



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

April 5, 2018 | Madita Nocon | JSC

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

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

- 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

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

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

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

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

- if $A_{r,t}$ Hermitian $\rightarrow U_{t,1}(\tau)$ unitary $\rightarrow$ 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:

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

- 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

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

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 $\rightarrow 2\times 2$ -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 $H = H_{\text{CPB}} + H_{\text{res}}$ with

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

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

- 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)

Applications

quantum annealer

- annealing Hamiltonian

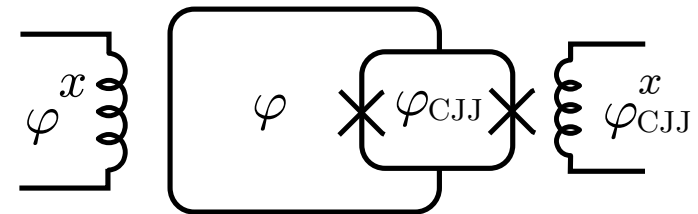
$$H(s) = A(s)H_{\text{init}} + B(s)H_{\text{final}}, \quad s = t/t_{\text{anneal}}$$

- 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

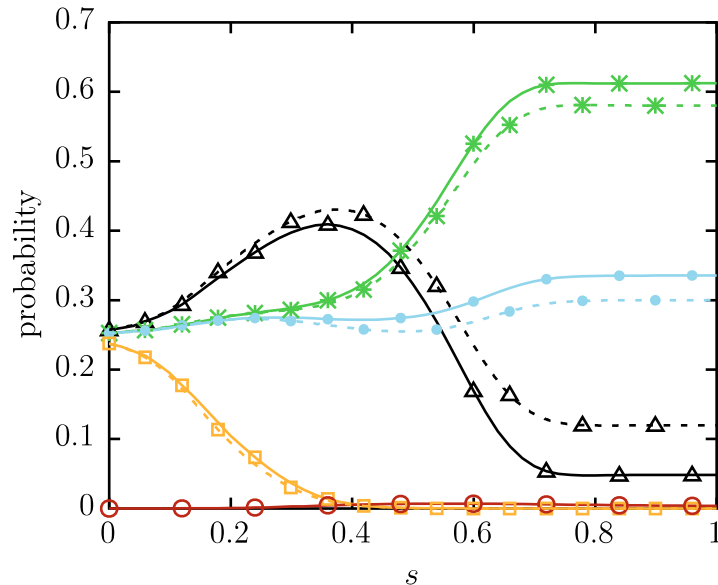


Figure 1: Probabilities of the states $|\uparrow\uparrow\rangle$ (Δ), $|\uparrow\downarrow\rangle$ (*), $|\downarrow\uparrow\rangle$ ($\bullet$), $|\downarrow\downarrow\rangle$ ($\square$), leakage ($\circ$) for the simulation of SQUIDs (solid) and 2-level systems (dashed)

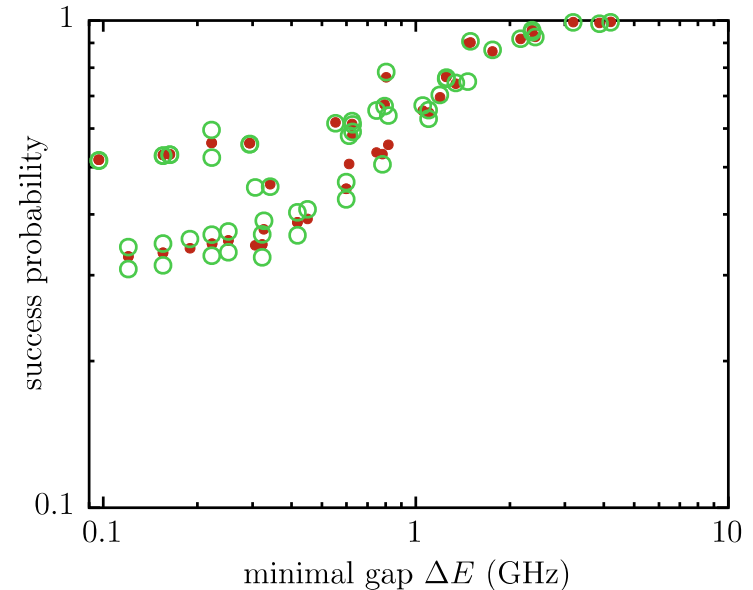


Figure 2: Success probability depending on the minimal gap for SQUIDs ($\circ$), 2-level systems ($\bullet$)

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
 - unconditionally stable
 - example for decomposition
 - other algorithms (not discussed)
- Application: Simulation of Transmon qubits
- Application: Simulation of a quantum annealer (SQUIDs)

**Thank you
for your attention!**