1.3 Spin-Qubit Shuttles for Scalable Semiconductor Quantum Computers: Modeling, Simulation and Optimal Control

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Quantum computers harness the principles of quantum mechanics to outperform classical computers in tackling certain mathematical problem classes. These problems encompass various tasks such as, e.g., integer factorization, searches in large unsorted databases, solving huge linear systems of equations and combinatorial optimization problems. Furthermore, a particular type of quantum computer—the quantum simulator—holds the potential for efficient simulations of large-scale quantum many-body systems, which are ubiquitous in materials research (e.g., high-temperature superconductors, catalysts, etc.) or pharmaceutical drug development.

In contrast to classical digital computers, where information is encoded in bits that can be either in the state 0 or 1, the information in quantum computers is encoded in so-called *quantum bits*, or *qubits* for short. These qubits represent abstract quantum mechanical two-level systems that are not limited to reside in one of the basis states[1] $|0\rangle$ or $|1\rangle$, but can also exist in any continuous superposition $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$. The information is encoded in the complex amplitudes $\alpha, \beta \in \mathbb{C}$, which describe a point on the unit sphere, the so-called *Bloch sphere*; see Figure 1. Accordingly, a quantum computer is more similar to an analog classical computer than to a digital one. The ability of a quantum system to be in a coherent superposition of different states simultaneously is a fundamentally non-classical property of the system that, however, requires careful shielding from its environment. Otherwise, coupling to external reservoirs might lead to uncontrolled disturbances or even to a "collapse of the wave function" into one of the two basis states when observing the qubit with a macroscopic measurement apparatus.

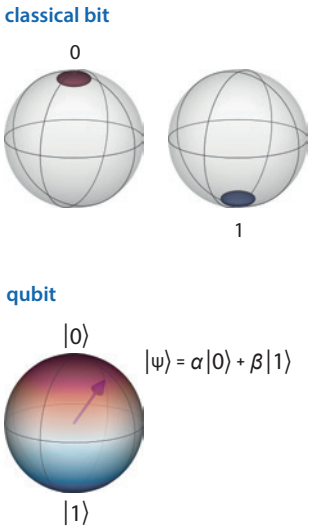

Fig. 1: *Bits in classical computers encode only digital information (state 0 or 1) whereas a qubit can be in a superposition of both states simultaneously (visualized as a point on the Bloch sphere)*

The true potential of quantum computers unfolds when a large number of qubits is considered. A system of N qubits can be in a superposition of up to 2^N states simultaneously, which means that a correspondingly large amount of information can be encoded in the associated 2^N amplitudes. The information stored in a qubit register thus scales exponentially with the system size, so that when a single new qubit is added, the size of the underlying state space doubles (and not just increases by +1 as with classical bits). It is this scaling behavior that limits the feasibility of simulating large quantum many-body systems on classical computers that inspired Richard Feynman in 1982 to the idea of using artificial quantum systems as novel type of computers. This led to the emergence of the new field of *quantum information theory* in the late 1980s and early 1990s, which quickly spawned several new algorithms such as the Shor algorithm for integer factorization (1994) that received enormous attention because of its potential to break widely used encryption methods.

The actual implementation of quantum algorithms requires new hardware realizations that have to meet very demanding and partly even complementary requirements. In 2000, David DiVincenzo published a list of criteria that potential hardware platforms for quantum computing must fulfill. This includes the ability to, e.g., initialize the qubit register with high precision in a specific state, control the system in a targeted manner to execute the actual computing steps (quantum gate operations) and to precisely measure the system in order to extract the results. Although each of

[1] Here, we use Dirac's notation, where $|\cdot\rangle$ denotes a Hilbert space vector.

these tasks requires a specific interaction of the qubits with the environment (preparation, manipulation, measurement), the register must be almost perfectly shielded from any other environmental influences, as otherwise the many-body wave function would dissipate into a classical mixture of states (known as *decoherence*), and the information encoded in the amplitudes would be lost.

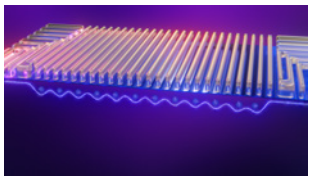

Fig. 2: *Schematic illustration of Intel's 12-qubit silicon quantum processor "Tunnel Falls" © Intel Corporation*

Electron spins in semiconductor nanostructures are among the most promising hardware platforms for the realization of universal quantum computers. In this technology, electrons are trapped in electrostatically defined quantum dots (QDs) resulting from a combination of epitaxial confinement in the vertical direction (a quantum well) and in-plane confinement generated by an electrostatic potential landscape shaped by gate electrodes on the top surface. Electrons bound in such QDs can reside only in discrete states, which can be selectively manipulated by adjusting the electrode voltages. In order to realize universal quantum algorithms, it is necessary to implement arbitrary one-qubit gates and a specific two-qubit gate. The former correspond to arbitrary rotations of the qubit on the Bloch sphere and can be realized via micromagnets or all-electrically using alternating current pulses to trigger the electron spin resonance. For the realization of two-qubit gates, the exchange interaction between electrons in neighboring QDs is used to build up non-classical correlations between them (known as *entanglement*). Both types of operations as well as initialization and readout have already been demonstrated with high fidelity exceeding 99% [1]. A key factor for the quality of these qubits is the use of isotopically purified ^{28}Si in the quantum well, which enables very long coherence times. The great prospect of this technology is its compatibility with industrial fabrication techniques that should enable scaling to a very large number of qubits just as it has been achieved with silicon transistors in classical computers. As a landmark step in this direction, Intel unveiled its first 12-qubit silicon quantum processor *Tunnel Falls* in June 2023; see Figure 2.

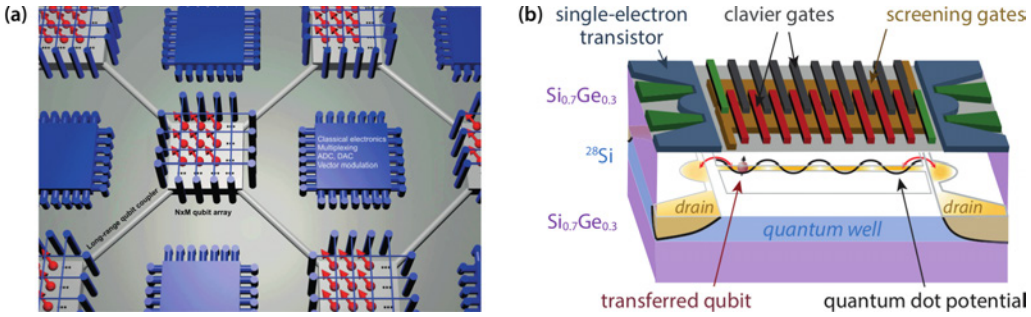

Fig. 3: *(a) Small-scale qubit arrays interconnected by links for coherent exchange of quantum information as a concept for a scalable quantum computing architecture [2]. (b) Concept for a spin-qubit shuttling device developed at RWTH Aachen/ FZ Jülich [3].*

Wiring of a large number of QDs on a chip, however, is a great challenge, as each QD requires several contact lines for confinement, readout, and signaling that must be stacked in multiple layers. This results in geometric limitations as well as the risk of unintentional self-heating due to high current densities. A potential remedy is a modular design with rather small qubit arrays that are interconnected by so-called *quantum links* [2]; see Figure 3 (a). These quantum links serve—in analogy to the bus system in classical computers—to exchange quantum information between qubit arrays, whereby even spatially far separated qubits can become entangled. One possible realization of such a quantum link is the quantum bus [3] that is currently being developed at Rheinisch-Westfälische Technische Hochschule (RWTH) Aachen and Forschungszentrum (FZ) Jülich; see Figure 3 (b). The WIAS Focus Platform SemQuTech *Simulation of Semiconductor Devices for Quantum Technologies* supports this development with mathematical modeling and numerical

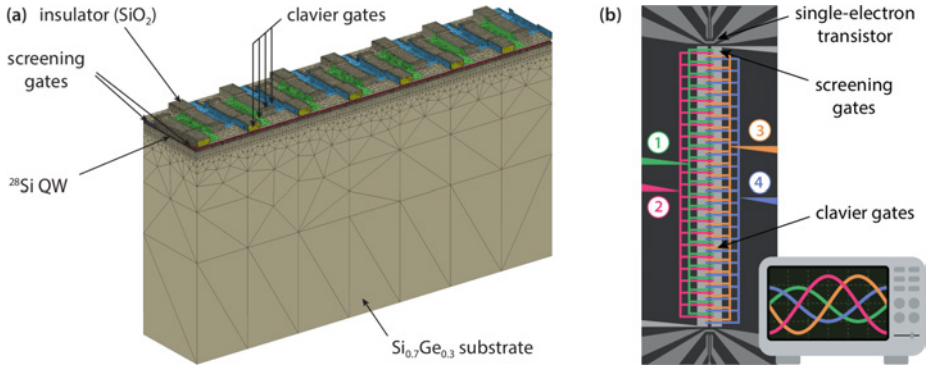

Fig. 4: *(a) Delaunay mesh of the Si-Qubus device with indicated gate electrodes, insulators, and ^{28}Si quantum well (QW). The computational mesh has about 20 million nodes and was generated using* `TetGen`*. (b) Top view on the quantum bus shown in Figure 3 (b), adapted from [3]. The four different clavier gate sets are indicated by color.*

simulation. The collaboration interlinks the two Clusters of Excellence *Matter and Light for Quantum Computing* (ML4Q) and *MATH+*.

Modeling and simulation of spin-qubit shuttling

The quantum bus shown in Figure 4 (a) forms a moving chain of QDs that can be propagated by suitable pulsing of the clavier gates like a conveyor belt. This enables shuttling of electrons inbetween qubit arrays. A key feature of the device concept is that there are only four different clavier gate sets, with every fourth being electrostatically connected to all the others in the chain; see Figure 4 (b). Hence, the number of required control signals is independent of the length of the shuttle, making the technology scalable. Moreover, the required classical control electronics can be integrated directly on the chip; see Figure 3 (a). Next to the clavier gates, there are two screening gates at the sides that can be used for lateral control of the shuttling trajectory; see Figure 4.

The starting point for numerical device simulation is the computation of the electrostatic potential distribution Φ to generate the QDs. The potential is given as the solution of the Poisson problem

$$\begin{aligned} -\nabla \cdot (\varepsilon(\mathbf{r}) \nabla \Phi(\mathbf{r},t)) = 0, \qquad & \Phi(\mathbf{r},t)|_{\Gamma_{D_k}} = U_k(t), \\ \mathbf{n} \cdot \nabla \Phi(\mathbf{r},t)|_{\Gamma_N} = 0, \quad & \Phi(\mathbf{r},t)|_{\Gamma_{\text{period}}} = \Phi(\mathbf{r}+\mathbf{e}_x L_x, t), \end{aligned} \tag{1}$$

with Dirichlet (at the gate contacts Γ_{D_k}), Neumann, and periodic (in propagation direction) boundary conditions. By exploiting the linearity of the problem, the system (1) can be reduced via

$$\Phi(\mathbf{r},t) = \sum_k U_k(t)\,\phi_k(\mathbf{r}) \tag{2}$$

to a stationary Poisson problem for each of the six independent electrode potentials ϕ_k; see Figure 5. The clavier gate voltage sequence for conveyor-mode qubit shuttling is

$$U_k(t) = U_k^{\text{DC}} + U_k^{\text{AC}} \sin\left(\frac{\pi}{2}k + 2\pi f_s t\right), \qquad k = 1 \ldots 4, \tag{3}$$

where f_s is the shuttling frequency. The problem (1) is discretized using a finite volume method and solved by Conjugate Gradient (CG) iteration. The numerical computation is based on the Julia package `VoronoiFVM.jl` [4].

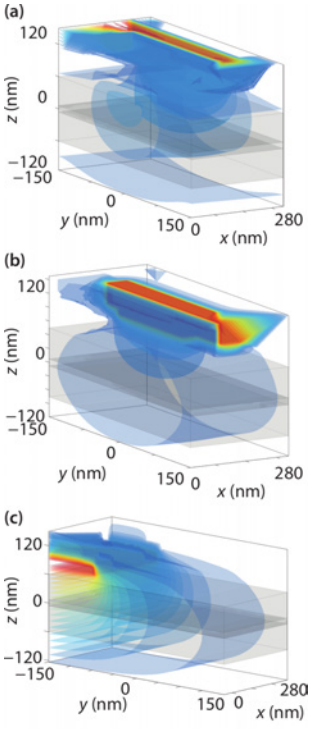

Fig. 5: *Normalized gate electrode potentials ϕ_k of the (a) upper clavier gates, (b) lower clavier gates, and (c) screening gates*

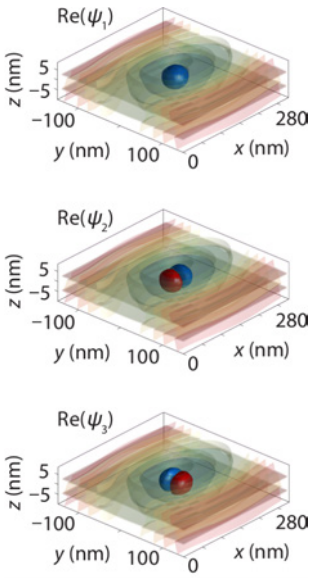

Fig. 6: *Isosurface plots of the three lowest energy quantum dot orbital eigenstates and the confinement potential*

Having the electrostatic potential generating the QDs at our disposal, we can turn to electron wave packet propagation that is described by the time-dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = H(\mathbf{r},t,\mathbf{u}(t))\,\Psi(\mathbf{r},t) = \left(H_0(\mathbf{r},t) - e_0\sum_k u_k(t)\,\phi_k(\mathbf{r})\right)\Psi(\mathbf{r},t)\,, \tag{4}$$

where Ψ is the wave function. The reference Hamiltonian

$$H_0(\mathbf{r},t) = -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m^*(\mathbf{r})}\nabla\right) - e_0\Phi(\mathbf{r},t) + V_{\mathrm{QW}}(\mathbf{r}) + V_{\mathrm{defect}}(\mathbf{r}) \tag{5}$$

describes the kinetic energy of the electron (with effective mass m^*), the electric potential of the gate electrodes, the quantum well confinement potential V_{QW} and the potential V_{defect} of charged defects. Because of the pulse sequence (3), the Hamiltonian H_0 is also time dependent. In addition, the full Hamiltonian in (4) includes an extra control part that describes a correction $u_k(t)$ to the nominal pulse sequence $U_k(t)$. A direct simulation of (4) by spectral and split-step methods is computationally expensive due to a large time-scale separation: While the envelope of the wave packet evolves only slowly during shuttling (typical time scale is tens of ns), the phase undergoes rapid oscillations that are several orders of magnitude faster. Therefore, an alternative approach is pursued that is based on an expansion of the wave function in instantaneous eigenfunctions ψ_n of H_0 (see Figure 6)

$$\Psi(\mathbf{r},t) = \sum_n c_n(t)\,\psi_n(\mathbf{r},t)\,.$$

With the help of the Hellmann–Feynman theorem, the TDSE (4) can be reduced to a system for the complex amplitudes $c_n(t)$, which has several advantages: It is directly interpretable, provides a dramatic reduction of the dynamical state space and, furthermore, allows to eliminate the rapid phase oscillations [5]. This approach, however, requires the (partial) eigendecomposition of H_0 for any point in time (and a suitable strategy for adaptive refinement) in a pre-processing step. Figure 7 shows the eigenvalue curves as a function of the shuttling phase featuring numerous avoided crossings, each of which can give rise to complex dynamics. Note that the spectrum can be strongly modified in the presence of a charged defect; see Figure 7 (b). Forward simulations of conveyor-mode shuttling depicted in Figure 8 show the impact of a charged defect within the channel that triggers undesired population transfer to excited states in a sequence of Landau–Zener transitions. Since the coupling of the spin to the external magnetic field is modified for excited states, this will lead to a randomization of the accumulated spin phase that must be avoided.

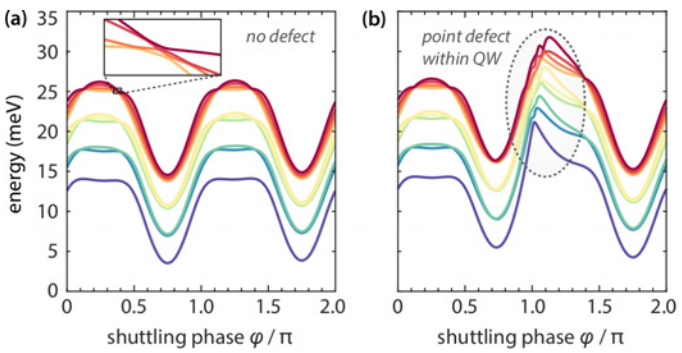

Fig. 7: *Eigenvalue branches as a function of the shuttling phase $\varphi = 2\pi f_s t$, cf. (3), (a) without a defect and (b) with a charged point defect in the QW center*

Quantum optimal control

Pontryagin's maximum principle [6] is employed to engineer control pulse sequences $u_k(t)$ to counteract the impact of charged material defects. This is achieved by minimizing a cost functional

$$J(\Psi, \mathbf{u}) \propto \int_{t_0}^{T} \mathrm{d}t \left(\langle \Psi(t) | \hat{H}^2(t, \mathbf{u}(t)) | \Psi(t) \rangle - \left(\langle \Psi(t) | \hat{H}(t, \mathbf{u}(t)) | \Psi(t) \rangle \right)^2 \right) \tag{6}$$

that penalizes the accumulated energy uncertainty of the electron during shuttling, which is proportional to the infidelity due to spin dephasing. The functional (6) is supplemented with the TDSE (4) as a dynamical constraint using the Lagrange multiplier method. Variation of the augmented functional yields evolution equations for the state and co-state that allow to construct gradients of the functional with respect to the controls. These equations are solved using structure-preserving propagation schemes to preserve the norm of the wave function. Functional minimization is carried out using a quasi-Newton method (L-BFGS) in a collaboration with Technische Universität Berlin (MATH+ project AA2-17). The controls obtained this way enable an almost deterministic passage of the electron through the channel without reducing the shuttling velocity [5].

Conclusions and outlook

Electron shuttling devices are new functional elements in modular concepts for spin-qubit based quantum computers that have promising prospects for scalability due to direct compatibility with industrial fabrication techniques. Numerical device simulation is crucial for understanding the limiting factors and performance bottlenecks of such devices and provides a means for further optimization. Quantum optimal control theory can be used to engineer pulse sequences that enable a high transfer fidelity of the qubit even in the presence of charged impurities and other defects. In the future, the model will be extended by further important aspects such as mechanical deformations (strain) and random alloy fluctuations at the Si/SiGe heterostructure interface.

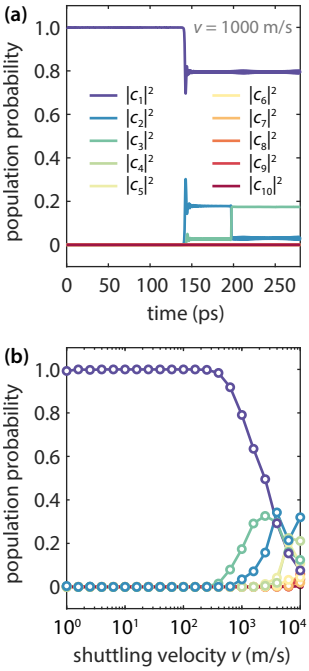

Fig. 8: *(a) Population dynamics of a qubit swept through a sequence of avoided crossings showing several Landau–Zener transitions. (b) Final state population probability vs. shuttling velocity $v = L_x f_s$ after propagation over one unit cell (four clavier gates).*

References

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