Coherent Spin-Qubit Shuttling in a SiGe Quantum Bus: Device-Scale Modeling, Simulation and Optimal Control

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Abstract

We present a framework for device-scale simulation of qubit shuttling in Si/SiGe along the interconnecting links of qubit registers. Propagation of the electron wave packet is modeled using a time-dependent Hamiltonian that describes the pulsing of the gate electrodes. Counterdiabatic driving is discussed from the viewpoint of expressibility and feasibility. An Outlook on the application of quantum optimal control theory is given.

Introduction

Spin qubits in gate-defined semiconductor quantum dots

- major candidates for the realization of fault-tolerant quantum computers
- long coherence time due to isotopically purified ^{28}Si quantum wells
- compatibility with industry standard fabrication technology
- small-scale devices have been demonstrated, which execute one- and two-qubit logic gates as well as initialization and read-out operations with high fidelity using all-electrical control
- scalable architecture with sparse 2D qubit-arrays interconnected by quantum bus shuttles

Quantum Bus: Coherent Shuttling of Spin-Qubits

- high-fidelity transfer of electron spin state between remote QD arrays along a channel
- scalability due to the design based on periodic segments
- channel length independent of number of gate electrode sets
- design provides sufficient space for QD wiring and classical on-chip control electronics, solving the fan-out problem [3]

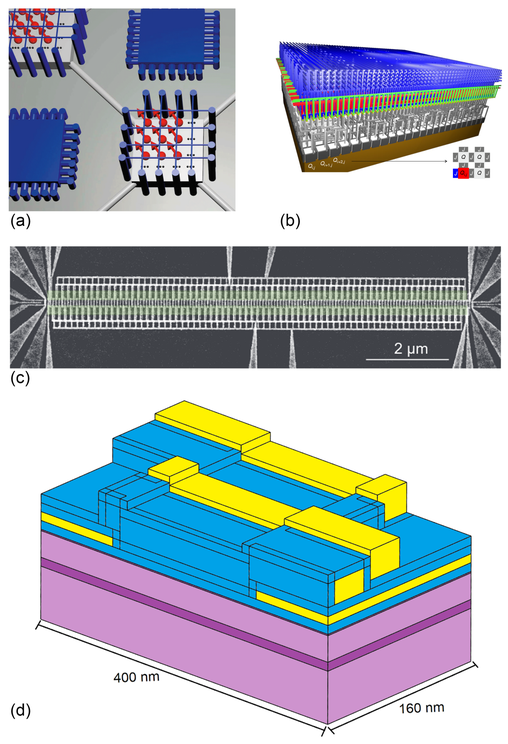

Fig. 1. (a) Sparse 2D qubit arrays interconnected by quantum links for coherent qubit shuttling [1]. (b) Side view of one qubit array [2]. (c) Scanning electron micrograph [3] and (d) schematic illustration of the SiGe-quantum bus.

Electrostatic Model

- electrostatic potential is the solution of the Poisson's equation

$$-\nabla \cdot (\varepsilon(\mathbf{r}))\nabla\Phi(\mathbf{r}, t)) = \rho(\mathbf{r}) \quad \text{on } \Omega \tag{1}$$

- mixed boundary conditions (Dirichlet and homogeneous Neumann)

$$\mathbf{n} \cdot \nabla\Phi + \lambda\Phi = \lambda U_i(t) \quad \text{on } \partial\Omega \tag{2}$$

- exploit linearity of the problem: splitting into separate contributions of individual electrodes and the defect potential

$$\Phi(\mathbf{r}, t) = \sum_i \Phi_i(\mathbf{r}) U_i(t) \tag{3}$$

- discretization of the equation with a Voronoi box based finite volume method using `VoronoiFVM.jl` [4]
- 3D Delauney mesh tetrahedralization with `TetGen.jl` [4]

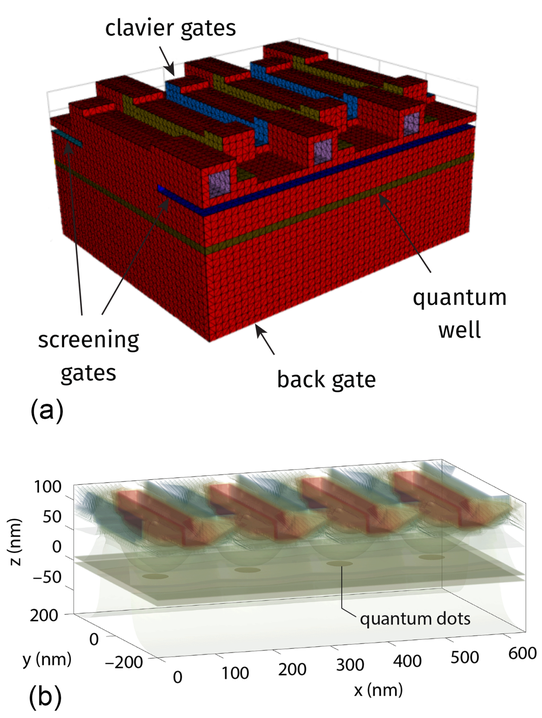

Fig. 2. (a) Boundary conforming Delaunay mesh of the quantum bus device geometry. (b) Numerically computed electrostatic confinement potential.

Bound States

- bound states of the wave function are the solutions of the stationary Schrödinger equation $\hat{H}\varphi_n = E_n\varphi_n$
- Hamiltonian consists of the kinetic part and the sum of potential energies:
  - conduction band gap of Si and SiGe in the quantum well V_{qw}
  - charge defect potential V_ρ
  - gate electrode potentials $-q\Phi(\mathbf{r}, t)$

$$\hat{H}\varphi_n = -\frac{\hbar^2}{2}\nabla \cdot \left(\frac{1}{m^*}\nabla\varphi_n\right) + \Big(V_{\text{qw}}(\mathbf{r}) + V_\rho(\mathbf{r}) - q\Phi(\mathbf{r}, t)\Big)\varphi_n \tag{4}$$

- solve with `WavePacket` [5] using a pseudospectral method (3D FFT grid)

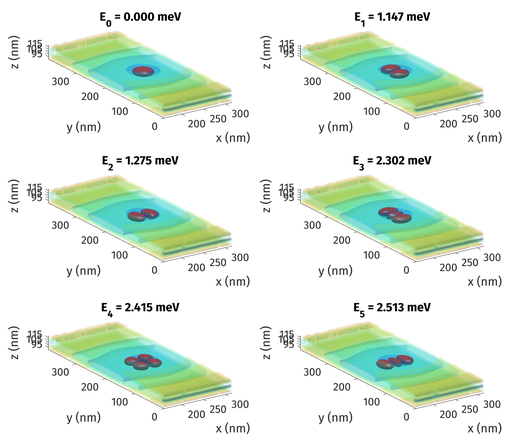

Fig. 3. Bound states of the lowest six eigenvalues for the stationary Schrödinger equation.

Instantaneous Eigenvalue Problem

- voltages at the clavier gates change slowly in time with sinusoidal protocol (conveyor belt mode)
- electron wave function is the solution of the time-dependent Schrödinger equation $i\hbar\partial_t\psi = \hat{H}(t)\psi$
- electron wave function is expanded in instantaneous eigenmodes of the Hamiltonian at each instant of time (adiabatic frame representation)

$$\psi(\mathbf{r}, t) = \sum_n c_n(t)\varphi_n(\mathbf{r}, t) \tag{5}$$

- where the eigenmodes obey the instantaneous eigenvalue problem

$$\hat{H}(\mathbf{r}, t)\varphi_n(\mathbf{r}, t) = E_n(t)\varphi_n(\mathbf{r}, t) \tag{6}$$

- obtain the complex amplitudes $\tilde{c}$ in the co-rotating frame by solving the nonautonomous differential equation for the dynamics

$$\dot{\tilde{c}}_n = \sum_{m\neq n} \frac{\langle\varphi_n(t)|\,\dot{\hat{H}}\,|\varphi_m(t)\rangle}{E_n(t) - E_m(t)} \times e^{-i(\theta(t)-\theta_m(t))}\tilde{c}_m(t) \tag{7}$$

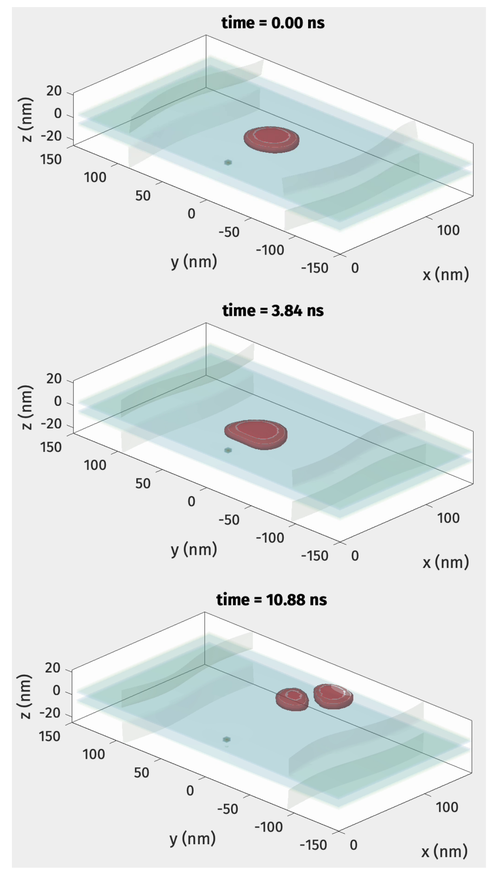

Fig. 4. Scattering of the electron interacting with a charge defect inside the channel. Simulation with periodic boundary conditions.

Counterdiabatic Driving

- suppression of non-adiabatic transitions
- compensate for the non-adiabatic part of the Hamiltonian with a reverse engineered control potential

$$\hat{V}_{\text{cd}}(t) = i\hbar\frac{d\hat{U}(t)}{dt}\hat{U}^\dagger(t) \tag{8}$$

- $\hat{U}(t)$ is the unitary operator that diagonalizes the uncontrolled Hamiltonian

$$\hat{U}^\dagger(t)\hat{H}(t)\hat{U}(t) = \text{diag}(E_1(t), E_2(t), \ldots)$$

- problem with expressibility by gate electrode voltages
- problem with rapidly changing electromagnetic field, that could alter the spin state

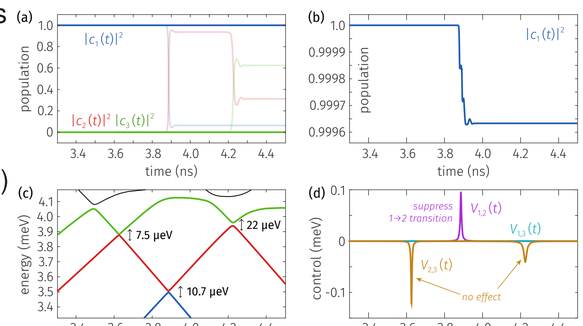

Fig. 5. (a) Population of the three lowest eigenstates calculated from Eq. 7 with (solid line) and without control (faint line) and (b) zoom on the ground state population. (c) Eigenvalue curves with defect-induced narrow spectral gaps that enable Landau–Zener transitions. (d) Control matrix elements over time.

Outlook: Quantum Optimal Control

- consider a control potential $\hat{V}_{\text{ctrl}}(t) = \sum_k \hat{V}_k(t)u_k(t)$
- Pontryagin's maximum principle: minimize the cost functional

$$J[\mathbf{u}] = \langle\psi(t_f)|\,\hat{R}\,|\psi(t_f)\rangle + \int_{t_i}^{t_f} dt\left(\frac{1}{2}\sum_k u_k^2(t) + \langle\psi(t)|\,\hat{Q}(t)\,|\psi_(t)\rangle\right) - \frac{2}{\hbar}\text{Im}\int_{t_i}^{t_f} dt\,\langle\chi(t)|\left(\left(\hat{H}(t) + \hat{V}_{\text{ctrl}}(t)\right)|\psi(t)\rangle - i\hbar\frac{d}{dt}|\psi(t)\rangle\right) \tag{9}$$

- solve two-point boundary value problem
  - controlled state equation with initial conditions

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \left(\hat{H}(t) + \hat{V}_{\text{ctrl}}(t)\right)|\psi(t)\rangle, \qquad |\psi(t_i)\rangle = |\psi_{\text{init}}\rangle \tag{10}$$

  - co-state equation with terminal conditions

$$i\hbar\frac{d}{dt}|\chi(t)\rangle = \left(\hat{H}(t) + \hat{V}_{\text{ctrl}}(t)\right)|\chi(t)\rangle + i\hbar\hat{Q}(t)\,|\psi(t)\rangle, \qquad |\chi(t_f)\rangle = -\hat{R}\,|\psi(t_f)\rangle \tag{11}$$

  - optimality condition

$$u_k(t) = \frac{2}{\hbar}\text{Im}\left(\langle\chi(t)|\,\hat{V}_k(t)\,|\psi(t)\rangle\right) \tag{12}$$

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This work received funding from the German Research Foundation under Germany's Excellence Strategy – EXC 2046: MATH+ (project AA2-17).