QUANTUM SIMULATION (introduction)

We discuss a few basic ideas to implement the simulation of dynamics and other properties of physical systems using quantum circuits.

While we will mainly illustrate the concepts via spin 1/2 systems (a prominent example being the quantum Transverse Field Ising Model TFIM) they readily apply to other many body or few body systems of interest in solid state physics, quantum chemistry, nuclear physics. Beside various combinatorial optimization problems can be formulated as spin systems and we will see

that the simulation methods discussed here have also found applications in combinatorial optimization (e.g. the minimum vertex cover problem in theoretical computer science).

I. Quantum spin models.

Consider a graph $G = (V, E)$ made of a set of vertices $V = \{1 \dots N\}$ and edges $E \ni \langle i, j \rangle$ $i, j \in V \times V$. We attach to each edge a quantum spin S which is a degree of freedom with Hilbert space $\mathbb{C}^{2S+1}$ spanned by the spin states $|S, m\rangle$ with $m = -S, \dots, +S$. Here we recall $S \in \frac{\mathbb{N}}{2}$ a half integer.

$\vec{S} = (S_x, S_y, S_z)$

The associated spin vector is an (three matrix)

$(2s+1) \times (2s+1)$ matrix satisfying

algebra

$$[S_x, S_y] = 2i S_z$$

$$S_x^2 + S_y^2 + S_z^2 = s(s+1)\,Id.$$

For spin $1/2$ this is realized through the Pauli matrices $S_i = \frac{1}{2}\sigma_i \qquad i = x, y, z$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For spin 1 we have

$S_x =$ $\qquad$ $S_y =$ $\qquad$ $S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

The Hilbert space for N spins on the graph $G = (V, E)$ is $\mathcal{H} = \left(\mathbb{C}^{2S+1}\right)^{\otimes N}$.

The Hamiltonian takes the form in general

$$H = \sum_{\langle i,j \rangle \in E} J_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta + \sum_{i \in V} h_i^\alpha S_i^\alpha$$

where here α, β run over x, y, z components.

Note that the notation here means:

$$S_i^\alpha = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes S_i^\alpha \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}.$$

$$S_i^\alpha S_j^\beta = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes S_i^\alpha \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes S_j^\beta \otimes \mathbb{1} \cdots \otimes \mathbb{1}$$

There are $(2S+1)^N \times (2S+1)^N$ matrices which act on the total Hilbert space:

$$\mathcal{H} = \underbrace{\mathbb{C}^{2S+1} \otimes \mathbb{C}^{2S+1} \otimes \cdots \otimes \mathbb{C}^{2S+1}}_{N \text{ times}}.$$

Of course this can be generalized to hypergraphs & multispin (beyond pairs) interactions.

For all the discussions that follow we will limit ourselves to spin 1/2 systems and our main illustrative example will be the TFIM (Quantum transverse field Ising model).

$$H = \sum_{\langle i,j \rangle \in E} J_{ij}\, \sigma_i^z\, \sigma_j^z \;-\; \Gamma \sum_{i \in V} \sigma_i^x .$$

directly written in terms of the Pauli matrices $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Again note the simplified notation: all terms are in fact tensor products as remarked above and are $2^N \times 2^N$ matrices.

The first term is diagonal in the computational basis $|s_1 \dots s_N\rangle$, $s_i = \pm 1$. :

$$\sigma_i^z \sigma_j^z \,|s_1 \dots s_N\rangle = s_i s_j \,|s_1 \dots s_N\rangle$$

while the second term introduces non diagonal elements

$$\sigma_i^x \, |s_1 \cdots s_N\rangle = |s_1 \cdots -s_i \cdots s_N\rangle$$

↑

a spin flip operator.

In particular:

$$\langle s_1' \cdots s_N' | H | s_1 \cdots s_N \rangle$$

$$= \sum_{(i'j') \in E} J_{i'j'} \, s_{i'} s_{j'} \, \delta_{s_1' s_1} \delta_{s_2' s_2} \cdots \delta_{s_N' s_N}$$

$$+ \Gamma \sum_{i' \in V} \delta_{s_1' s_1} \cdots \delta_{s_{i'-1}' s_{i'-1}} \, \delta_{s_{i'}' -s_{i'}} \, \delta_{s_{i'+1}' s_{i'+1}} \cdots \delta_{s_N' s_N}$$

Note that instead of $2^N \times 2^N = 2^{2N}$ elements this matrix has "only" $(N+1)\,2^N$ elements. This can be exploited beneficially in numerical computations

Remarks:

- For the spin 1/2 hamiltonians we directly have a system of qubits with Hilbert space

$$\underbrace{\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2}_{N \text{ times}} \quad \text{of dim} = 2^N.$$

The computational basis $|b_1 \cdots b_N\rangle$, $b_i = 0,1$ is equivalent to $|s_1 \cdots s_N\rangle$, $s_i = \pm 1$ through the mapping $b_i = 0 \leftrightarrow s_i = +1$, $b_i = 1 \leftrightarrow s_i = -1$

so $s_i = (-1)^{b_i} = 1 - 2b_i$. or $b_i = \frac{1 - s_i}{2}$.

- Higher spin systems correspond to qudits. To work in terms of qubits one has to set up a suitable correspondence and the choice may depend on the problem at hand.
- Fermionic systems (electrons) → see next class for Fermion ↔ qubit correspondences.

II. Quantum dynamics.

We focus on the problem of solving the time dependent Schroedinger equation for spin systems. We analyze here only the case of time-independent hamiltonians.

II.1 Naive Taylor expansion method.

For a static Hamiltonian the time evolved state which solves the Schroedinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

is $$|\psi(t)\rangle = e^{-i\frac{Ht}{\hbar}} |\psi(0)\rangle$$

Let Δ be a small time step and consider the Taylor expansion of the exponential (set $\hbar = 1$)

$$|\psi(t+\Delta)\rangle = \left(1 - i\Delta H - \frac{\Delta^2}{2} H^2 - i\frac{\Delta^3}{6} H^3 + \dots\right) |\psi(t)\rangle$$

Taking the first S orders in Taylor's expansion garantees a scheme of order $O(\Delta^S)$ which can be efficiently implemented for sparse Hamiltonians (because products of H are efficiently computable). A simple iterative formulation is:

$$\begin{cases} |\Gamma_k\rangle = -\frac{i\Delta}{k} H |\Gamma_{k-1}\rangle \\ |\Delta_k\rangle = |\Delta_{k-1}\rangle + |\Gamma_k\rangle \end{cases}$$

for $k = 1, 2, \dots, S$ with initial condition $|\Gamma_0\rangle = |\Delta_0\rangle = |\psi(t)\rangle$. Then

$$|\psi(t+\Delta)\rangle = |\Delta_S\rangle$$

This scheme is memory friendly as we only have to store $|\Delta_k\rangle$ & $|\Gamma_k\rangle$ at each step.

Exercise : check the iterative scheme above reproduces the Taylor expansion of the evolution operator up to order $O(\Delta^5)$.

Remark : a default of this scheme is that unitarity is not preserved due to the truncation of the exponential. Thus $|\psi(t+1)\rangle$ may not be normalized to exactly one.

II. 2 Trotter-Suzuki decomposition.

We present an alternative scheme at the basis of many developments which preserves the unitarity of time-evolution.

First let us discuss the general idea before illustrating particular applications.

Let $H = \sum_{k=1}^{K} h_k$ with <u>non-commuting terms</u>

The Trotter-Suzuki decomposition begins with

$$\exp(-iH\Delta) = e^{-ih_1\Delta} e^{-ih_2\Delta} \cdots e^{-ih_K\Delta} + O(\Delta^2)$$

for a small time step Δ. Then we use:

$$e^{-iHt} = \left(e^{-iH\Delta}\right)^M$$

where we take M large and $\Delta = \frac{t}{M}$ small given t. Thus we get the approximation:

$$e^{-iHt} \approx \left(e^{-ih_1\Delta} e^{-ih_2\Delta} \cdots e^{-ih_K\Delta}\right)^M$$

with $\Delta = \frac{t}{M}$.

The error term here is $M\, O(\Delta^2) = O\left(\frac{t^2}{M}\right)$

$= O(t\Delta)$.

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Improved second order scheme of Trotter-Suzuki:

We have

$$e^{-iH\Delta} = \left(e^{-ih_1\frac{\Delta}{2}} \cdots e^{-ih_K\frac{\Delta}{2}}\right)\left(e^{-ih_K\frac{\Delta}{2}} \cdots e^{-ih_1\frac{\Delta}{2}}\right) + O(\Delta^3)$$

Note here the error term is smaller. Then again we get with $\Delta = \frac{t}{M}$, M large:

$$\boxed{e^{-itH} \simeq \left(\left(e^{-ih_1\frac{\Delta}{2}} \cdots e^{-ih_K\frac{\Delta}{2}}\right)\left(e^{-ih_K\frac{\Delta}{2}} \cdots e^{-ih_1\frac{\Delta}{2}}\right)\right)^M}$$

The error term now is $M\, O(\Delta^3) = O\left(\frac{t^3}{M^2}\right)$

$= O(t\Delta^2)$.

The special case $k = 2$ where the Hamiltonian is split in two terms is particularly important.

$$H = h_1 + h_2 \quad .$$

First order scheme :

$$e^{-itH} = \left(e^{-ih_1 \Delta} \, e^{-ih_2 \Delta} \right)^M$$

with $\Delta = \frac{t}{M}$ and $O(t\Delta)$.

Second order scheme :

$$e^{-itH} = \left(e^{-ih_1 \frac{\Delta}{2}} \, e^{-ih_2 \Delta} \, e^{-ih_1 \frac{\Delta}{2}} \right)^M$$

with $\Delta = \frac{t}{M}$ and $O(t\Delta^2)$

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II.3 Transverse Field Ising Model.

For the TFIM we take two terms $K=2$ with

$$h_1 = \sum_{\langle ij\rangle \in E} J_{ij}\, \sigma_i^z \sigma_j^z$$

$$h_2 = -\Gamma \sum_{i\in V} \sigma_i^x .$$

These do not commute $[h_1, h_2] = h_1 h_2 - h_2 h_1 \neq 0$.

However terms <u>within</u> h_1 and <u>within</u> h_2 commute and can be easily exponentiated.

$$e^{-i\Delta h_1} = \prod_{\langle ij\rangle \in E} e^{-i\Delta J_{ij}\sigma_i^z\sigma_j^z}$$

$$= \prod_{\langle ij\rangle\in E} \left\{ (\cos \Delta J_{ij})\, \mathbb{1}_{4\times 4} - i(\sin \Delta J_{ij})\, \sigma_i^z \otimes \sigma_j^z \right\}.$$

or also:

$$e^{-i\Delta h_1} |s_1 \cdots s_N\rangle = \prod_{\langle ij\rangle\in E} e^{-i\Delta J_{ij} s_i s_j} |s_1 \cdots s_N\rangle$$

For the spin-flip terms:

$$e^{-i\Delta h_2} = \prod_{i\in V} e^{+i\Delta\Gamma\sigma_i^x}$$

and using $(\sigma_i^x)^2 = \mathbb{1}$ & the Taylor expansion we prove (exercise):

$$e^{i\Delta\Gamma\sigma_i^x} = \cos(\Delta\Gamma)\,\mathbb{1} + i(\sin\Delta\Gamma)\,\sigma_i^x$$

Thus

$$e^{-i\Delta h_2}|s_1\cdots s_N\rangle = \bigotimes_{i\in V}\Big\{(\cos\Delta\Gamma + i\sigma_i^x\sin\Delta\Gamma)\,|s_i\rangle\Big\}$$

$$= \bigotimes_{i\in V}\Big\{(\cos\Delta\Gamma)\,|s_i\rangle + i(\sin\Delta\Gamma)\,|-s_i\rangle\Big\}$$

$$= \sum_{I\subset V} (\cos\Delta\Gamma)^{|V\setminus I|}\,(i\sin\Delta\Gamma)^{|I|}\,|s_{V\setminus I}, -s_I\rangle$$

$$= \sum_{f=0}^{N} (\cos \Delta\Gamma)^{N-f} (i \sin \Delta\Gamma)^{f} \sum_{I : |I|=f} | s_{V \setminus I}, -s_I \rangle$$

where here f = number of spin-flips.

$$\simeq_{\uparrow} i \Delta\Gamma \sum_{i=1}^{N} | s_1 \cdots -s_i \cdots s_N \rangle$$

to order $O(\Delta^2)$.

With these formulas one can easily compute

$$\exp(-i t H) \simeq \left((\exp -i \Delta h_1)(\exp -i \Delta h_2) \right)^M$$

with $\Delta = \frac{t}{M}$ either we use matrix multiplications or apply the time evolution to an initial state expanded in the computational basis.

III. Quantum circuit implementation.

The preceding discussion is at the basis of path integral formulations of quantum dynamics. Here however our goal is to go in another direction : the quantum circuit implementation.

We proceed still within the example of the TFIM. In principle exponential speedup can be obtained as we do not have to deal with the proliferation of terms (as seen in the previous formulas due to the spin flips).

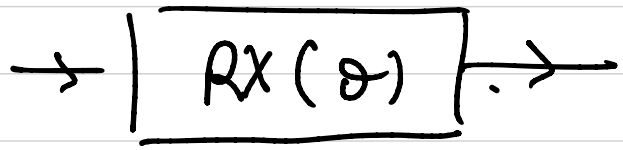
$$H = \underbrace{-\Gamma \sum_{i \in V} \sigma_i^x}_{h_1} + \underbrace{\sum_{\langle ij \rangle \in E} J_{ij} \sigma_i^z \sigma_j^z}_{h_2}$$

The time evolution of the spin flip terms

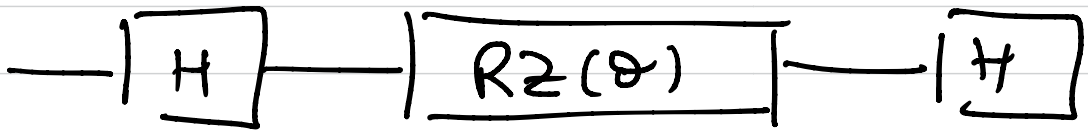
$$e^{i\Delta\Gamma\,\sigma_i^x}$$

$e^{-\frac{i}{2}\theta\sigma^x}$;

is easy to implement from a rotation gate around the x-axis with angle $-2\Delta\Gamma = \theta$:



with $\theta = -2\Delta\Gamma$. If only an $RZ(\theta)$ rotation around Z is available one can implement a basis change thanks to the Hadamard matrix



indeed $H\sigma^x H = \sigma^z$ and thus :

$$\underbrace{RX(\theta)}_{e^{-\frac{i}{2}\theta\sigma_x}} = H^2 RX(\theta) H^2 = H \underbrace{HRX(\theta)H}_{RZ(\theta)=e^{-\frac{i}{2}\theta\sigma_z}} H$$

The I_{ij} diagonal term is implemented via a 2-qubit gate as it involves two qubits.

Note that:

$$e^{-i\Delta J_{ij}\sigma_i^z\sigma_j^z} = \text{CNOT}\left(\mathbb{1}\otimes e^{i\Delta J_{ij}\sigma_j^z}\right)\text{CNOT}$$

Indeed applying on a computational basis state $|s_i, s_j\rangle$ the left hand side gives:

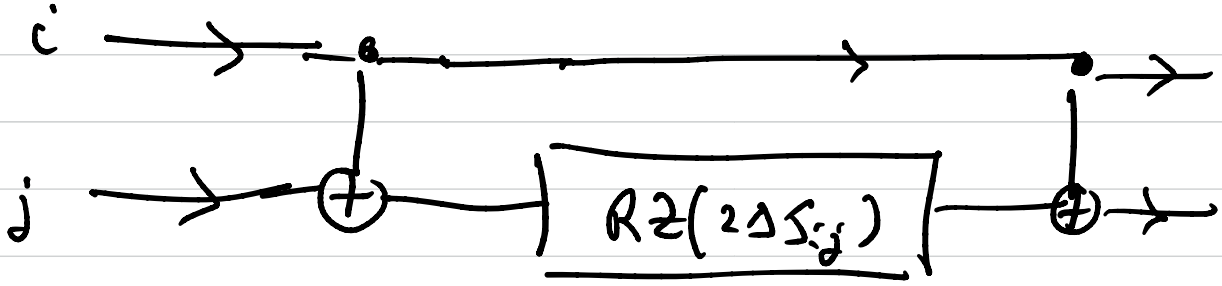
$$e^{-i\Delta J_{ij} s_i s_j}|s_i s_j\rangle$$

and the right hand side gives:

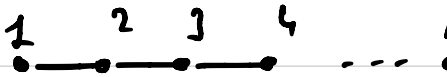
$$\underbrace{\text{CNOT}\left(\mathbb{1}\otimes e^{-i\Delta J_{ij}\sigma_j^z}\right)\underbrace{\text{CNOT}\,|s_i\, s_j\rangle}_{|s_i,\, s_j s_i\rangle}}_{e^{-i\Delta J_{ij} s_j s_i}|s_i,\, s_j s_i\rangle}$$

$$e^{-i\Delta J_{ij} s_j s_i}|s_i, s_j \underbrace{s_i s_i}_{\mathbb{1}}\rangle \quad \checkmark .$$

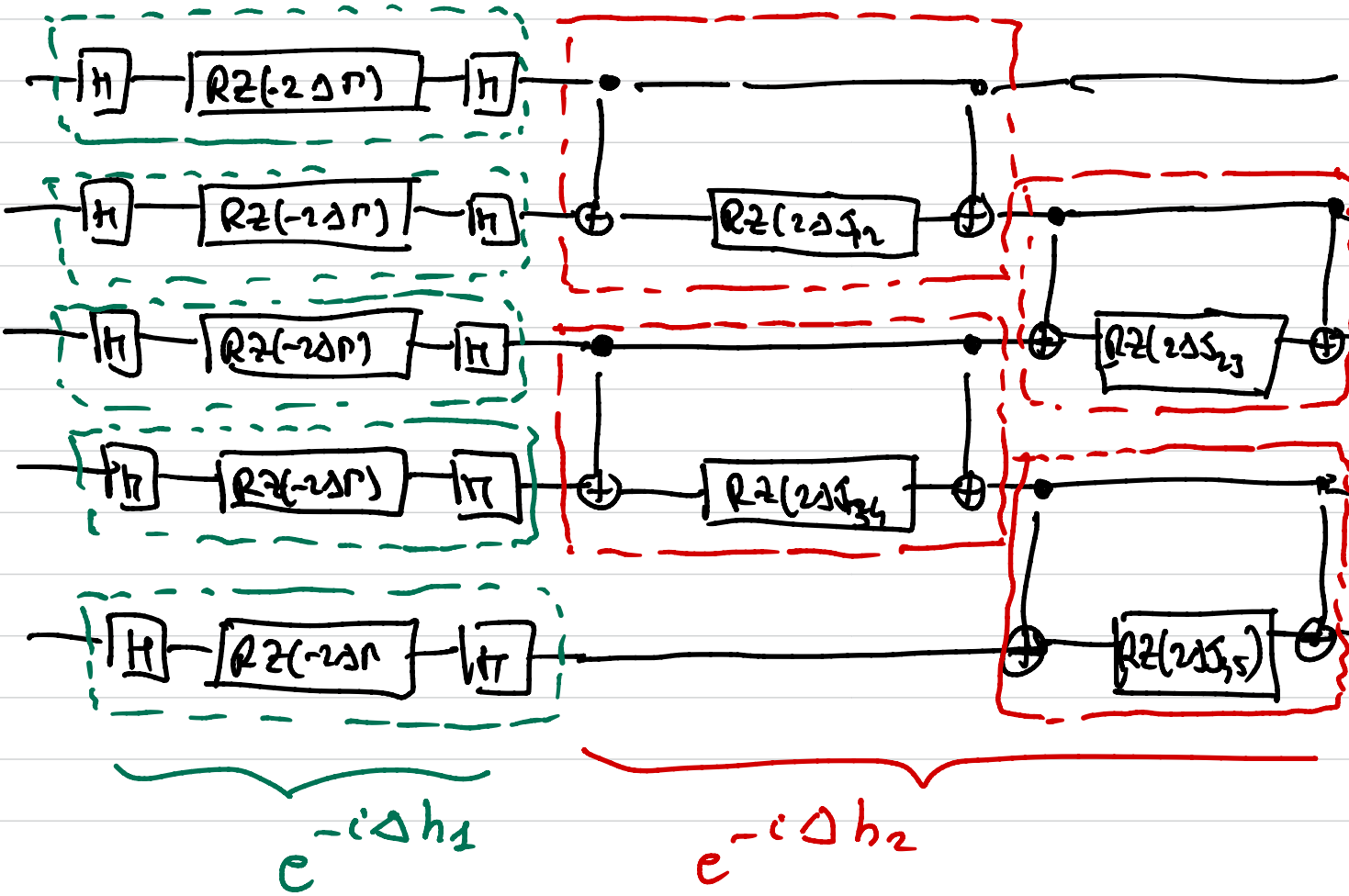
The circuit corresponding to this identity is



As an example consider now a spin chain. The graph

is $G = (V, E) =$ 

A possible circuit with $M = 1$ Trotter step would be:



Note that the two qubit gates enclosed in red commute since they implement $e^{-i\Delta J_{ij} \sigma_i^z \sigma_j^z}$ terms. So there is no ambiguity in this circuit design for $e^{-i\Delta h_2} e^{-i\Delta h_1} \simeq e^{-i\Delta H}$ up to order $O(\Delta^2)$.

For M trotter steps we simply have to append the same circuit M times. We see that the depth of this circuit will be essentially proportional to M. The width is equal to N.

Exercise: design a circuit corresponding to the second order Trotter-Suzuki approximation:

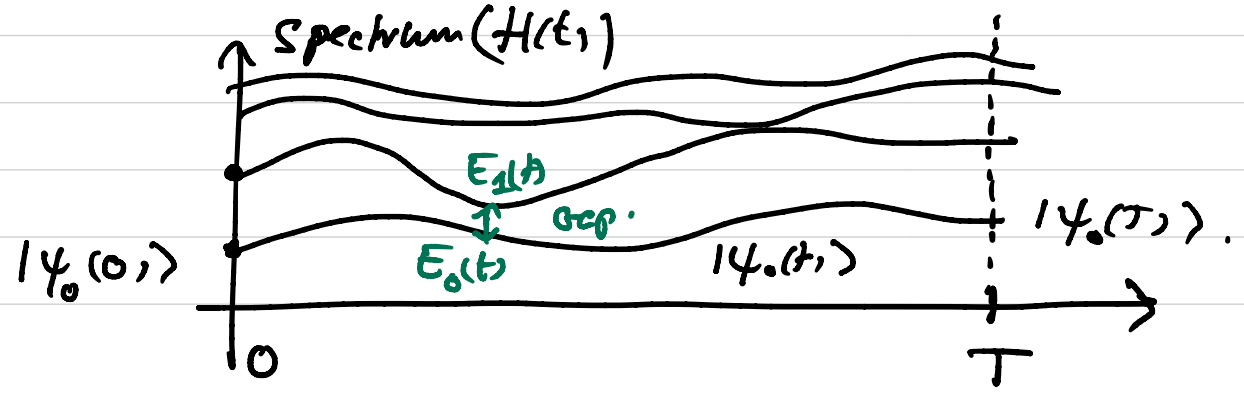
$$e^{-i\Delta H} \simeq e^{-i\frac{\Delta}{2}h_1} e^{-i\Delta h_2} e^{-i\frac{\Delta}{2}h_1} + O(\Delta^3)$$

$$e^{-itH} = \left(e^{-i\Delta H}\right)^M \quad ; \quad \Delta = \frac{t}{M}.$$

IV. Quantum adiabatic method

The adiabatic theorem of quantum mechanics can be used as an inspiration to develop new algorithms or simulation methods. We discuss here the main ideas of this approach.

Informally, the adiabatic theorem states that if we have a Hamiltonian family $\hat{H}(t)$ parametrized by time (say with a time dependent parameter, see later) and we vary time slowly enough the system will remain in the ground state $|\psi_0(t)\rangle$ all along the time evolution as long as the GS is separated from the rest of the spectrum by a gap



More formally if $U(t,0)$ is the true evolution for $H(t)$:

We should have:

$$U(t,0)\,|\psi_0(0)\rangle \simeq |\psi_0(t)\rangle$$

as long as $T \gg O\left(\frac{1}{\min_{t\in[0,T]} |E_1(t)-E_0(t)|}\right)$.

minimal gap in spectral family.

A typical example of application is a Hamiltonian family of the form:

$$H(t) = \left(1-\frac{t}{T}\right) H_0 + \frac{t}{T} H_1$$

where $H(0) = H_0$ is an "easy hamiltonian" with known eigenstates/GS and $H(T) = H_1$ is a "hard hamiltonian" with hard to find or prepare eigenstates/GS. By applying the adiabatic theorem we can find the GS of H_1.

However in practice for many body systems we expect $T \sim e^N$ as a result of exponentially closing of the minimum gap along the path $H(t)$.

V. Quantum alternating method

The above adiabatic state preparation method can be used as an inspiration for quantum algorithms. Suppose we want to find the GS of the TFIM. We use the following Hamiltonian family:

$$\hat{H}(t) = \left(1 - \frac{t}{T}\right) h_1 + \frac{t}{T}\left(h_1 + h_2\right)$$

where again $\begin{cases} h_1 = -\Gamma \sum_i \sigma_i^x \\ h_2 = \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z \end{cases}$.

Note that here $\vec{H}(t) = h_1 + \frac{t}{T} h_2$.

$\vec{H}(0) = h_1$, $\vec{H}(T) = h_1 + h_2$.

We have $|\psi_0(0)\rangle = \bigotimes_i \frac{|0\rangle + |1\rangle}{\sqrt{2}}$

(if $\Gamma > 0$ say) with $E_0(0) = -N\Gamma$.

The first excited state has $E_1(0) = -N\Gamma + 2\Gamma$
$= -(N-1)\Gamma + \Gamma$.

ect... corresponding to one place flip:

$$\left(\bigotimes_{\text{rest}} \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} .$$

Inspired by the adiabatic theorem we imagine that we implement the time evolution slowly by making small steps Δ from $t=0$ to $t=T$. We use on this a "Trotter splitting" with two terms h_1 and $\frac{t}{T} h_2$:

We thus consider the following heuristic approximation for the time evolution operator:

$$\left(e^{-i\Delta h_1}\, e^{-i\Delta \frac{t}{T} h_2}\right) \cdots \left(e^{-i\Delta h_1}\, e^{-i\Delta \frac{t}{T} h_2}\right)$$

Note: here $\vec{H}(t) = h_1 + \frac{t}{T} h_2$ is time dependent so the time evolution operator is not given by the exponential of $\vec{H}(t)$.

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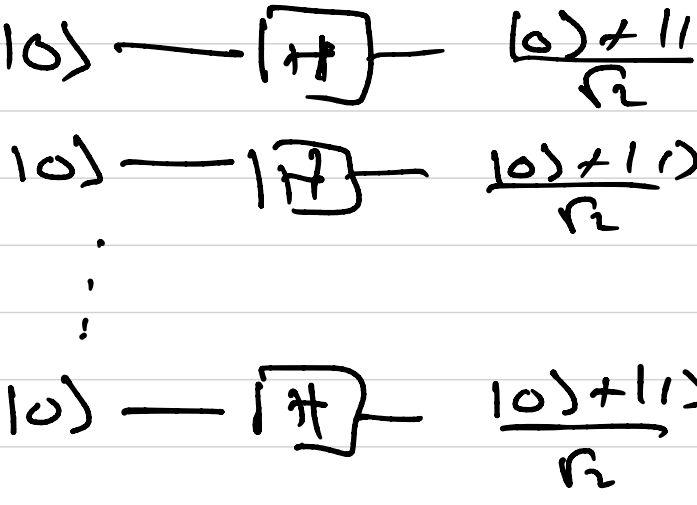
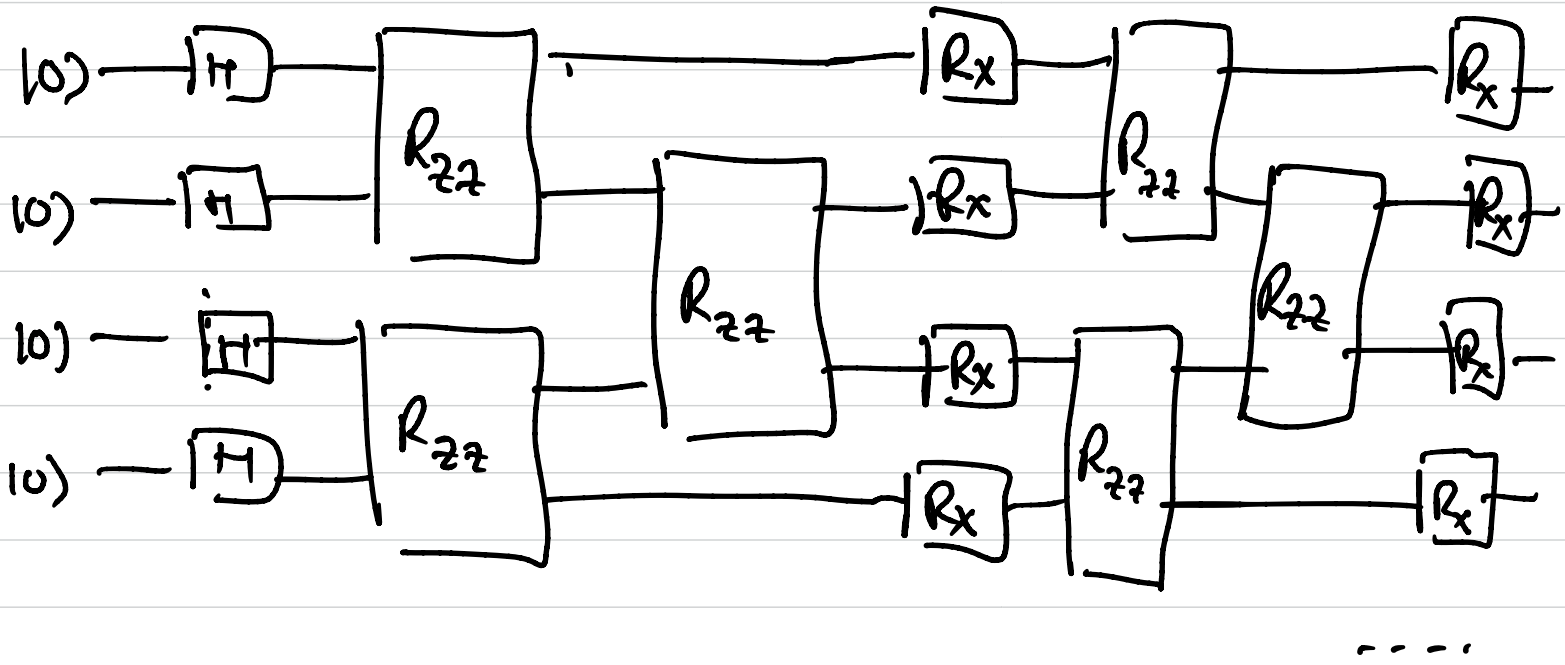
We start with the GS of $H(0) = h_1$. This is prepared from the circuit



The circuit of the algorithm is thus :



with initial state preparation and then two Trotter-Suzuki steps with gate RZZ and RX discussed in the previous paragraphs.

Remarks:

- The time parametrization can be changed which would correspond to make Δ time dependent along the "Trotter steps".
- One could also turn the "Δ's" into parameters that one has to be optimized. This leads to the QAOA algo for optimization (NEXT CLASS)

VI. Fermion systems.

Fermionic systems are ubiquitous physical systems in solid state, chemistry, nuclear physics, whose dynamics we also want to simulate.

These systems have Hamiltonians expressed in terms of creation & annihilation operators satisfying anticommutation relations:

$$\{c_i^\dagger, c_j\} = c_i^\dagger c_j + c_j c_i^\dagger = \delta_{ij}$$

$$\{c_i, c_j\} = c_i c_j + c_j c_i = 0$$

$$\{c_i^\dagger, c_j^\dagger\} = c_i^\dagger c_j^\dagger + c_j^\dagger c_i^\dagger = 0$$

For example typical Hamiltonians have the form

$$H = \sum_{i,j} t_{ij} c_i^\dagger c_j + \sum_{k,l,m,n} V_{klmn} c_k^\dagger c_l^\dagger c_m c_n$$

(with $t_{ij} = t_{ji}^*$ & $V_{klmn} = V_{mnlk}^*$ to ensure hermiticity)

There exist mappings for fermions to Spins 1/2 which for us serve to map a fermion system on a qubit system. Using these mappings we reformulate the Hamiltonian as a spin system. However this spin system is not necessarily a sum of simple "local monomials" in which case the methods exposed before are hard to use. But when the reformulated spin Hamiltonian is a sum of local simple monomials we can use the simulation methods outlined in previous paragraphs. This works typically for one dimensional lattices or for "small" molecules modelled as fermion systems on small graphs.

Here we discuss the most common of these mappings namely the Jordan-Wigner transformation. Another popular mapping is the Kitaev transformation.

Jordan-Wigner transformation:

We order the vertices $\ell \in \{1, 2, \dots, N\}$ of the graph. The transformation is then:

$$\begin{cases} c_\ell = \sigma_1^z \otimes \sigma_2^z \otimes \cdots \otimes \sigma_{\ell-1}^z \otimes \underbrace{\sigma_\ell^-}_{\frac{1}{2}(\sigma_\ell^x - i\sigma_\ell^y)} \\ c_\ell^\dagger = \sigma_1^z \otimes \sigma_2^z \otimes \cdots \otimes \sigma_{\ell-1}^z \otimes \underbrace{\sigma_\ell^+}_{\frac{1}{2}(\sigma_\ell^x + i\sigma_\ell^y)}. \end{cases}$$

To check that the "strings" on the r.h.s satisfy fermionic anticommutation algebra one proceeds as follows for $l \geq m$:

$$\{c_l^+, c_m\} = \left\{ \prod_{j=1}^{l-1} \sigma_j^z \, \sigma_l^+ \, , \prod_{j=1}^{m-1} \sigma_j^z \, \sigma_m^- \right\}$$

$$= \prod_{j=1}^{l-1} \sigma_j^z \prod_{j=1}^{m-1} \sigma_j^z \, \sigma_l^+ \sigma_m^- + \prod_{j=1}^{m-1} \sigma_j^z \prod_{j=1}^{m-1} \sigma_j^z \cdot \sigma_m^- \prod_{j=m}^{l-1} \sigma_j^z \, \sigma_l^+$$

$$= \begin{cases} \sigma_l^+ \sigma_l + \sigma_l \sigma_l^+ = 1 & \text{for } l = m \\ \left(\prod_{j=m}^{l-1} \sigma_j^z \right) \underbrace{(\sigma_l^+ \sigma_m^- - \sigma_m^- \sigma_l^+)}_{0} . & \text{for } l > m \end{cases}$$

For $\{c_l^+, c_m^+\} = \{c_l, c_m\} = 0$.

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