Simulation of a Quantum Annealer Based on Superconducting Flux Qubits

Madita Nocon[1], Dennis Willsch[1], Fengping Jin[1], Hans De Raedt[2], Kristel Michielsen[1,3]
[1] *Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[2] *Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, NL-9747AG Groningen, The Netherlands*
[3] *RWTH Aachen University, D-52056 Aachen, Germany*

Quantum Annealing

A quantum annealer is prepared in the known ground state of the initial Hamiltonian H_{initial} and then adiabatically transformed to the problem Hamiltonian H_{final}

$$H(s) = A(s)H_{\text{initial}} + B(s)H_{\text{final}}.$$

The functions $A(s)$ and $B(s)$, where $s = t/T_{\text{max}}$ and T_{max} is the annealing time, determine the annealing scheme and satisfy

$$A(0) > 0 \quad A(1) \approx 0$$
$$B(0) \approx 0 \quad B(1) > 0.$$

During the annealing process, the system is supposed to stay in its ground state (adiabatic theorem) such that the final state gives the solution (ground state) of the problem Hamiltonian.
For the quantum annealer built by D-Wave Systems Inc., the Hamiltonian is given by the Ising spin Hamiltonian

$$H(s) = -A(s)\sum_k \sigma_k^x - B(s)\Big(\sum_k h_k\sigma_k^z + \sum_{l<k} J_{lk}\sigma_k^z\sigma_l^z\Big), \qquad (1)$$

where h_k, $J_{lk} \in [-1,1]$ have to be chosen according to the problem, and σ_k^x, σ_k^z are Pauli matrices acting on qubit (2-level system) k.

Suzuki-Trotter Product-Formula Algorithm

De Raedt, Comp. Phys. Rep. 7, 1, 1987

To solve the time-dependent Schrödinger equation

$$i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

numerically, we approximate the Hamiltonian to be piecewise constant in time and treat the time as a parameter.
The vector $|\psi(t)\rangle$ is then updated for each time step τ

$$|\psi(t+\tau)\rangle = e^{-iH_{t+\tau/2}\tau}|\psi(t)\rangle.$$

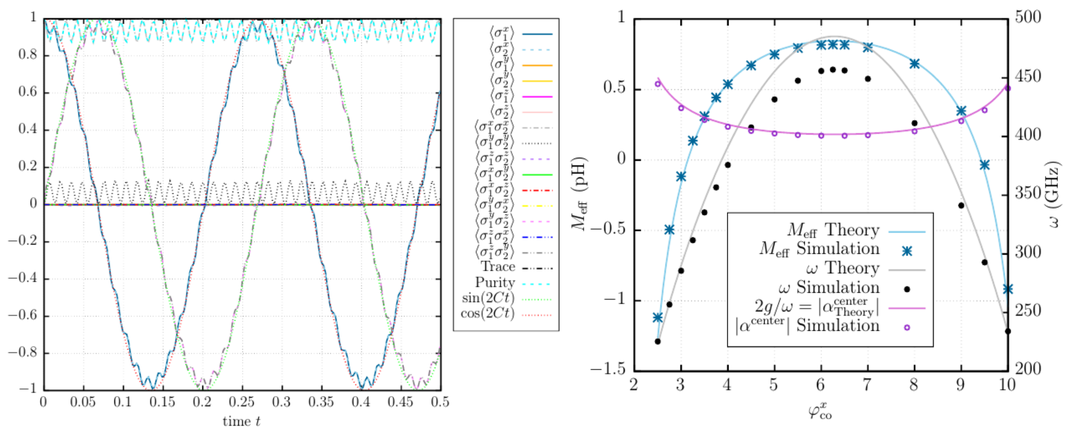
For sufficiently small τ, the time-evolution operator $e^{-iH_t\tau}$ can be approximated by $e^{-iH_t\tau} = e^{-i\sum_k A_{k,t}\tau} \approx \prod_k e^{-iA_{k,t}\tau}$ where the decomposition $H_t = \sum_k A_{k,t}$ is ideally chosen such that the exponentials can be performed in two-component updates of the vector $|\psi(t)\rangle$.

Simulation Results

To investigate whether the effective Hamiltonian describes the evolution of the system of two qubits and one coupler, the initial state is set to $|{+}{+}\rangle$ for the qubits and $|0\rangle$, i.e., the ground state of the harmonic oscillator, for the coupler. The state $|{+}{+}0\rangle$ evolves a time t with the time evolution operator for fixed $s = 1$. In the case that $h_1 = h_2 = 0$, the expectation values of the Pauli matrices in that state at time t are

$$\langle\sigma_1^x\rangle = \langle\sigma_2^x\rangle = \cos(2cBt),\ \langle\sigma_1^y\sigma_2^z\rangle = \langle\sigma_1^z\sigma_2^y\rangle = \sin(2cBt),\ \langle\sigma_1^x\sigma_2^x\rangle = 1,$$

and otherwise zero. The dependence of c on φ_{co}^x can be determined for different values of φ_{co}^x. The figures show an example for $\varphi_{\text{co}}^x = 6$ of the expectation values, and the dependence of $M_{\text{eff}} \propto cB$ on φ_{co}^x.
The oscillations in the purity can be traced back to the coupler being in a coherent state $|\alpha\rangle$ if the qubits are in the state $|{\uparrow}{\uparrow}\rangle$ or in the state $|{\downarrow}{\downarrow}\rangle$.



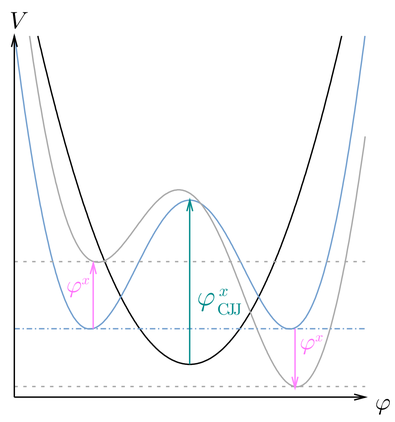
Superconducting Flux Qubits (rf-SQUID)

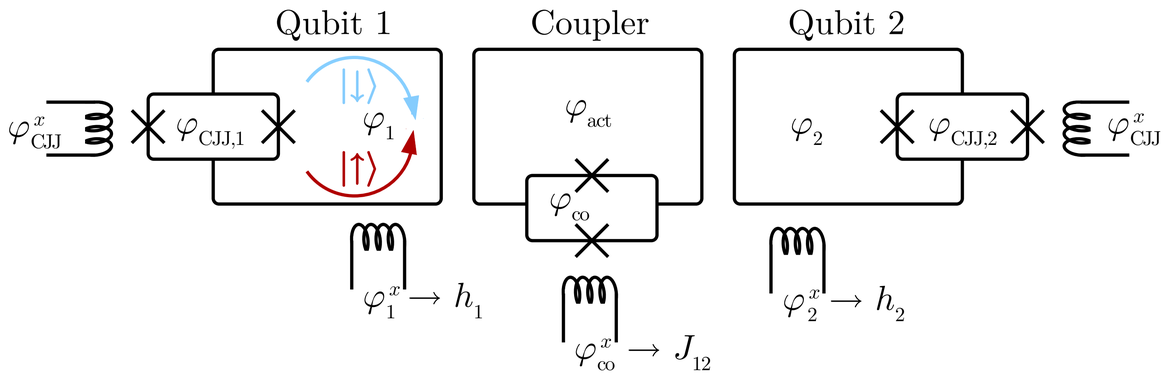
Harris *et al.*, Phys. Rev B 81, 134510, 2010
Johnson *et al.*, Nature 473, 194, 2011
Boixo *et al.*, Nat. Comm. 7, 10327, 2016

The Hamiltonian of a single rf-SQUID is given by

$$H(s) = -E_C\partial_\varphi^2 + E_L(\varphi-\varphi^x(s))^2/2 + E_J\cos(\varphi)\cos(\varphi_{\text{CJJ}}/2)$$
$$-E_{C\text{CJJ}}\partial_{\varphi_{\text{CJJ}}}^2 + E_{L\text{CJJ}}(\varphi_{\text{CJJ}}-\varphi_{\text{CJJ}}^x(s))^2/2, \qquad (2)$$

where the external fluxes $\varphi^x{}_{\text{CJJ}}(s)$ and $\varphi^x(s)$ determine the functions $A(s)$ and $B(s)$ for the annealing procedure. Additionally, $\varphi^x(s)$ depends on the parameter of the problem Hamiltonian for this qubit.
The flux φ_{CJJ} allows for a tunable Josephson-Junction such that the potential for the flux φ, which determines the 2 qubit states, changes from monostable to bistable.





Coupling 2 Qubits via rf-SQUID

Maassen van den Brink *et al.*, New J. Phys. 7, 230, 2005
Harris *et al.*, Phys. Rev B 80, 052506, 2009

In addition to the single rf-SQUID Hamiltonians for each qubit and coupler, the coupling terms have to be considered:

$$H_{\text{int}} = (M/L_{\text{eff}})E_L(\varphi_1-\varphi_1^x)(\varphi_{\text{act}}-\varphi_{\text{act}}^x) + (M/L_{\text{eff}})E_L(\varphi_2-\varphi_2^x)(\varphi_{\text{act}}-\varphi_{\text{act}}^x)$$
$$+ (M^2/L_qL_{\text{eff}})E_L(\varphi_1-\varphi_1^x)(\varphi_2-\varphi_2^x)$$

Effective Hamiltonian

Taking into account only the 2 lowest energy states of the Hamiltonian describing qubit i (Eq. (2)) for $\varphi_i^x = 0$, a 2-level subspace can be defined such that

$$H_i(s) \approx -A(s)\sigma_i^x - B(s)h_i\sigma_i^z.$$

The rf-SQUID describing the coupler can be approximated as a harmonic oscillator $H_{\text{coupler}}(s) \approx \omega a^\dagger a$ such that

$$H_{\text{int}} = -mB(s)\big(h_2\sigma_1^z + h_1\sigma_2^z\big) + jB(s)\sigma_1^z\sigma_2^z + g(s)(\sigma_1^z + \sigma_2^z - \xi(s))(a^\dagger + a),$$

where m and j are constants, and $g(s)$ and $\xi(s)$ contain some constants but also depend on s. For $s \approx 1$, $A(s) \approx 0$ and a Schrieffer-Wolff transformation gives the effective Hamiltonian

$$H_{\text{eff}} = c(\varphi_{\text{co}}^x)B(s)\sigma_1^z\sigma_2^z - B(s)\big((h_1 + mc(\varphi_{\text{co}}^x)(h_2 + h_1/\beta(\varphi_{\text{co}}^x)))\sigma_1^z$$
$$+ (h_2 + mc(\varphi_{\text{co}}^x)(h_1 + h_2/\beta(\varphi_{\text{co}}^x)))\sigma_2^z\big) + \omega a^\dagger a,$$

where $c(\varphi_{\text{co}}^x) =: J$ is the tunable coupling constant, and correction terms in m can be neglected such that we get the Hamiltonian from Eq. (1).

Conclusion and Outlook

- For the investigated case, the simulation results of the effective coupling agree with the theory and the experiment. Thus, the analytical approximations can be justified, and the experimental setup can be sufficiently described by this Hamiltonian.
- The discrepancy in ω does not affect the tunable coupling.
- Further examination is in progress for cases with $h_i \neq 0$ and s < 1, and for the annealing process itself. The focus will be on the effects caused by the fact that the tunable coupling is a consequence of the dynamics of the system only. To this end, comparisons with the simulation of directly coupled qubits is planned.