Gate Control of Single-Electron Spins in GaAs/AlGaAs semiconductor quantum dot

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Among recent proposals for next-generation, non-charge-based logic is the notion that a single electron can be trapped and its spin manipulated through the application of gate voltages (Rev. Mod. Phys.79, 1217 (2007)). In this talk we present numerical simulations of such Spin Single Electron Transistors (SSET) in support of experimental work at the University at Albany, State University of New York aimed at the practical development of post-CMOS concepts and devices. We use COMSOL based Multiphysics finite element simulation strategy to solve the Schrödinger-Poisson equations (with and without exchange-correlation effects) self-consistently to obtain realistic confining and gating potentials for realistic device geometries. We will discuss the calculation of the gate-tuned ``g-factor" for electrons and holes (Phys. Rev. B 68, 155330 (2003)) in electro-statically defined quantum dots including the Rashba and Dresselhaus spin-orbit interactions numerically from realistic wave functions for asymmetric and symmetric confining potentials. This work is supported through funding from the DARPA/NRI INDEX center.

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The semiconductor industry is driving the development of optoelectronics devices with smaller and smaller feature sizes according to Moore's law. A variety of efforts to use the electron spin rather than, or in combination with, its charge for information processing or, even more ambitiously, quantum information processing are being considered [1]. One of the challenging problems for such applications is to obtain sufficient control over the spin dynamics at large QD radius nanostructures in single electron Transistors.

Based on finite element simulation work, it is possible to design a quantum dot spin quantum computer for large quantum dot radius where the g-factor can be engineered by manipulating the spin-orbit coupling through external gates. A spin polarized electron is injected into the dot from one of the ferromagnetic layers which is trapped by Coulomb blockade. Its spin orientation encodes a qubit and its arbitrary directions are brought in resonance and out of resonance with global ac magnetic fields by applying a suitable electric field or voltage into the dot which eventually alters the g-value. [2]

Mathematical Model:

The Hamiltonian for a single electron bound to a heterojunction quantum dot can be written as [3]

$$H = H_0 + H_z + H_R + H_{D1} + H_{D2} \tag{1}$$

The first term corresponds to the motion of a conduction band electron confined in a two dimensional parabolic well in an external perpendicular magnetic field B

$$H_0 = \frac{\vec{P}^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 r^2 + \frac{1}{2} g_0 \mu_B \sigma_z B \tag{2}$$

Where the kinetic momentum $\vec{P} = \vec{p} + \frac{e}{c}\vec{A}$ is written with the canonical momentum $\vec{p} = -i\hbar\left(\partial_x, \partial_y, 0\right)$ and $\vec{A} = \frac{B}{2}(-y, x, 0)$ is the vector potential confined to the 2D plane. Here e is the electron charge, c is the velocity of light, m* is the conduction band edge effective mass, ω_0 is the parabolic confining frequency, g_0 is the bulk g-factor and σ_z is the diagonal Pauli matrix. The eigenstates of such a Hamiltonian and corresponding self energies were determined analytically by Fock and Darwin long before the appearance of nanostructures [4]. H_0 is diagonal when written as a function of the Fock-Darwin number operators $n_\pm = a_\pm^\dagger a_\pm$

$$H_0 = \hbar\omega_+\left(n_+ + \frac{1}{2}\right) + \hbar\omega_-\left(n_- + \frac{1}{2}\right) + \frac{1}{2}g_0\mu_B\sigma_z B \qquad (3)$$

Where

$$a_\pm^\dagger = \frac{1}{2\ell}(x \pm i y) - \frac{\ell}{2}\left(\partial_x \pm i\partial_y\right) \qquad (4)$$

$$a_\pm = \frac{1}{2\ell}(x \mp i y) + \frac{\ell}{2}\left(\partial_x \mp i\partial_y\right) \qquad (5)$$

Here $\omega_\pm = \Omega \pm \frac{\omega_c}{2}$ with $\Omega = \sqrt{\omega_0^2 + \frac{\omega_c^2}{4}}$ and $\omega_c = \frac{eB}{m^*c}$ being renormalized dot frequency and cyclotron frequency respectively. $\ell = \sqrt{\frac{\hbar}{m^*\Omega}}$ being the Fock Darwin radius [3].

The second term in Hamiltonian (1) represents the Quantum well confinement in the growth direction, $H_z = \frac{P_z^2}{2m^*} + V(z)$ where $V(z)$ is a triangular well, $V(z) = eEz$ for $z \geq 0$ and $V(z) = \infty$ for $z < 0$. A numerical calculation leads to the H_z ground state

$$\Psi_{0z} = 1.4261\,\kappa^{1/2}\mathrm{Ai}(\kappa z + \xi_1) \qquad (6)$$

Where $\zeta_1 = -2.3381$ is the first zero of the Airy function Ai, while the inverse length scale κ is set by

$$\kappa = (2m^* e E/\hbar^2)^{1/3} \qquad (7)$$

And the ground state energy is $E_{0Z} = -\zeta_1 eE/\kappa$. In the discussion below, we will make use of the average momentum squared in the state (6) $\langle P_z^2\rangle = 0.7794\,(\hbar\kappa)^2$ and the average position $\langle z\rangle = 1.5587/\kappa$ (which is the thickness of the 2DEG).

We now turn to the spin orbit interactions, third to fifth terms in Eq. (1). A k.p band structure calculation for zinc blend materials leads to the bulk conduction-band spin-orbit interaction [5]

$$H_{Bulk} = \frac{\gamma_c}{2\hbar^3}\sigma\cdot P \qquad (8)$$

Where $\widetilde{P}_x = P_x\left(P_y^2 - P_z^2\right) + H.c$. This equation is Hermitian and guage invariant. By averaging Eq (8) over the Quantum well ground state, we will get two spin orbit terms, linear and cubic in momenta [6].

$$H_{D1} = \frac{0.7794\,\gamma_c\,\kappa^2}{\hbar}\left(-\sigma_x P_x + \sigma_y P_y\right) \tag{9}$$

$$H_{D2} = \frac{\gamma_c}{\hbar^3}\left(-\sigma_x P_x P_y^2 - \sigma_y P_y P_x^2\right) + H.c. \tag{10}$$

The structural inversion asymmetry in V(z) leads to the Rashba interaction [7]

$$H_R = \frac{\alpha_R\, e\, E}{\hbar}\left(\sigma_x P_y - \sigma_y P_x\right) \tag{11}$$

TABLE 1 Parameters used in our calculations [3, 7, 8]

Parameter		**GaAs**
g_0		-0.44
m^*/m_e		0.067
α_R	[$Å^2$]	4.4
γ_c	[eV $Å^3$]	26

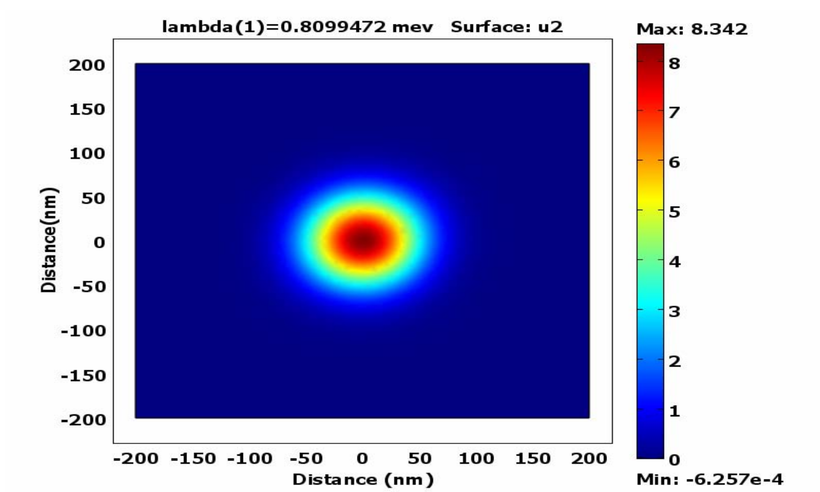

Figure 1: Illustration of Quantum Dot for spin up in a symmetric confining potentials at electric field 10^6 v/cm, 1 T magnetic field and QD radius equal to 120nm.

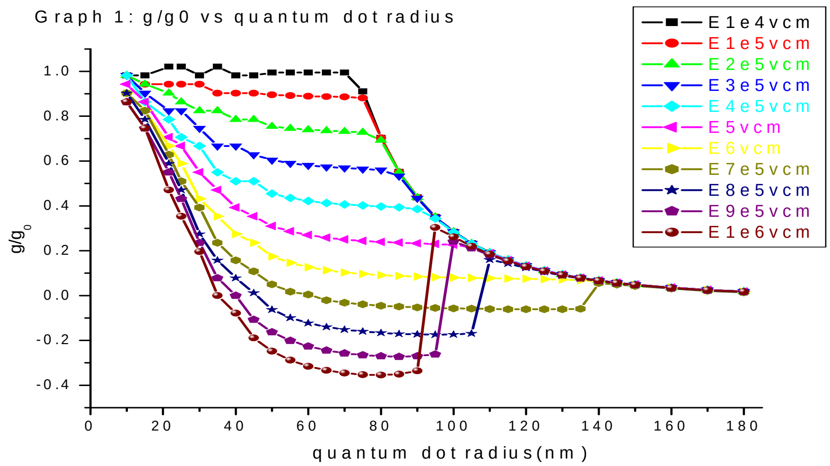

Figure 2: g-factor switching vs. quantum dot radius for symmetric quantum Dots

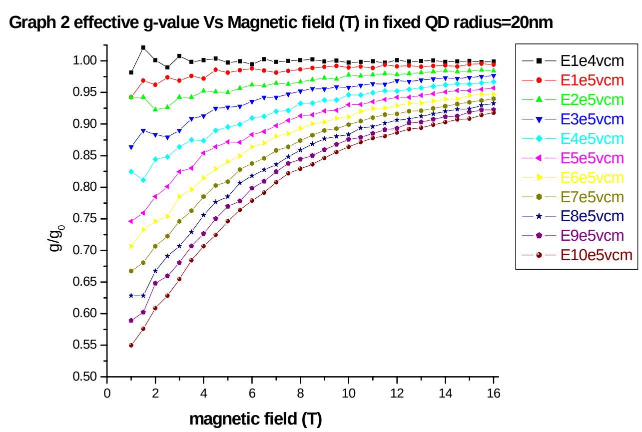

Figure 3: effective g-value verses magnetic filed in 20 nm fixed QD radius at different electric fields in symmetric confining potential

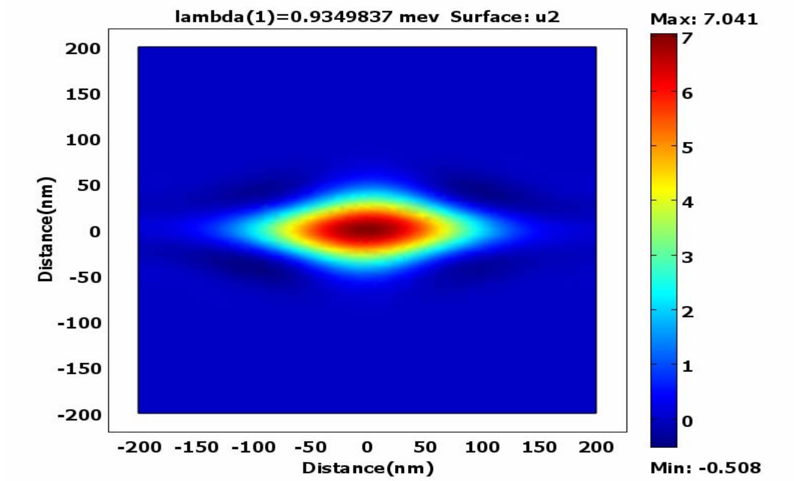

Figure 4: Illustration of Quantum dot for spin up in asymmetric confining potentials (y-axis confining potential is twice bigger than x-axis) at 10^6 v/cm electric field, 1Tesla magnetic field and QD radius equal to 120nm

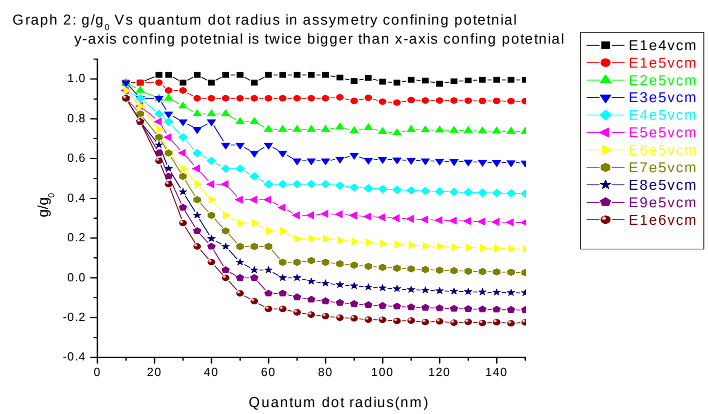

Figure 5: effective g-value verses magnetic filed in 20 nm fixed QD radius at different electric fields in Asymmetric confining potential

Results and Discussions:

The full Hamiltonian (1) is solved by using COMSOL Multiphysics Commercial software to find the ground and first excited state of GaAs QD in 2D plane for symmetric and asymmetric confining potentials which eventually leads us to calculate the electron g-value

$$g = \frac{E_2 - E_1}{\mu_B B}$$

Where E_1 and E_2 are the ground and first excited states including the spin, μ_B is the Bohr magneton and B is the applied magnetic field. We study the g-factor behavior at the range of electric fields from 10^5 v/cm to 10^6 v/cm and various quantum dot radius by restoring the exact diagonalization of the full Hamiltonian (eq^n.1) by finite element method (similar work for GaAs QD can be found in [3]. Figure 1 is the illustration of Quantum Dots for spin up in symmetric confining potentials at 10^6v/cm, 1 T magnetic field and QD radius equal to 120nm. Figure 4 is the illustration of Quantum dots for spin up in asymmetric confining potentials (y-axis confining potential is twice bigger than x-axis) at 10^6v/cm electric field, 1Tesla magnetic field and QD radius equal to 120nm.

Figure 2 shows the results of g-value calculation for the different values of electric fields and GaAs QD radius in symmetric confining potentials. It is clearly indicating that level crossing (two lowest energy states have the same spin) is mainly depends on the electric fields. We can switch the positive g-value to negative g-value at high electric fields (around $7*10^5$ v/cm to $10*10^5$ v/cm) and then we are getting level crossing at high QD radius. So the proposed device might work at high electric fields and lower Quantum Dot radius than level crossing. We estimated for a GaAs QD with $\ell_0 = 21.58$ nm, ΔE ~ 0.12 mev and $g - g_0 \sim -0.23$ at 10^6 v/cm for symmetric confining potentials. Figure 2 is a plot of effective g-value verses magnetic filed in 20 nm fixed QD radius at different electric fields in symmetric confining potential by solving full Hamiltonian 1 numerically. Instead controlling the g-value electrically, we can also control the g-value magnetically at high electric fields.

Figure (5) is a plot of effective g-value Vs QD radius in asymmetric confining potential where y-axis confining potential is twice bigger than x-axis confining potential. From figure it is clearly indicating that we are losing level crossing by applying asymmetric confining potential and we can still switch the positive g-value to negative g-value at high electric fields (around $7*10^5$ v/cm to $10*10^5$ v/cm). So the proposed device might work at large Quantum Dot radius by applying asymmetric confining potential in either x or y directions. We estimated for a GaAs QD with ℓ_0=21.58 nm, ΔE ~ 0.015mev and $g-g_0 \sim -0.18$ at 10^6 v/cm for asymmetric confining potential (y axis is twice than x-axis confining potential).

In this section, we comment on some of the features exhibited by the results of this work and will comment on some of our calculations and will point out the future directions for realistic design of the post CMOS process. Our results agree with the results of Das Sarma [3] for the case of symmetric confining potentials. For realistic geometries one must consider asymmetric confining potentials. In this case the Rashaba term dominates over the Dresselhauss term in the full Hamiltonian.
GaAs QD g-factor can be controlled electrically even in the absence of wave function overlap with a different material. These parameters show a striking dependence with dot radius when the 2DEG confinement is strong (`10^5v/cm). For example, the g-factor changes sign. This result establishes the versatility of III-V quantum dots as units for spin manipulation.

A related finding of interest in our work is the dual importance of both Dresselhauss (i-e the Bulk inversion symmetry inherent in zinc blend structures of II-V semiconductors) and Rashba (i-e the real space structural inversion asymmetry present in a heterostructure due to external electric fields).

Conclusions:

The relative quantitative importance of the Dresselhauss effect in the III- V nanostructures should have considerable significance in the g-factor engineering to the spin quantum computer architecture (that we consider in this work) but also in fabrication of the Datt-Das spintronic transistor where spin orbit coupling is used to modulate a spin – polarized current in field effect transistor configuration.
Eigen values and g- value calculation for different size of the GaAs QDs in different electric fields in symmetric confining potentials are consistent with previous findings by Das Sharma [3] where Dresselhauss terms were found to dominate.

Our new results based on finite element simulation show the importance of both types of spin orbit coupling (Rashba and Dresselhous) as well as a significant effect resulting from asymmetric confining potentials. These simulations are helping to guide experimental efforts by a providing realistic, engineering level description of the devices.

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