, Zawadski and Wlasak 1984). The increasing depth of the donor state in InSb with increasing magnetic field has also been observed quantitatively by electrical measurements of transport properties (Sladek 1958, Zawadski and Wlasak 1984) and by the use of the dependence of the donor depth on magnetic field in InSb as a magnetically tunable photovoltaic infrared detector (Kimmet and Niblett 1963).

Magnetic fields produce similar but orientation-dependent effects in silicon and germanium. Silicon and germanium are multivalley semiconductors and the wavefunctions of donors are combinations of states derived from the individual valleys. The details of the effects of a magnetic field depend on the crystallographic direction of the field; the effects of the field on a valley depend on its direction with respect to the axis of the valley. In addition to changing the form of a wavefunction the magnetic field will in general destroy the symmetry degeneracy of the valleys, further altering the wavefunction by changing the contributions of the various valley wavefunctions to the bound donor wavefunction.

Table 1 shows the expected scale of the effects on ρ_c for silicon and germanium in a worst case, when the magnetic field is aligned with the long axis of a valley and m is the transverse effective mass. The shrinking of donor wavefunctions and the decrease in their overlap is evidenced in germanium by a large ($\Delta R/R \sim 1$) magnetoresistance in the hopping conductivity regime at low temperature when ρ_c approaches the average donor–donor separation (Sladek and Keyes 1961). Zwerdling *et al* (1959) found similar effects at higher magnetic fields in the exciton spectrum of germanium.

With the exception of the technique of Stoneham *et al* (2003), the contacts between the wavefunctions of neighbouring donors are essential to the interactions used in the operations of the proposed quantum computers. The separations between donors are in the range tens of nanometres to hundreds of nanometres, comparable to the values of ρ_c in table 1. By diminishing the value of the wavefunction at distances of order ρ_c and larger, the magnetic fields will reduce the exchange energy of the wavefunctions of donors separated by distances approaching or exceeding ρ_c to values smaller than those calculated by Herring and Flicker (1964).

The changes in the donor wavefunctions of semiconductors caused by a magnetic field will increase their densities at the donor nuclei and their interaction with a nuclear magnetic resonance signal and may weaken the interaction between neighbouring donors. The modifications of the electronic wavefunctions of multivalley semiconductors by the applied magnetic field must be taken into account in the design of quantum computing systems.

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