Valley degree of freedom in classical and quantum bits

PhD Thesis Booklet

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Introduction, motivation

Exponential growth of computational capability cannot be sustained only by miniaturization of electrical circuits. On the one hand, reaching the atomic-scale limit results in increased importance of leakage current; on the other hand, heat dissipation of the circuits significantly increases with growing transistor density. To solve these problems, it seems necessary to change the present computer architecture.

Classical bits are often realized using the charge of electrons, but an electron has spin degree of freedom as well, furthermore in certain crystalline solids, the so-called valley degree of freedom is also present. The former is studied by spintronics from the aspect of information processing and data storage, the latter is researched by valleytronics for the same purpose. The rise of valleytronics occurred due to the isolation of two-dimensional multivalley materials (e.g. graphene, transition metal dichalcogenide monolayers). From the perspective of information technology, the key parameter for realizing a new valley-based computer architecture is the valley polarization: the generation and detection of which are of fundamental concern.

Another possible computer architecture would be the quantum computer, which exploits the superposition and entanglement of quantum mechanics. The elementary unit of a quantum computer is the quantum bit (qubit) which is invoked to perform quantum algorithms. In principle, certain problems can be solved much faster using quantum algorithms than using the known classical algorithms. For instance, these kinds of problems are the simulation of
a many body quantum system, prime factorization and searching in an unsorted list.

Three well-separated processes have to be executed to realize classical or quantum computation: initialization of the bits, performing single- and two-bit logic gates, and readout of the result. The question is what system can physically realize this? To obtain the answer we have to study physical mechanisms which affect the classical or quantum bits, and the operations performed on them.

My doctoral thesis is based on three publications in which I studied systems that can physically realize classical [1] or quantum bits [2, 3]. In these works, the valley degree of freedom plays a crucial role. In the papers [1, 2] that I investigated, the presence of the valley degree of freedom can be considered as a carrier of information, whereas in the work [3] I found that the most dominant information loss mechanism is derived from the valley degree of freedom.

In my first work [1] I studied how valley polarization of an ensemble of electrons is lost under the influence of randomly distributed charged impurities located under the graphene sheet and how this is affected by the screening effects due to the electron-electron interaction. In my second paper [2], the valley qubit realized in silicon quantum dot is investigated for the purpose of showing how a single-atom high step at the silicon-barrier interface can be exploited to electrically control the qubit, and how the usability of the valley qubit is affected by relaxation and dephasing. In my third work [3] I examined the charge, flip-flop and electronic spin relaxation of a donor-dot system realized by a phosphorus donor in silicon.
Models and methods

The key consideration in choosing the theoretical models, which solve the above specified problems, was to be minimal in some sense, i.e. the models had to contain all necessary physical details of the systems while remaining solvable by analytical or numerical methods as effortlessly as possible. The appointed theoretical tasks were performed using the toolboxes of quantum mechanics and solid state physics.

Valley relaxation in graphene [1]

To investigate the valley relaxation due to charged impurities in graphene, a special model of graphene was applied, where the $p_z$ orbitals of graphene electrons were approximated by two-dimensional Gaussian functions. Charged impurities were assumed to be located in a plane parallel with the graphene sheet, distributed randomly. I obtained the valley relaxation rate by solving the Boltzmann equation: for the case of noninteracting electrons, as well as for the case when the impurity potential is screened due to electron-electron interaction. For the screened case, I applied linear response theory to evaluate the dielectric and polarizability matrix in the random phase approximation, and local-field effects were also taken into account. Inter-valley transition rates were evaluated using Fermi’s golden rule.
Dynamics of valley qubit in silicon quantum dots [2]

The silicon quantum dot was treated with a hybrid model, where the electronic wave function is described by a one-dimensional tight-binding model perpendicular to the interface, and by using an envelope function approximation parallel to the interface. The proper geometry and material composition of the quantum dot were achieved by setting the parameters (effective mass, electrostatic potentials, on-site energies and hopping amplitudes) of the model. The eigenenergies and eigenstates were obtained by exact diagonalization of the model Hamiltonian. The Rabi oscillation of the valley qubit due to an ac electric field, the cavity-mediated two-qubit coupling, just as the phonon-induced relaxation, and the dephasing due to quasi-static noise were described by the transverse and longitudinal matrix elements of the model. The phonon-induced relaxation process was treated using the silicon-specific Herring-Vogt electron-phonon coupling.

Relaxation of the flip-flop qubit in the donor-dot system [3]

The donor-dot system was described by an $8 \times 8$ effective Hamiltonian, where the spatial part of the electronic wave function was obtained by projection into the donor and dot states. Valley compositions of these two states were determined by means of Kohn-Luttinger theory. Coupling between electronic and nuclear spin was described by an isotropic interaction term, and spin-orbit coupling and $g$-tensor modulation were regarded as source mechanisms of electronic spin relaxation. The charge, flip-flop and
electronic spin relaxation were investigated. The electron-phonon interaction was described by Herring-Vogt coupling, and the transition rates were obtained from Fermi’s golden rule. The various relaxation rates were calculated analytically using perturbation theory and numerically using exact diagonalization.

**Thesis points**

**Valley relaxation in graphene [1]**

I theoretically studied the time evolution of a non-equilibrium ensemble of valley-polarized electrons due to charged impurities in graphene.

- I determined the valley relaxation rate for the case of noninteracting electrons, as well as for the case when the impurity potential is screened due to electron-electron interaction.

- To describe the inter-valley scattering, I determined the polarizability, the dielectric and the inverse dielectric matrix at the wave vector corresponding to inter-valley scattering.

- I showed that the inter-valley scattering rate is proportional to density of states at the Fermi-energy.

- I pointed out, in the case of inter-valley scattering, that the local-field effects have significant impact on the screening mechanism and valley relaxation time influenced by screening.

- I showed that the valley relaxation time is sensitive to atomic-scale details of the electronic wave functions for both unscreened and screened cases.
Dynamics of valley qubit in silicon quantum dots [2]

I proposed a way of manipulation of the valley qubit by means of an atomic step and electric field in silicon quantum dots.

- I showed that the basis states of the valley qubit are deformed differently by the interface step (valley-to-charge conversion), allowing nondemolition qubit readout.
- I pointed out that an ac gate-induced electric field together with the interface step enables fast electric control of the valley qubit (electrically driven valley resonance).
- I determined the single-qubit gate times enabled by the above mechanism, as well as the cavity-mediated two-qubit gate times.
- I calculated the phonon-induced relaxation time $T_1$ and inhomogeneous dephasing time $T_2^*$ due to charge noise.
- I determined the critical noise level, below which the single- and two-qubit gate times can be shorter than the relaxation and dephasing times.

Relaxation of the flip-flop qubit in the donor-dot system [3]

I investigated the relaxation processes of the flip-flop qubit realized in a donor-dot system based on a phosphorus atom in silicon.

- I determined the charge, flip-flop and electron spin relaxation times as a function of the electric and magnetic fields.
• I pointed out that the relaxation processes around the ionization point are boosted by the significant modifications of the electronic spectrum and wave functions, the nontrivial valley structure of the electron–phonon interaction, and the different valley compositions of the donor and interface electronic states.

• The obtained flip-flop relaxation time ($\sim 100 \, \mu$s) is 8 orders of magnitude shorter than the value for an on-donor electron in bulk silicon.

• I showed that the spin relaxation due to the spin-orbit interaction and $g$-tensor modulation leads to leakage from the flip-flop qubit subspace, although the proper alignment of the magnetic field suppresses these processes.

The publications providing the basis for the thesis points


Further publications

