Simulating realizations of quantum computers by solving the time-dependent Schrödinger Equation

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Formal solution of the time-dependent Schrödinger equation

- in QT, systems for quantum computers obey the time-dependent Schrödinger equation (TDSE)

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

- where the solution is given by

$$|\psi(t+\tau)\rangle = U(t+\tau,t)|\psi(t)\rangle$$

- with the time-evolution operator

$$U(t+\tau,t) = \mathcal{T}\exp\left(-i\int_t^{t+\tau} H(t')\mathrm{d}t'\right)$$

- for small enough τ, Hamiltonian $H(t)$ assumed to be piece-wise constant

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

Solving the TDSE numerically

- “simple” solution: numerically exact diagonalization (e.g. LAPACK)

- Problem: memory and CPU time needed grow with $\mathcal{O}(N^2)$
  → only for “small” systems (validation!)

- Idea: make use of the Lie-Trotter-Suzuki product formula

$$e^{-i\sum_{r=1}^{R} A_r t} = \lim_{m\to\infty}\left(\prod_{r=1}^{R} e^{-iA_r t/m}\right)^m$$

Trotter, *Proc. Am. Math. Soc.* **10**, 545 (1959)
Suzuki et al., *Prog. Theor. Phys.* **58**, 1377 (1977)

- find decomposition $H_t = \sum_{r=1}^{R} A_{r,t}$ and apply first order approximation

$$e^{-iH_t\tau} = e^{-i\sum_{r=1}^{R} A_{r,t}\tau} \approx \prod_{r=1}^{R} e^{-iA_{r,t}\tau} =: U_{t,1}(\tau)$$

Stability and higher order approaches of the Suzuki-Trotter product-formula algorithm

- if $A_{r,t}$ Hermitian → $U_{t,1}(\tau)$ unitary → algorithm unconditionally stable
- error is bounded and controlled by τ: $||U_t(\tau) - U_{t,1}(\tau)|| \leq c_1\tau^2$
- second order such that $U_{t,2}(\tau)$ unitary:

$$U_{t,2}(\tau) = U^{\dagger}_{t,1}(-\tau/2)U_{t,1}(\tau/2) = \prod_{r=R}^{2} e^{A_r\tau/2} \times e^{A_1\tau} \times \prod_{r=2}^{R} e^{A_r\tau/2}$$

- error vanishes with τ^3: $||U_t(\tau) - U_{t,2}(\tau)|| \leq c_2\tau^3$

De Raedt et al., *Phys. Rev. A* **28**, 3575 (1983)
De Raedt, *Comp. Phys. Rep.* **7**, 1 (1987)

How to choose the decomposition

- time-evolution operator is product of matrix exponentials: $U_{t,1}(\tau) = \prod_{r=1}^{R} e^{-iA_{r,t}\tau}$
- ideally: analytical expression
- diagonal matrix: clear
- Example: tridiagonal Hamiltonian

$$\begin{pmatrix} 0 & x & & & & & & \\ x & 0 & x & & & & & \\ & x & 0 & x & & & & \\ & & x & 0 & & & & \\ & & & & \ddots & & & \\ & & & & & 0 & x & \\ & & & & & x & 0 & x \\ & & & & & & x & 0 \end{pmatrix} = \begin{pmatrix} \boxed{\begin{matrix} 0 & x \\ x & 0 \end{matrix}} & 0 & & & & \\ 0 & \boxed{\begin{matrix} 0 & x \\ x & 0 \end{matrix}} & & & & \\ & & \ddots & & & \\ & & & \boxed{\begin{matrix} 0 & x \\ x & 0 \end{matrix}} & 0 \\ & & & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & & & & \\ 0 & \boxed{\begin{matrix} 0 & x \\ x & 0 \end{matrix}} & 0 & & & \\ & 0 & 0 & & & \\ & & & \ddots & & \\ & & & & 0 & 0 \\ & & & & 0 & \boxed{\begin{matrix} 0 & x \\ x & 0 \end{matrix}} \end{pmatrix}$$

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How to choose the decomposition

- blocks are proportional to $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- using Euler's formula
$$e^{ix\mathbf{n}\cdot\boldsymbol{\sigma}} = \cos(x)\mathbb{I} + i\sin(x)\mathbf{n}\cdot\boldsymbol{\sigma}$$
- exponentials of 2×2-block matrices → 2×2-block matrices
- 2-component update rule for state vector:
$$\psi_k = \cos(x)\psi_k + i\sin(x)\psi_{k+i}$$
$$\psi_{k+i} = i\sin(x)\psi_k + \cos(x)\psi_{k+i}$$
- $\mathcal{O}(RN)$
- also possible: $j\times j$ -blocks with $j \ll N$
  (analytically or by diagonalization of smaller blocks, j-component updates)

Applications

Transmon qubits

- Hamiltonian given by $H = H_{\mathrm{CPB}} + H_{\mathrm{res}}$ with

$$H_{\mathrm{CPB}} = \sum_{i=1}^{N} \left[E_{Ci}(\hat{n}_i - n_{gi}(t))^2 - E_{Ji} \cos \hat{\varphi}_i \right],$$

$$H_{\mathrm{res}} = \omega_r \hat{a}^\dagger \hat{a} + \sum_{i=1}^{N} g_i \hat{n}_i (\hat{a} + \hat{a}^\dagger).$$

- state vector $|\psi(t)\rangle = \sum_{k,n_1,n_2} a_{kn_1n_2}(t) |k\rangle |n_1 n_2\rangle$ (Fock and charge basis)

- tridiagonal matrices

- Transmon basis $a_{km_1m_2}(t) = \sum_{n_1,n_2} (B_{n_1m_1})^* (B_{n_2m_2})^* a_{kn_1n_2}(t)$

Willsch et al., *Phys. Rev. A* **96**, 062302 (2017)

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Applications

quantum annealer

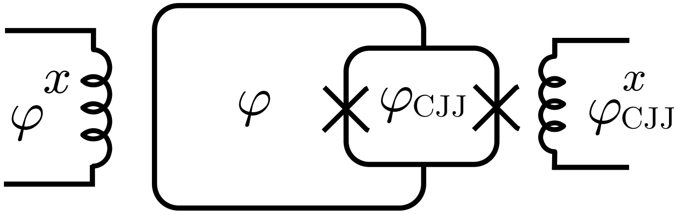
- annealing Hamiltonian

$$H(s) = A(s)H_{\text{init}} + B(s)H_{\text{final}}, \qquad s = t/t_{\text{anneal}}$$

- qubits and coupler elements modeled by SQUIDs

$$H(s) = -E_C\frac{\partial^2}{\partial\varphi^2} + E_L\frac{(\varphi-\varphi^x(s))^2}{2} - E_{C_{\text{CJJ}}}\frac{\partial^2}{\partial\varphi_{\text{CJJ}}^2} + E_{L_{\text{CJJ}}}\frac{(\varphi_{\text{CJJ}}-\varphi_{\text{CJJ}}^x(s))^2}{2} + E_J\cos(\varphi)\cos\left(\frac{\varphi_{\text{CJJ}}}{2}\right)$$

+ interaction terms



- tridiagonal matrices in φ -space

Applications

quantum annealer

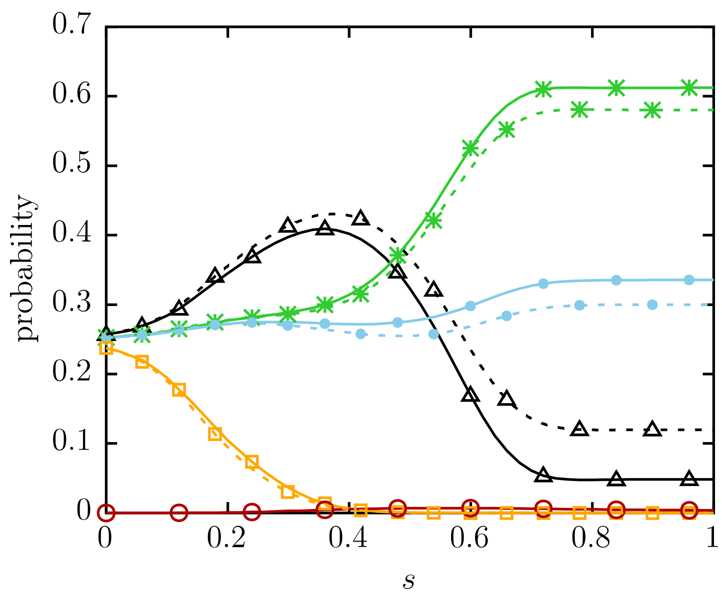


Figure 1: Probabilities of the states $|\uparrow\uparrow\rangle$ (△), $|\uparrow\downarrow\rangle$ (✳), $|\downarrow\uparrow\rangle$ (●), $|\downarrow\downarrow\rangle$ (□), leakage (○) for the simulation of SQUIDs (solid) and 2-level systems (dashed)

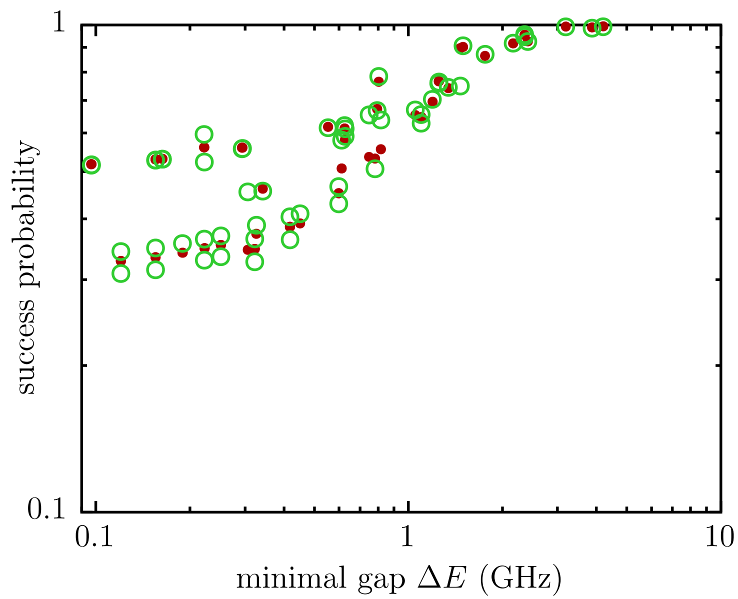


Figure 2: Success probability depending on the minimal gap for SQUIDs (○), 2-level systems (●)

Summary

- Physical hardware can be simulated by solving the TDSE

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

- Suzuki-Trotter product-formula algorithm

  $\rightarrow$ unconditionally stable

  $\rightarrow$ example for decomposition

  $\rightarrow$ other algorithms (not discussed)

- Application: Simulation of Transmon qubits

- Application: Simulation of a quantum annealer (SQUIDs)

Thank you
for your attention!