QuanTech QTsolver Part: Qbit in planar Ge

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This part aim for the creation of a quantum dot in a Ge planar heterostructure. To this end a home-made quantum transport solver (QTSolver) will be used based on the kp approximation. The students will have to modify QTSolver source code to account for anisotropic part of the magnetic Hamiltonian as well as for the strain originating from the cooling of the structure to cryogenic temperature.

1 Before starting

Start by reading QTSolver manual to get acquainted with the simulation inputs/outputs and the implemented simulation approach. Then read the following source [1] to get a theoretical understanding of the kp method (Chapter 1 to 3 suffice).

2 Compile QTSolver on your machine

Download the CLion package from Jetbrains (`https://www.jetbrains.com/shop/eform/students`) using your student account. Copy the folder containing the QTSolver installation to your home directory.
`cp -r /home/bouqueti/Documents/PhD/QTSolver/QTSolver_v17_LK /your_home_directory/`
Remove the CMakeCache file and the CMakeFiles folder and move the QTSolver executable outside of the folder. Launch CLion and open a new project at the location of your QTSolver folder. The Cmake application should allow you to pass the pass of the c and c++ compiler directly when congiguring your project. You can also do it manually from the terminal going to your installation folder and running the two commands:
`cmake ./ -DCMAKE_C_COMPILER=/usr/local/mpich-3.3.2/gcc/bin/mpicc`
`-DCMAKE_CXX_COMPILER=/usr/local/mpich-3.3.2/gcc/bin/mpicxx`
`make QTSolver`
If you encounter any difficulties while compiling do not hesitate to ask questions.

3 Example simulation: Double Dot quantum device

3.1 Simulation

This example is meant for you to get a first taste of the type of simulation we will be working on during this project and to build your python scripts to plot the results. Start by creating a directory on the scratch of your machine where you will store the outputs of your simulation. For example:
`mkdir /scratch/username/double_qd/` Ssh to one of the tortin machines (check first the load average) and move to the directory you have just created.
Copy the double QD command file from the gitlab into the directory. Open the command file with your preferred text editor (emacs or vim for example) and read through the file to get familiar with the different simulation inputs. Set the number of threads to 8 by typing the terminal command `setenv OMP_NUM_THREADS 8`. Run your first simulation by typing
`path-to-executable/QTSolver double_qd_cmd`
The simulation uses an already converged potential and should just need two iterations to converge.

3.2 Plots of the results

Start by downloading all the matlab and python functions from Gitlab into your home directory. Plot the following data:

- Device geometry in 3D
- Charge density
- Electrostatic potential
- Qbit ground state eigenvectors (`SP_Z` whose energy is above Ef = 0 eV)

4 Modification of QTSolver kp Hamiltonian

For this section you will have to introduce a new set of parameters to be read from the command file (ask when you are so far).

4.1 Magnetic field

To understand how the influence of an applied magnetic field is accounted for in the kp formalism read the following source [2] (read until equation (45)) and the Chapter 5.4.2 and 5.4.3 of [3] (read until page 102). We will use the equation (5.70) as model for the implementation in QTSolver. Your task will be to modify the already existing function `add_magnetic_field` in the source code to add the anisotropic contribution (q parameter) to the Hamiltonian.

4.2 Strain

The second modification deals with introducing a strain Hamiltonian to the kp Hamiltonian. Refer to the strain part of [1] to get a formulation of the strain Hamiltonian. The idea is to adapt the function `find_strain, add_Pikus_Bir_6x6 and get_H_PB` of HAMILTONKP.H into the lower basis set 2 and 4.

5 Qbit in planar Ge

5.1 Structure

Create the heterogenous SiGe/Ge/SiGe structure based on the following sources [4, 5, 6, 7]

- Find parameters (kp and electrostatics)
- Decide on device size and discretization steps
- Place the top gate

5.2 Simulation

Once you have a prototype of the structure and you could plot it in matlab you can run the simulation:

- Set `mat_trans` for non-active region
- SP simulation (Temp, bias, number of modes)
- Plot results

5.3 Post-processing

The goal of post-processing is to retrieve device metrics that can be compared with the actual experimental device in order go towards optimization. Your task is to get the following metrics:

- g-factor/g-tensor (python function already written)
- Lamor frequencies
- Rabi frequencies (to do using the method describe in

6 Strain

To start you will have to construct the same structure you have been simulated but this time in COMSOL. To simulate the cooling of the device you can inspire yourself from the 2D layered plate example (`https://www.comsol.com/model/thermal-stresses-in-a-layered-plate-273`).

1. Simulate the cooling. Decide on:
    - Materials parameters
    - Boundary conditions
2. Simulation with homogeneous strain
3. Simulate with discretized strain

References

[1] Igor Ivashev. Theoretical investigations of Zinc Blende and Wurtzite semiconductor quantum wells on the rotated substrates.

[2] J. M. Luttinger. Quantum Theory of Cyclotron Resonance in Semiconductors: General Theory. *Physical Review*, 102(4):1030–1041, May 1956.

[3] Morten Willatzen and Lok C. Lew Yan Voon. *The k p Method: Electronic Properties of Semiconductors*. Springer Berlin Heidelberg, Berlin, Heidelberg, 2009.

[4] Stefano Bosco, Mónica Benito, Christoph Adelsberger, and Daniel Loss. Squeezed hole spin qubits in Ge quantum dots with ultrafast gates at low power. *Physical Review B*, 104(11):115425, September 2021.

[5] Amir Sammak, Diego Sabbagh, Nico W. Hendrickx, Mario Lodari, Brian Paquelet Wuetz, Alberto Tosato, LaReine Yeoh, Monica Bollani, Michele Virgilio, Markus Andreas Schubert, Peter Zaumseil, Giovanni Capellini, Menno Veldhorst, and Giordano Scappucci. Shallow and Undoped Germanium Quantum Wells: A Playground for Spin and Hybrid Quantum Technology. *Advanced Functional Materials*, 29(14):1807613, April 2019.

[6] N. W. Hendrickx, D. P. Franke, A. Sammak, G. Scappucci, and M. Veldhorst. Fast two-qubit logic with holes in germanium. *Nature*, 577(7791):487–491, January 2020.

[7] Michele Virgilio and Giuseppe Grosso. Type-I alignment and direct fundamental gap in SiGe based heterostructures. *Journal of Physics: Condensed Matter*, 18(3):1021–1031, January 2006.