Russian-Chinese International School
"Superconducting functional materials for advanced quantum technologies"

Quantum simulation of spin systems using digital quantum computers
(educational lecture)

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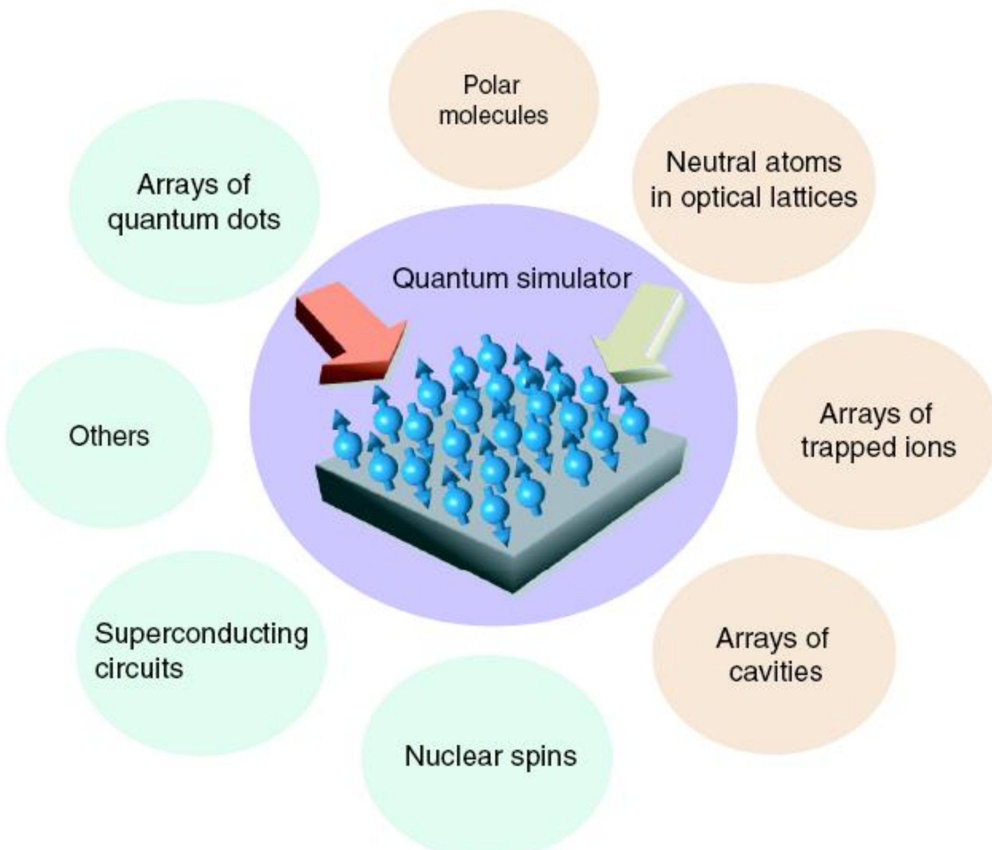
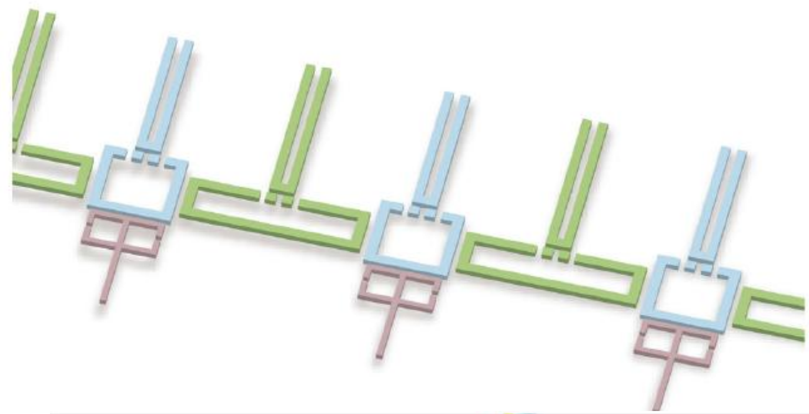
Outline

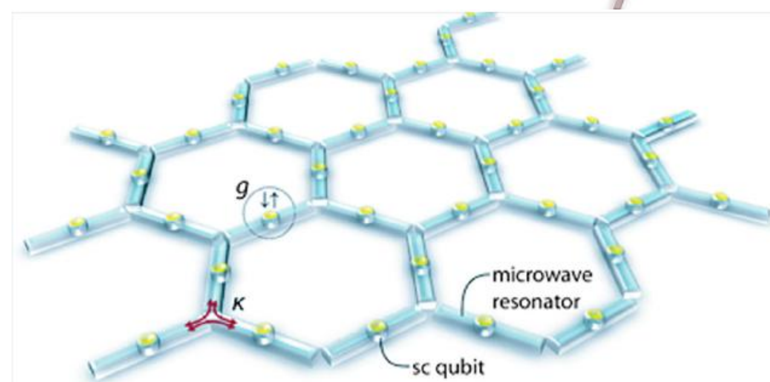
1. Introduction
2. Quantum logic gates
3. Illustration: simulation of the central spin model
4. Phase estimation algorithm

1. Introduction

21st century: dramatic progress in the construction of quantum computers and simulators based on different physical realizations (superconducting Josephson circuits, trapped ions, neutral atoms, quantum dots, etc.)



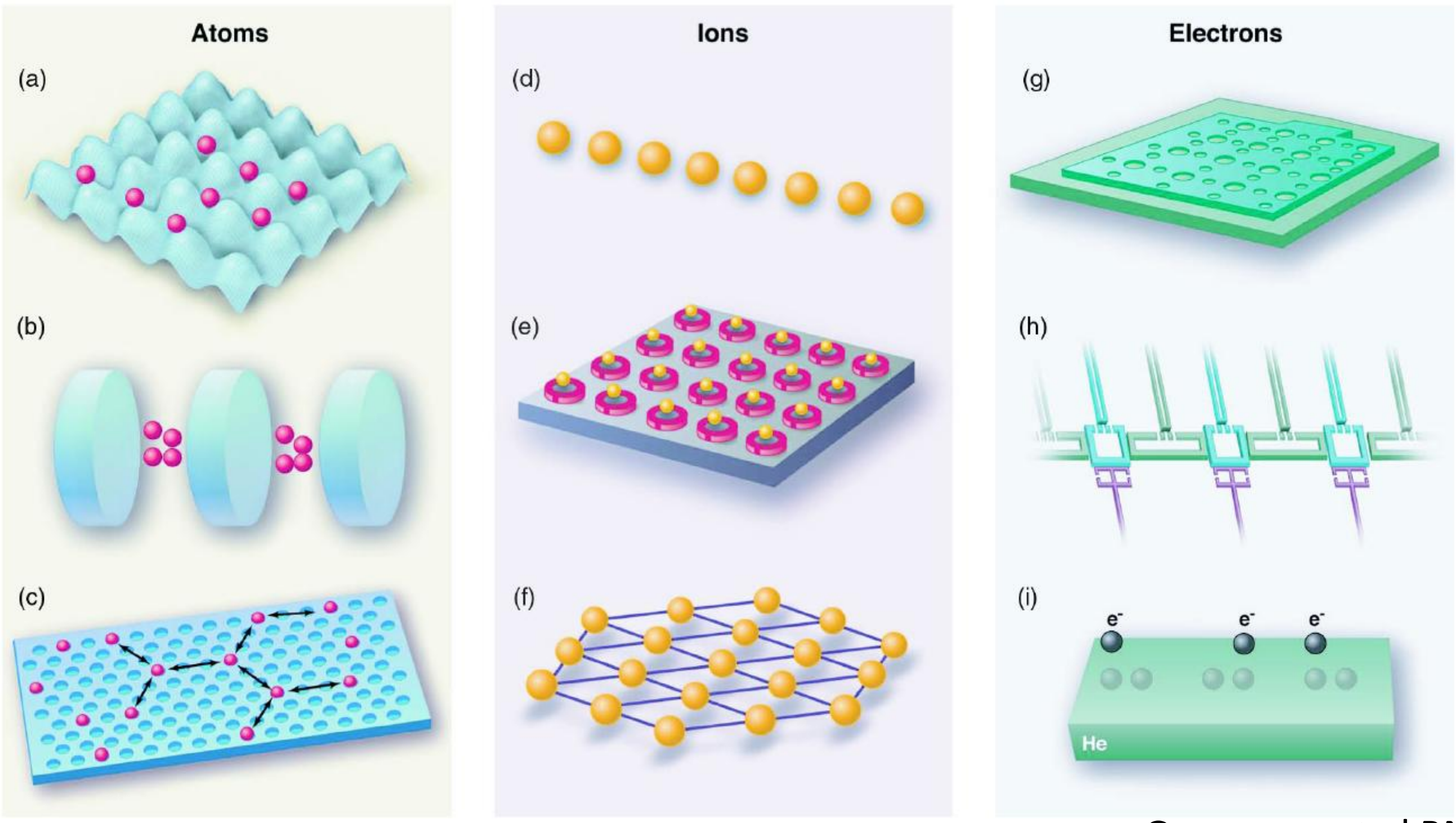




Georgescu et al, RMP (2014)

Quantum simulation: artificial quantum systems are believed to be extremely useful in simulation of quantum many-body systems - novel materials, molecules, drugs. Arguments: first-principle simulation of quantum systems is difficult due to the exponential “explosion” of the Hilbert space size (2^N states for N-spin system).

(Yu. Manin 1980, R. Feynman 1982)

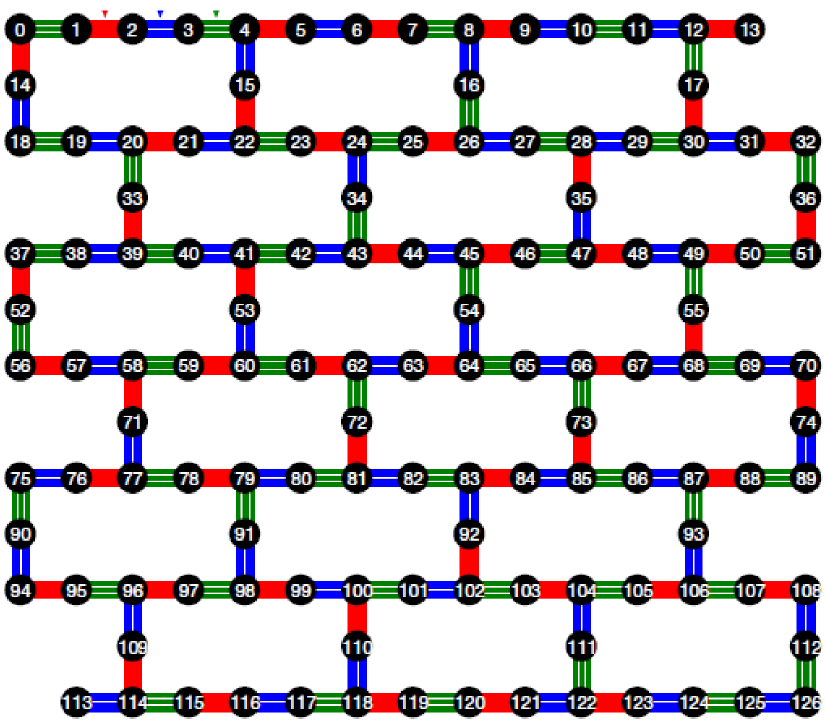


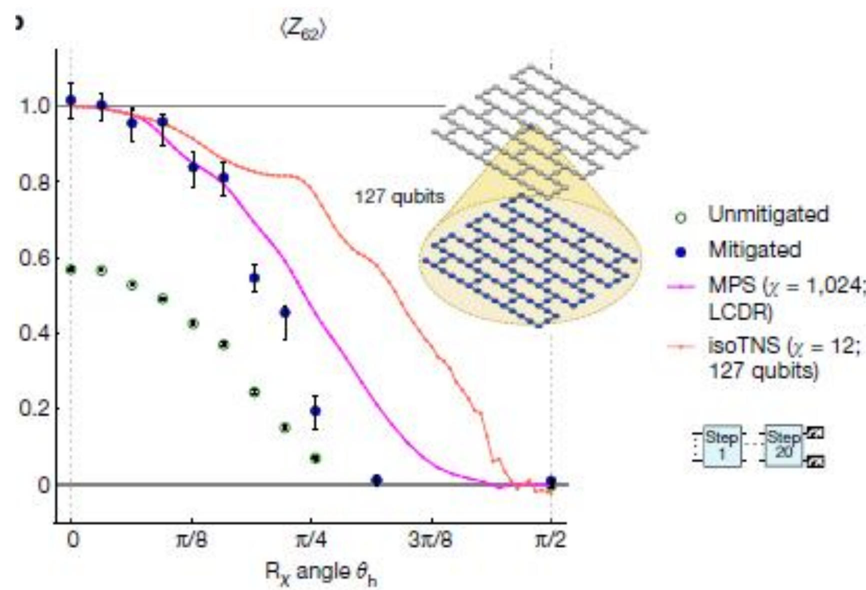
Georgescu et al RMP (2014)

IBM experiment with 127-qubit device: the utility of quantum computing before the fault tolerance

- Transverse-field Ising model

$$H = -J \sum_{\langle i,j \rangle} Z_i Z_j + h \sum_i X_i,$$

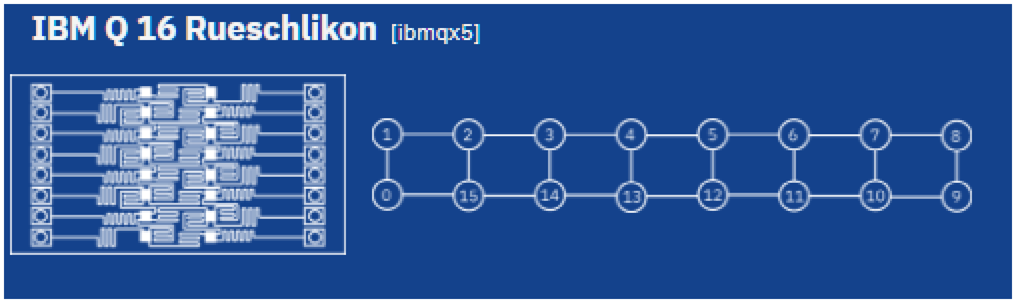




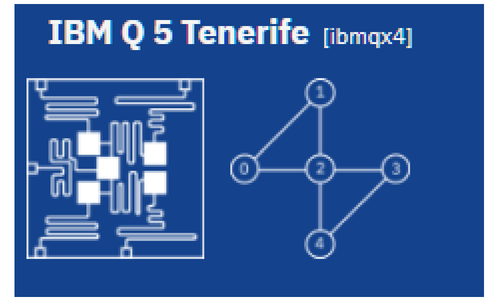
Kim, et al., Nature (2023)

IBM Quantum Experience

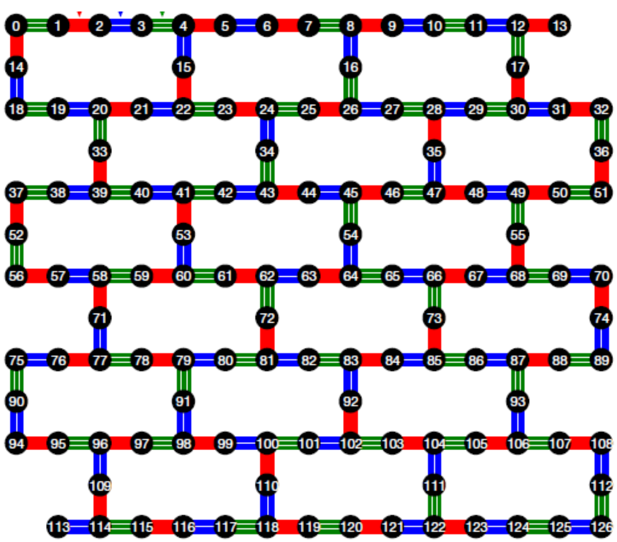
16-qubit chip (QISKIT)



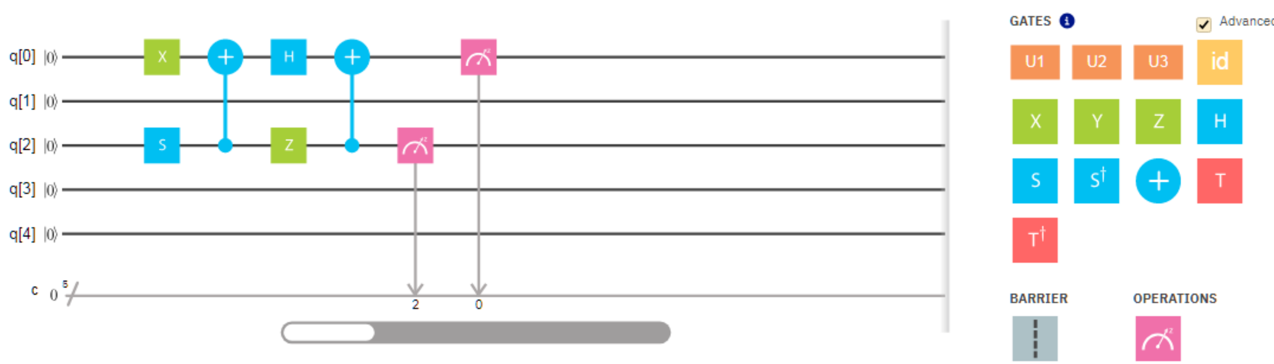
5-qubit chip (composer)



127 qubit chip

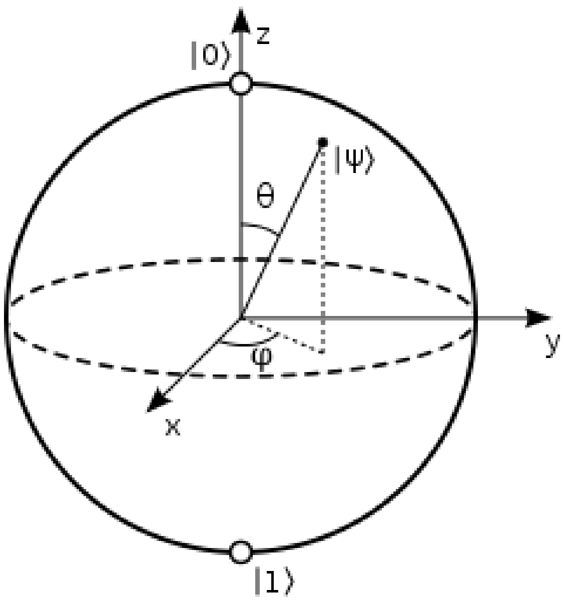


Composer



https://quantumexperience.ng.bluemix.net/qx/editor

Bloch sphere representation



$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

Probabilities to measure 0 or 1:

$$P_0 = \cos^2\left(\frac{\theta}{2}\right) \qquad P_1 = \sin^2\left(\frac{\theta}{2}\right)$$

A matrix representation:

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

2. Quantum logic gates

- *single-qubit gates*
- *two-qubit gates*

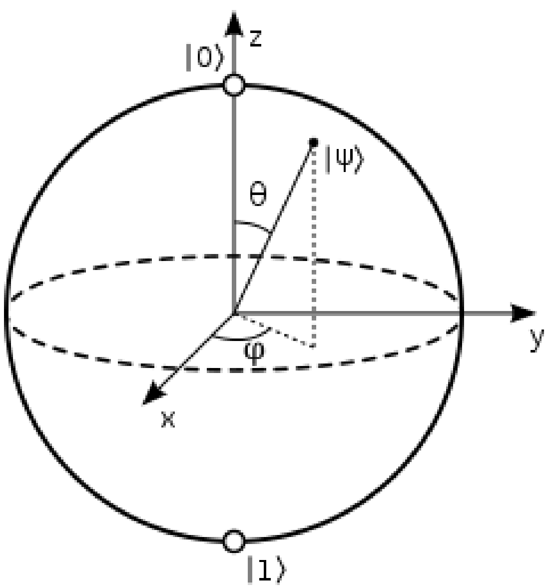
Pauli X gate

$$X \equiv NOT = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The Pauli $\boldsymbol{X}$ gate is a π-rotation around the $\boldsymbol{X}$ axis and has the property that $\boldsymbol{X} \to \boldsymbol{X}$, $\boldsymbol{Z} \to -\boldsymbol{Z}$. Also referred to as a bit-flip.

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$X(\alpha|0\rangle + \beta|1\rangle) = (\alpha|1\rangle + \beta|0\rangle)$$



$$X^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Pauli *Y* gate

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Y

The Pauli Y gate is a π-rotation around the Y axis and has the property that $X \to -X, Z \to -Z$. This is both a bit-flip and a phase-flip, and satisfies $Y = XZ$.

Pauli *Z* gate

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Z

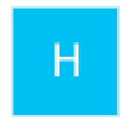
The Pauli Z gate is a π-rotation around the Z axis and has the property that $X \to -X, Z \to Z$. Also referred to as a phase-flip.

$$XY - YX = 2iZ \qquad YZ - ZY = 2iX \qquad ZX - XZ = 2iY$$

Hadamard gate

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$
$$|1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$



The Hadamard gate has the property that it maps $X \rightarrow Z$, and $Z \rightarrow X$. This gate is required to make superpositions.

- Hadamard gate produces quantum superpositions
- Rotation on π around x-axis followed by rotations on $\pi/2$ around y-axis

Rotations around *x, y, z axes*

$$R_x(\theta) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R_y(\theta) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R_z(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

IBM Q single qubit gates

$$U = \begin{pmatrix} \cos(\theta/2) & -e^{i\lambda}\sin(\theta/2) \\ e^{i\phi}\sin(\theta/2) & e^{i\lambda+i\phi}\cos(\theta/2) \end{pmatrix}$$

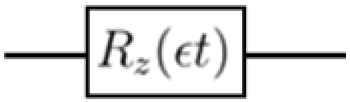
$$u1(\lambda) = U(0,0,\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix}$$

$$u2(\phi,\lambda) = U(\pi/2,\phi,\lambda) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -e^{i\lambda} \\ e^{i\phi} & e^{i\lambda+i\phi} \end{pmatrix}$$

Toy model

$H = \epsilon\sigma_z$ Hamiltonian of a single spin-1/2 particle

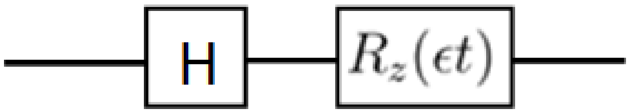
$e^{-it\epsilon\sigma_z}$ - Evolution operator



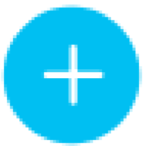
$$R_z(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

The action of the evolution operator is equivalent to the rotation around *z*-axis

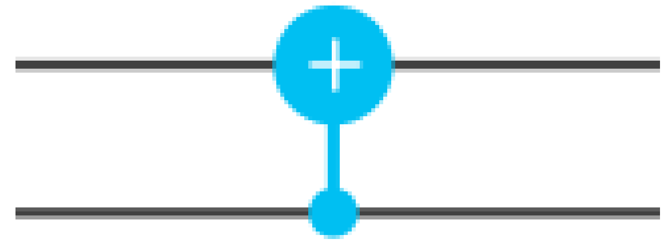
An example of the quantum circuit:



Two-qubit gate CNOT

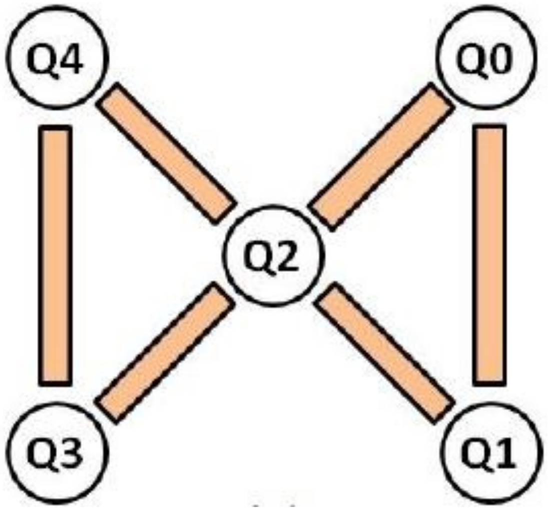


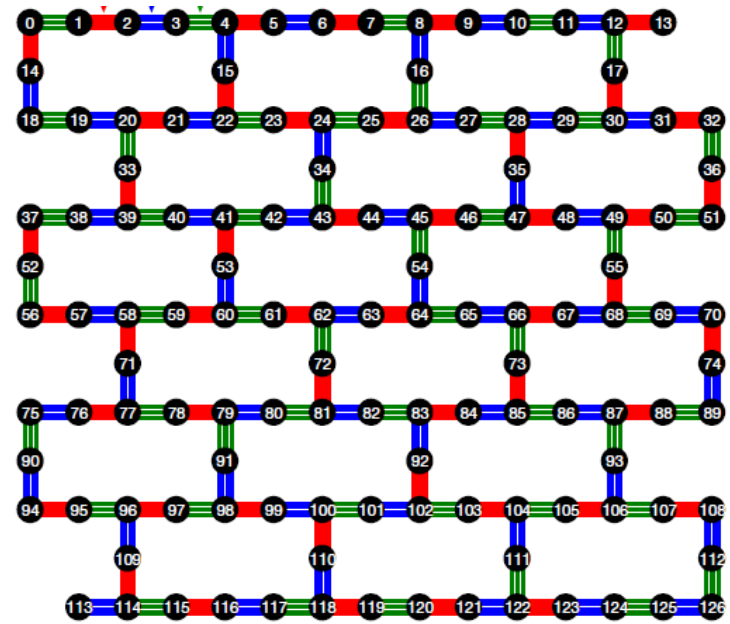
Controlled-NOT gate: a two-qubit gate that flips the target qubit (i.e. applies Pauli X) if the control is in state 1. This gate is required to generate entanglement and is the physical two qubit gate.

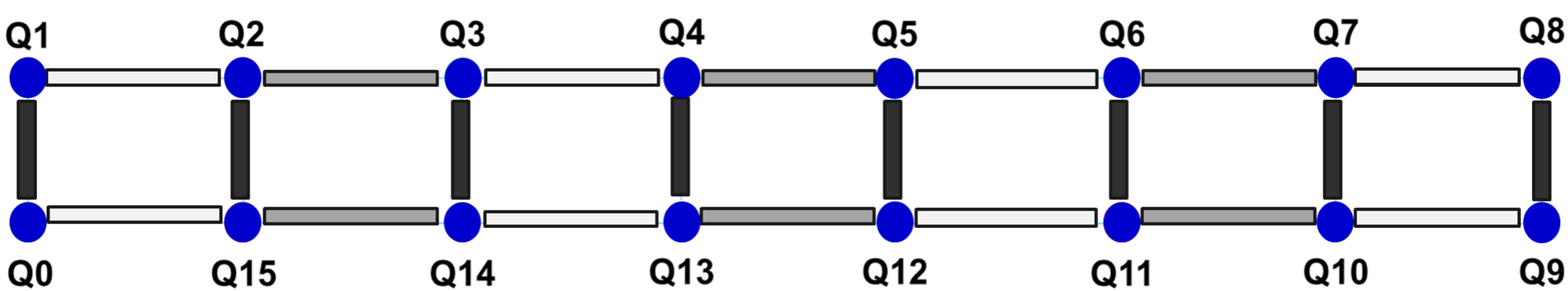


- Control qubit and target qubit
- CNOT does not change the state of the target qubit provided control qubit is in the state 0
- CNOT inverts the state of the target qubit provided control qubit is in the state 1

CNOTs on real superconducting quantum chips







A set of quantum logic gates

- CNOT produces entanglement between qubits.
- It is crucial for *algorithmic* simulation of many-body systems.
- With arbitrary single-qubit unitarities and CNOT you can construct a universal quantum computer.

Fidelities in superconducting realization

-Single-qubit gates: error rates are already low – 10^{-4}
-Two-qubit gates: error rates in multiqubit chips are relatively large, > 10^{-2}.
- Readouts: Errors are also relatively large, > 10^{-2}.
- Error rates are very important characteristics of a quantum computing hardware apart of longitudinal and transversal relaxation times of qubits (T_1 and T_2).

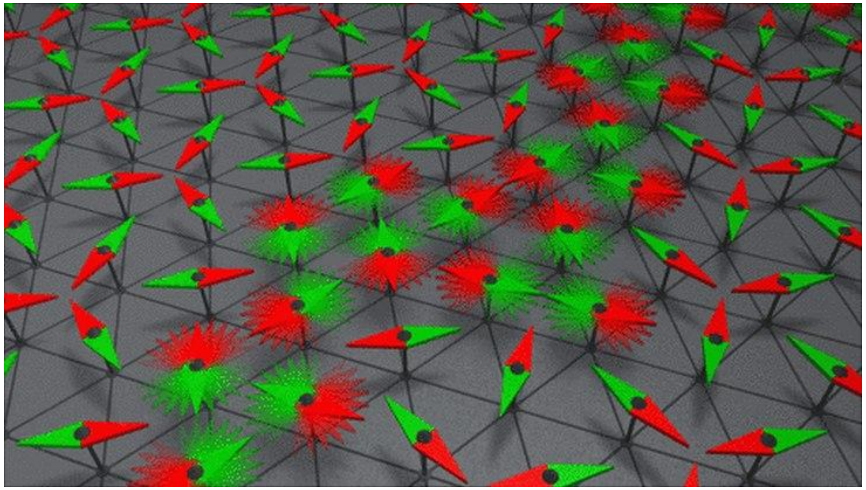
Quantum simulation: material science

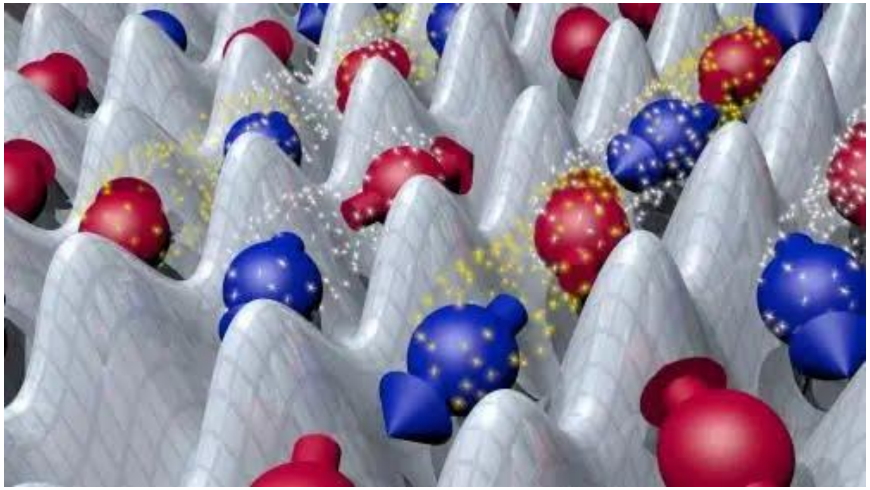
Magnetic materials & quantum magnets

- In certain cases you may forget fermionic (electronic) origin of the initial Hamiltonian and concentrate on spin-1/2 Hamiltonians. Spins of electrons or nucleons.

- Spin-1/2 Hamiltonians also appear in certain limits of more sophisticated Hamiltonians (Hubbard model etc.)

- Spin Hamiltonians are used to describe a magnetic order and quantum phase transitions.





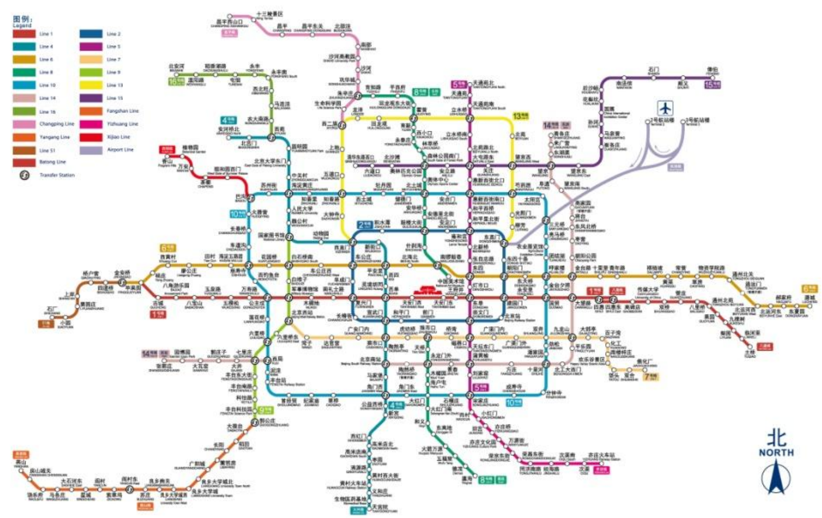
Quantum simulation: optimization problems

- In many binary optimization problems there appears a problem of minimization of a function of many variables, which has a lot of local minima.
- Such problems can be often mapped on long-range Ising model.

$$\mathcal{H}(t) = -\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z - h\sum_i \sigma_i^z$$

- Example: travelling salesman problem (NP-hard prtoblem). Need to visit a list of cities exactly once with the return to the original city. Minimization of cost function.

Moscow and Beijing metro maps as examples of real-world graphs



Quantum simulation of the unitary evolution

I. Correspondence between the degrees of freedom of a modeled system and qubits of the chip depending on the connectivity topology of the chip and the model.

II. Preparation of the initial state in real quantum device.

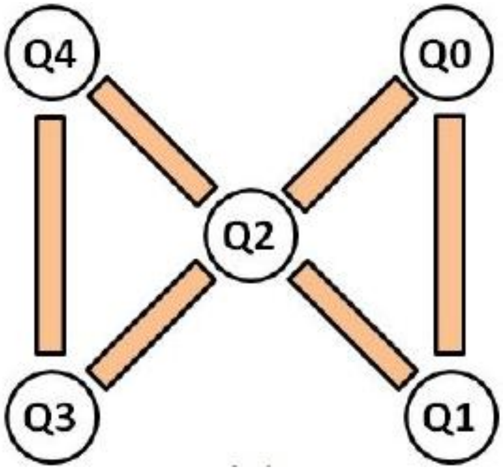
III. Simulation of unitary (free) evolution in real quantum device using evolution operator representation and Trotterization technique.

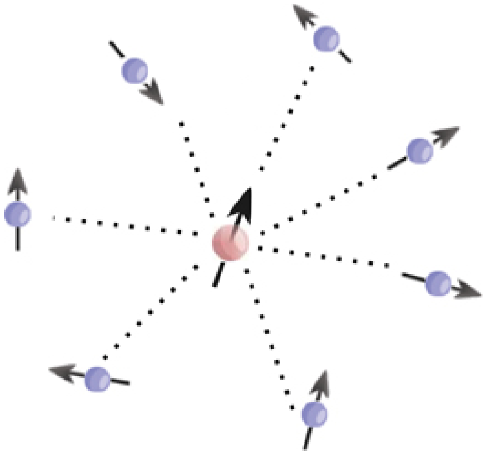
IV. Possible determination of ground state energy using phase estimation algorithms.

3. Illustration: simulation of the central spin model

Central spin model

- Direct mapping between degrees of freedom of a modeled system and degrees of freedom of the physical qubits of the chip





$$H_{cs} = \sum_{j=1}^{L} \epsilon_j(\sigma_{j,z} + 1/2) + \epsilon_c(\sigma_{c,z} + 1/2) + g\sum_{j=1}^{L}(\sigma_c^+\sigma_j^- + \sigma_c^-\sigma_j^+)$$

- Central particle with spin = 1/2 interacting with four similar particles of the “bath”.
- One-to-one correspondence (analog-like)
- Interaction between particles is simulated using CNOTs and Trotterization via discrete operations (digital modeling)
- CNOTs are also utilized to initiate the system, i.e., to encode quantum states of modeled system into quantum states of physical qubits. CNOTs produce entangled states.

Encoding initial condition to the chip

- Example: initial state of the system – entangled “bath”

$$\Psi(0) = |\downarrow\rangle \otimes \frac{1}{\sqrt{2}} \left(|\downarrow\uparrow\rangle + e^{i\varphi} |\uparrow\downarrow\rangle \right)$$

where φ is a tunable phase parameter.

Central particle dynamics can be suppressed due to the negative quantum interference of contributions from two qubits.

One of the eigenstates of *H* corresponds to the above formula with

$$\varphi = \pi$$

$$H = g \sum_{j=1}^{L} (\sigma_c^+ \sigma_j^- + \sigma_c^- \sigma_j^+)$$

Encoding initial condition to the chip

- Example: initial state of the system – entangled "bath"

$$\Psi(0) = |\downarrow\rangle \otimes \frac{1}{\sqrt{2}} \left(|\downarrow\uparrow\rangle + e^{i\varphi} |\uparrow\downarrow\rangle \right)$$

where φ is a tunable phase parameter.

Central particle dynamics can be suppressed due to the negative quantum interference of contributions from two qubits.

$$\sum_{j=1}^{2} (\sigma_c^+ \sigma_j^- + \sigma_c^- \sigma_j^+) |\downarrow\rangle \otimes \left(|\downarrow\uparrow\rangle + e^{i\varphi} |\uparrow\downarrow\rangle \right) = |\uparrow\rangle \otimes \left(|\downarrow\downarrow\rangle + e^{i\varphi} |\downarrow\downarrow\rangle \right)$$

$\varphi = \pi$ - Cancellation of two contribution coming from two different spins.

- No central spin dynamics. "Dark" state from quantum optics.

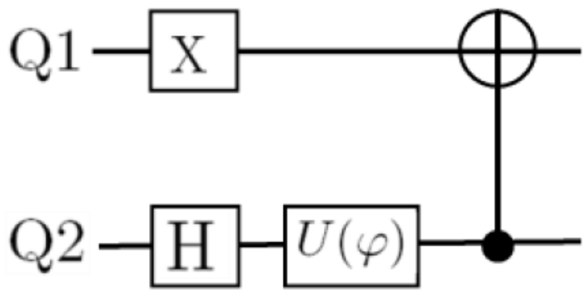
- Excitation blockade in the bath due to the quantum interference.

Encoding initial condition to the chip

- Example: initial state of the system – entangled "bath"

$$\Psi(0) = |\downarrow\rangle \otimes \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle + e^{i\varphi}|\uparrow\downarrow\rangle\right)$$

Quantum circuit



$$U(\varphi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{bmatrix}$$

Modeling dynamics

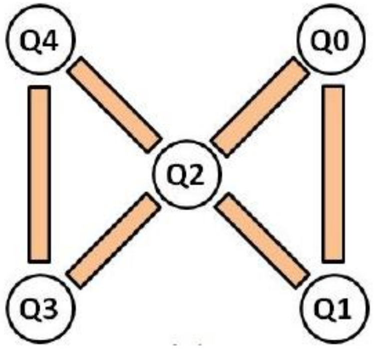
- Free evolution (through evolution operator)

$$\Psi(t) = e^{-iHt}\Psi(0)$$

This representation is needed for quantum computer and not for us

Natural mission of a quantum computer is to make unitary rotations in the multidimensional Hilbert space

$$H = \frac{g}{2}\sum_{j=1}^{L}(\sigma_c^x\sigma_j^x + \sigma_c^y\sigma_j^y)$$



Trotter-Suzuki decomposition

$$e^{i(H_A+H_B)t} = 1 + i(H_A + H_B)t + \frac{(it)^2}{2!}(H_A + H_B)(H_A + H_B) + \ldots$$

$$e^{iH_At} = 1 + iH_At + \frac{(it)^2}{2!}H_A^2 + \ldots$$

$$e^{iH_Bt} = 1 + iH_Bt + \frac{(it)^2}{2!}H_B^2 + \ldots$$

$$e^{iH_At}e^{iH_Bt} = 1 + i(H_A + H_B)t + \frac{(it)^2}{2!}(H_A^2 + 2H_AH_B + H_B^2)\ldots$$

$$e^{i(H_A+H_B)t} - e^{iH_At}e^{iH_Bt} = \frac{(it)^2}{2!}[H_A, H_B] + \ldots$$

Trotter-Suzuki decomposition

$$e^{-it(H_A+H_B)} = e^{-itH_A}e^{-itH_B} + \frac{(it)^2}{2!}[H_A, H_B] + \dots$$

$$e^{-it(H_A+H_B)} \simeq \left(e^{-iH_At/n}e^{-iH_Bt/n}\right)^n$$

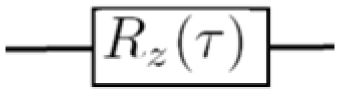
exact in the limit $n \to \infty$

The larger number of Trotter steps for the fixed time, the smaller (mathematical) Trotterization error

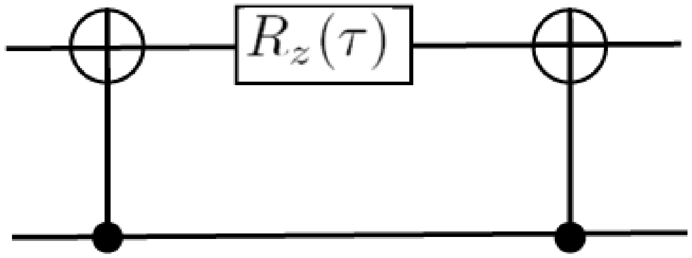
Trotter number = 1 – some initial dynamics
Trotter number = 2 – slightly longer time interval
Etc.

Main building blocks of a circuit

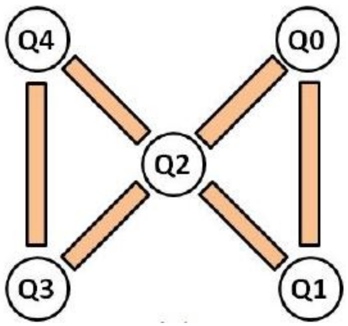
$$\epsilon\sigma_j^z \rightarrow \exp(-i\tfrac{\tau}{2}\sigma_j^z)$$



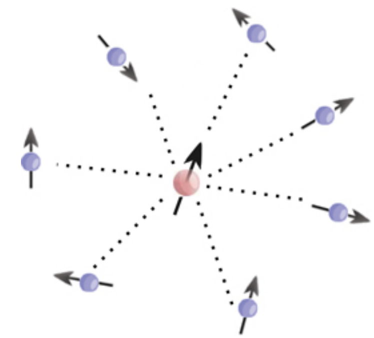
$$J\sigma_c^z\sigma_j^z \rightarrow \exp\left(-i\tfrac{\tau}{2}\sigma_c^z \otimes \sigma_j^z\right)$$



Central spin model: one-step Trotter decomposition



$$H = \frac{g}{2}\sum_{j=1}^{L}(\sigma_c^x\sigma_j^x + \sigma_c^y\sigma_j^y)$$



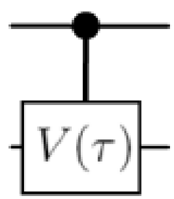
$$\Psi(\tau) \approx \prod_{j=1}^{L} \exp\left(-i\frac{\tau}{2}\sigma_c^x \otimes \sigma_j^x\right)\exp\left(-i\frac{\tau}{2}\sigma_c^y \otimes \sigma_j^y\right)\Psi(0)$$

$\tau = gt$ $\qquad\qquad$ $\tau \ll 1 \; (t \ll 1/g)$

Condition of applicability of a one-step Trotter decomposition

- Main building block for modeling interaction

$$H = \frac{g}{2}\sum_{j=1}^{L}(\sigma_c^x\sigma_j^x + \sigma_c^y\sigma_j^y)$$



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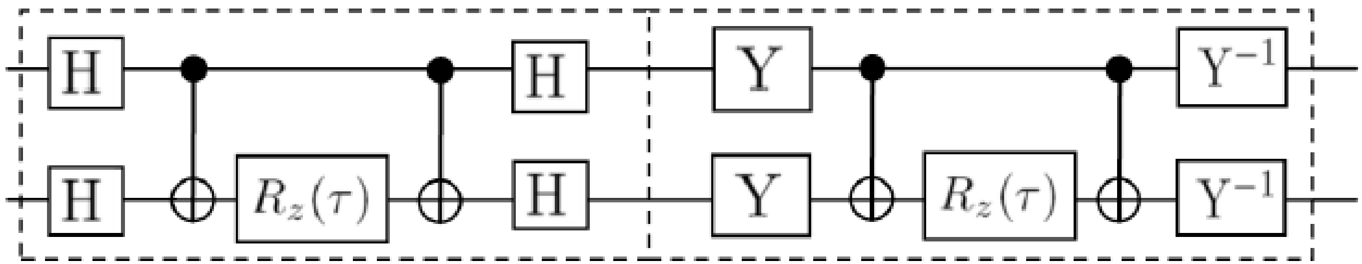


$\exp\left(-i\frac{\tau}{2}\sigma_c^x \otimes \sigma_j^x\right)$ $\quad$ $\exp\left(-i\frac{\tau}{2}\sigma_c^y \otimes \sigma_j^y\right)$

FIG. 7: Quantum circuit for $\exp\left(-i\frac{\tau}{2}\sigma_c^x \otimes \sigma_j^x\right)\exp\left(-i\frac{\tau}{2}\sigma_c^y \otimes \sigma_j^y\right)$ (see in the text).

change-of-basis gate $\hat{Y}$ is defined as $\hat{R}_x(-\pi/2)$

Full quantum circuit

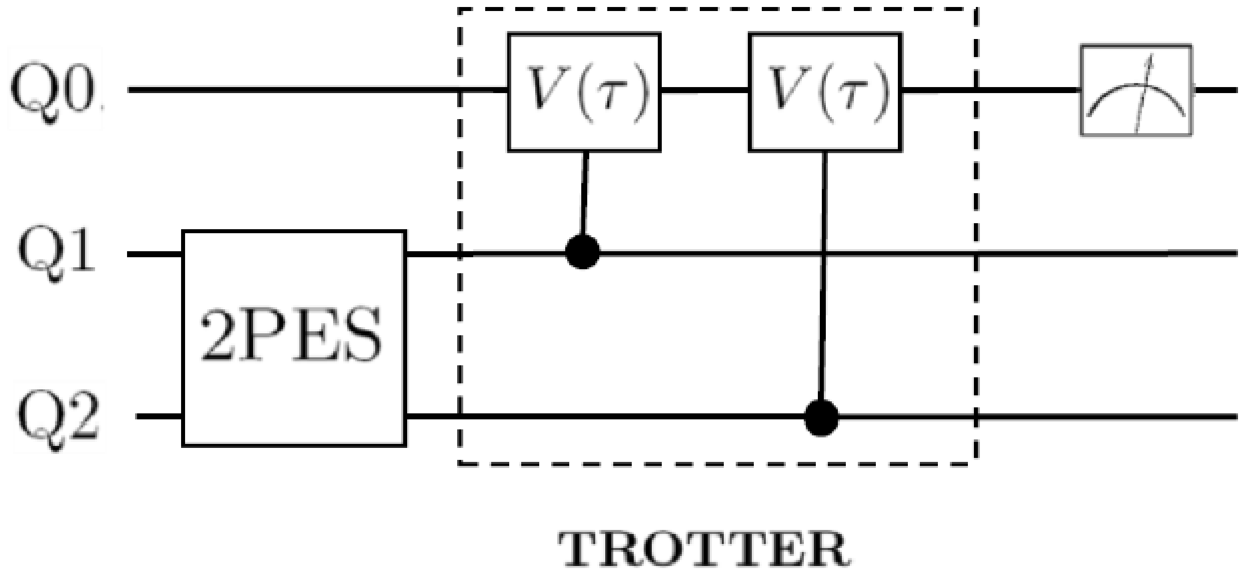
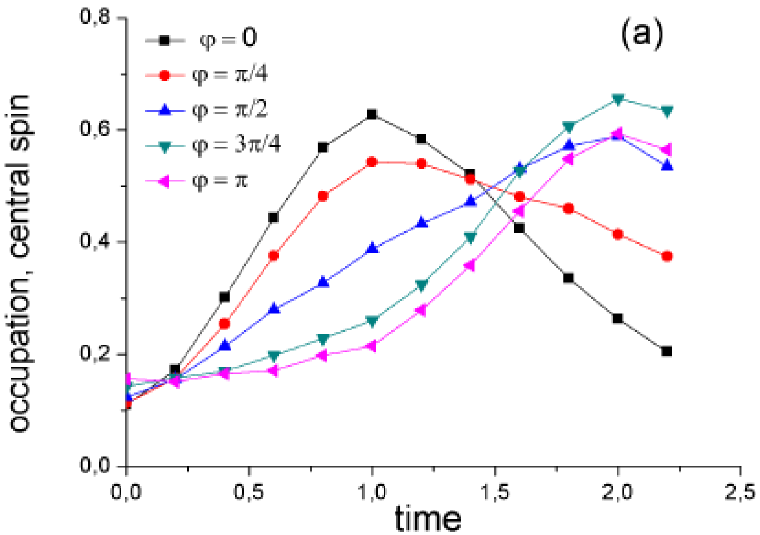


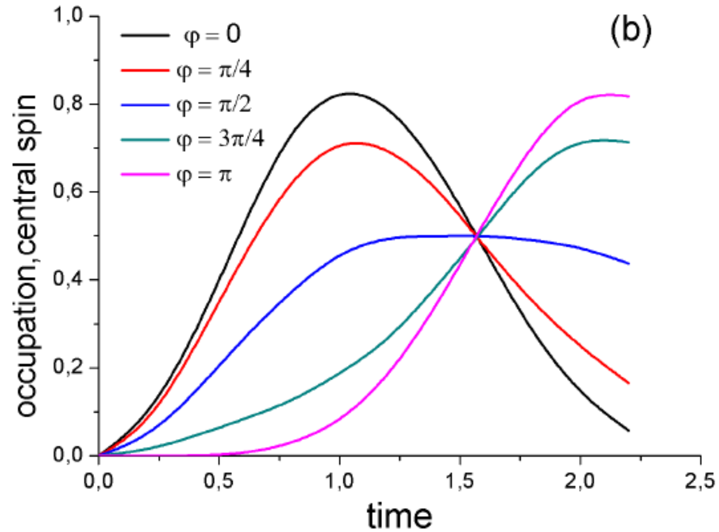
FIG. 12: Quantum circuit for the evolution of the system starting from the initial state of two-particle entangled state of the bath and unexcited central spin.

Two-particle entangled state: Population of the central particle

experiment (8128 runs per point)



theory



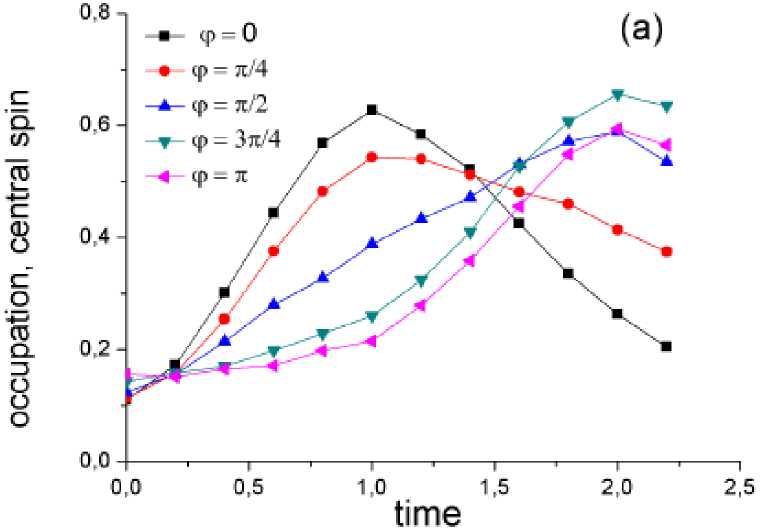
*Theory is not exact. Approximation of the same level – **one-step Trotter decomposition***

$$\Psi(0) = |\downarrow\rangle \otimes \frac{1}{\sqrt{2}} \left(|\downarrow\uparrow\rangle + e^{i\varphi} |\uparrow\downarrow\rangle \right)$$

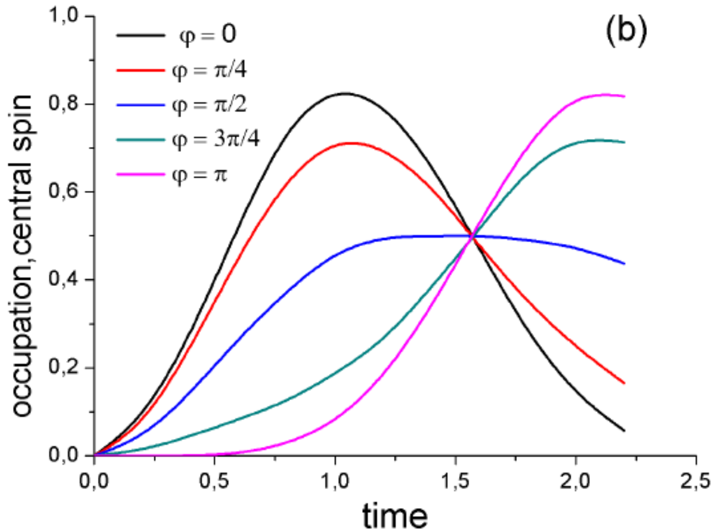
- Dark and bright states known from quantum optics
- Entanglement in the bath and quantum interference effects block excitation transfer to the center

Two-particle entangled state: Population of the central particle

experiment (8128 runs per point)



theory



- Noisy “background” is independent on time
- Many gates – randomization of wrong outputs.

Error mitigation: 2 Trotter steps

$$\Delta n_c(\tau) = n_c(\tau) - n_c(\tau = 0)$$ - analyzing differences

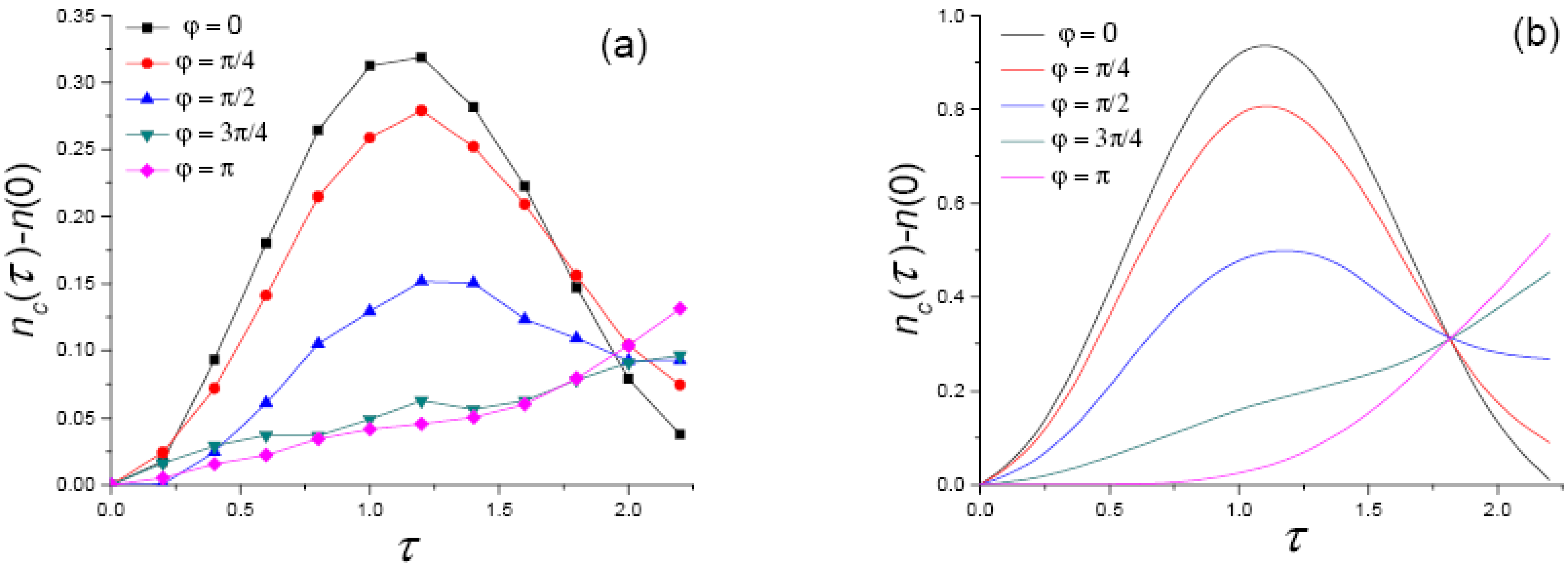


Fig. 9 (Color online) The results of our experiment (a) and theory (b) for $\Delta n_c(\tau)$ as a function of the dimensionless time τ for the Trotter number $N = 2$. Different curves correspond to different values of phase parameter φ entering the initial state (4).

Error mitigation: 3 Trotter steps

$$\Delta n_c(\tau) = n_c(\tau) - n_c(\tau = 0)$$ - analyzing differences

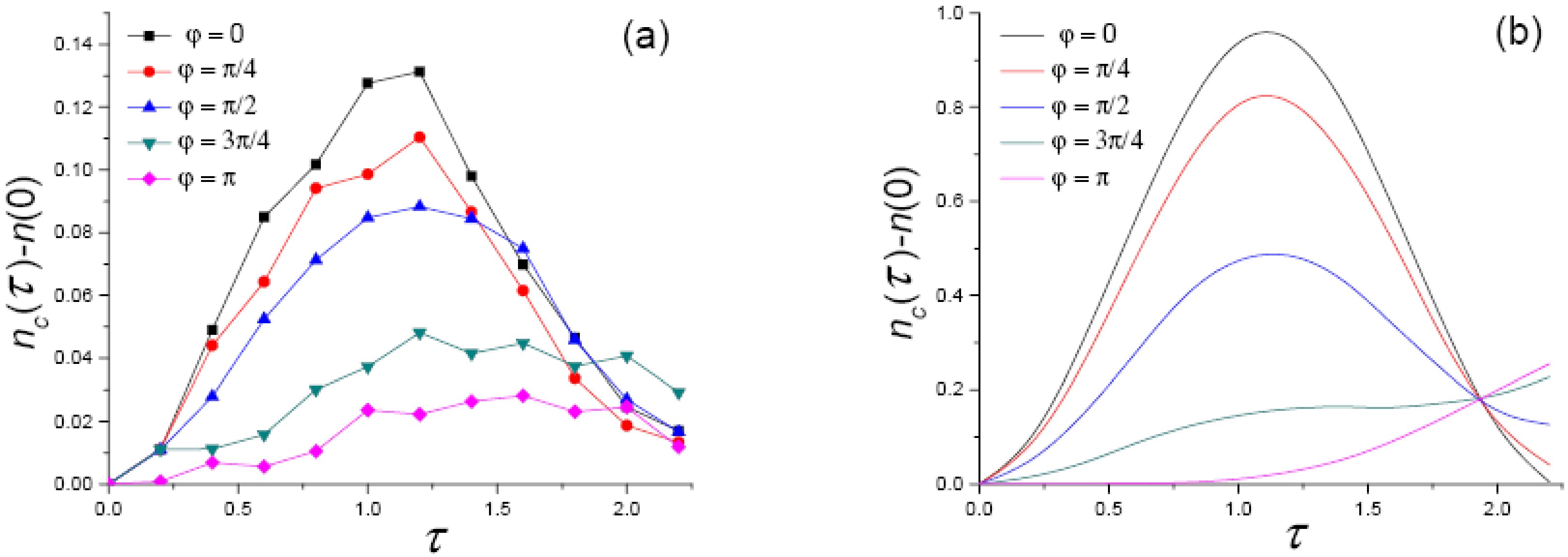


Fig. 10 (Color online) The results of our experiment (a) and theory (b) for $\Delta n_c(\tau)$ as a function of the dimensionless time τ for the Trotter number $N = 3$. Different curves correspond to different values of phase parameter φ entering the initial state (4).

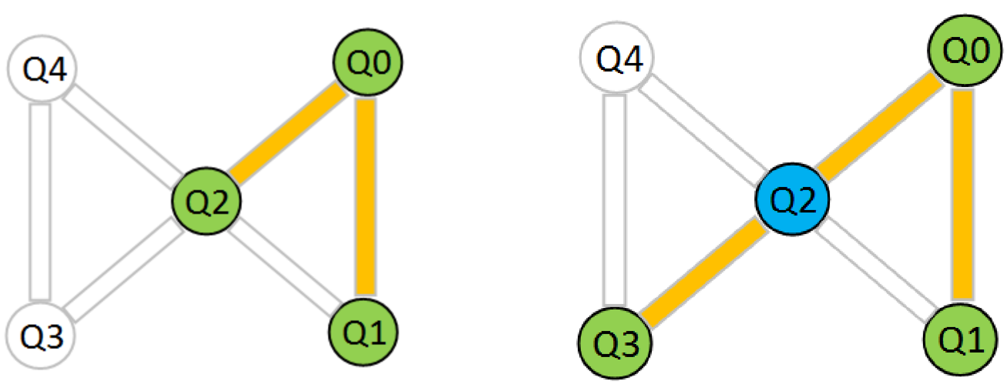
Example: initial state of the system – entangled “bath” of *three* particles

$$\Psi(0) = |\downarrow\rangle \otimes \frac{1}{\sqrt{6}} \left(|\downarrow\downarrow\uparrow\rangle - 2e^{i\chi} |\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\rangle \right)$$

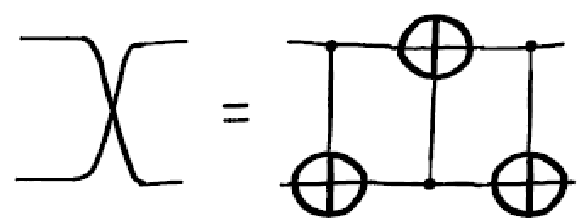
where χ is a tunable phase parameter.

Dynamics of the central spin can be suppressed due to the negative quantum interference of contributions from three qubits.

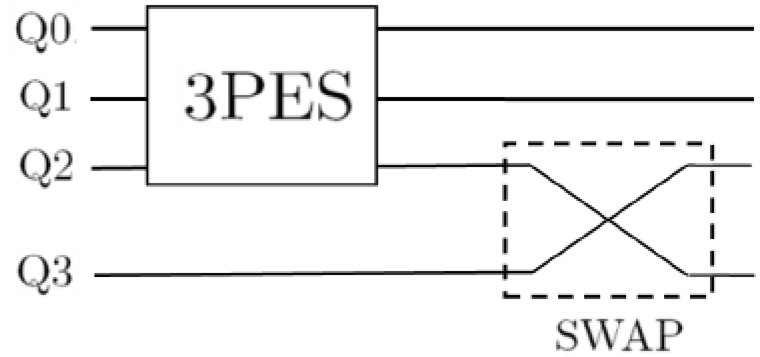
Two-step encoding



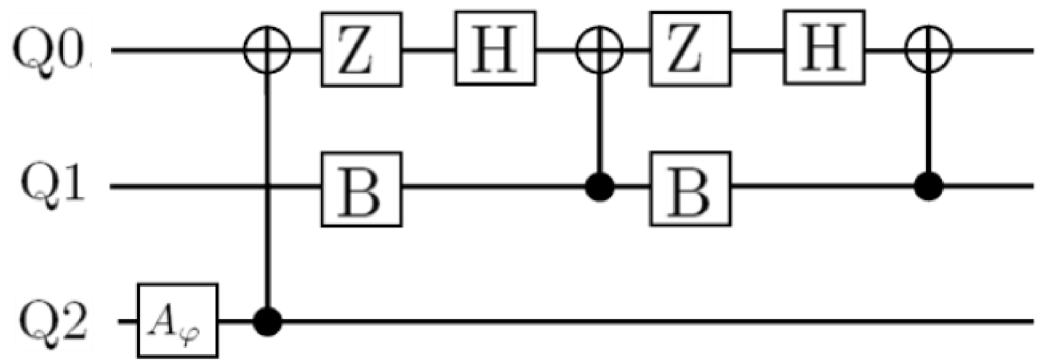
SWAP



Full circuit for encoding

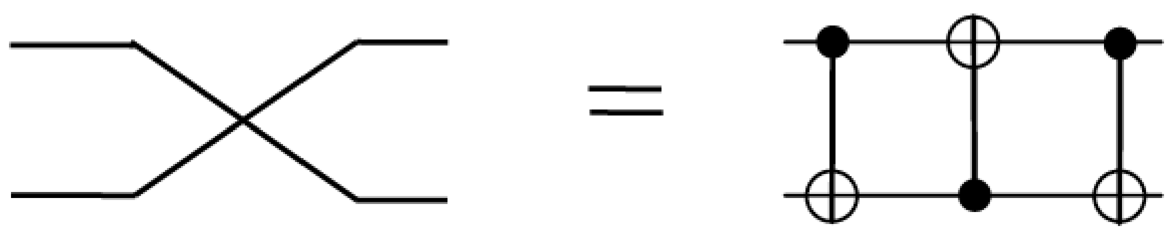


3PES



$$A_\varphi = U_3(\theta = 2\arccos\tfrac{1}{\sqrt{3}}, \varphi, \lambda = 0),$$
$$B = U_3(\theta = \tfrac{\pi}{4}, \varphi = 0, \lambda = 0);$$

SWAP



Full circuit for the whole algorithm

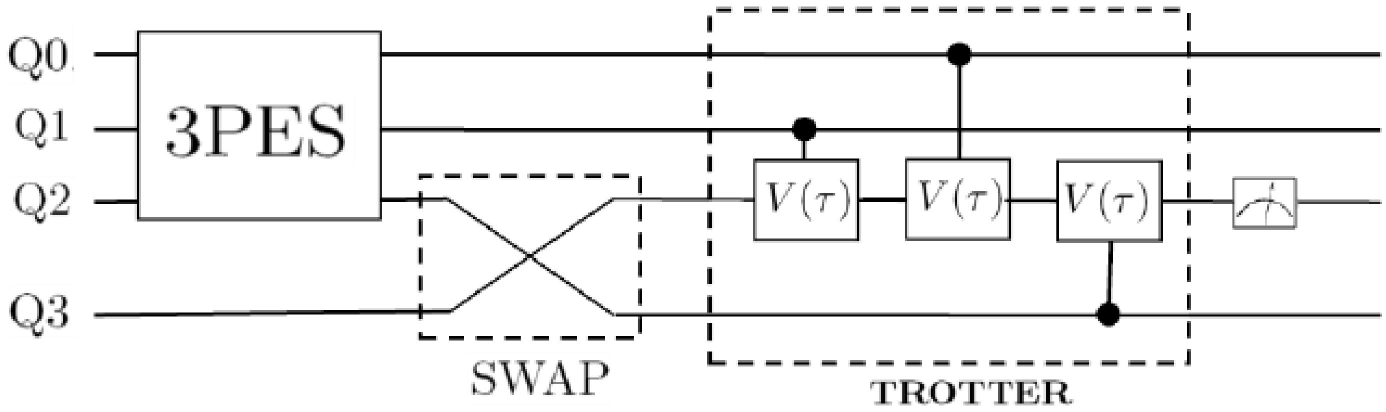
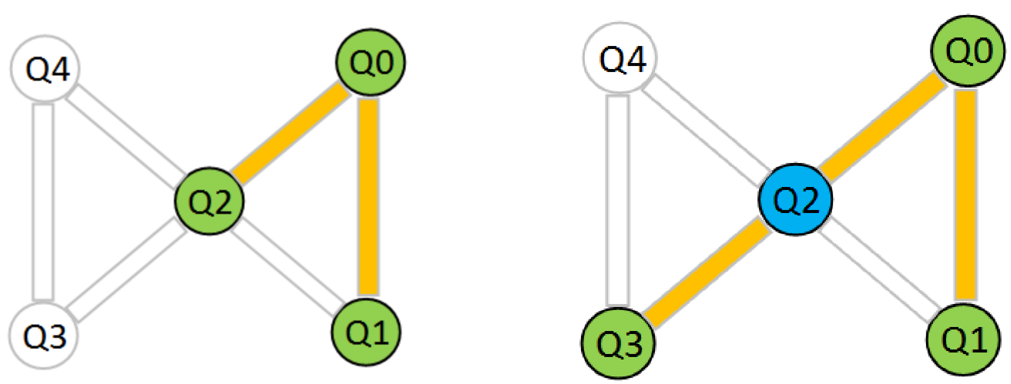
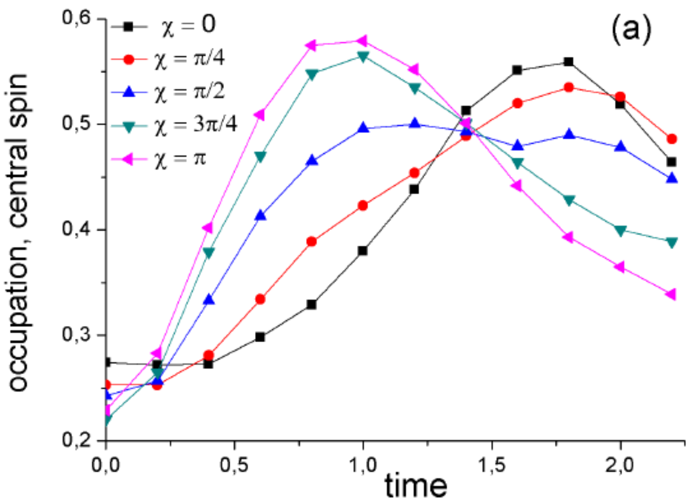


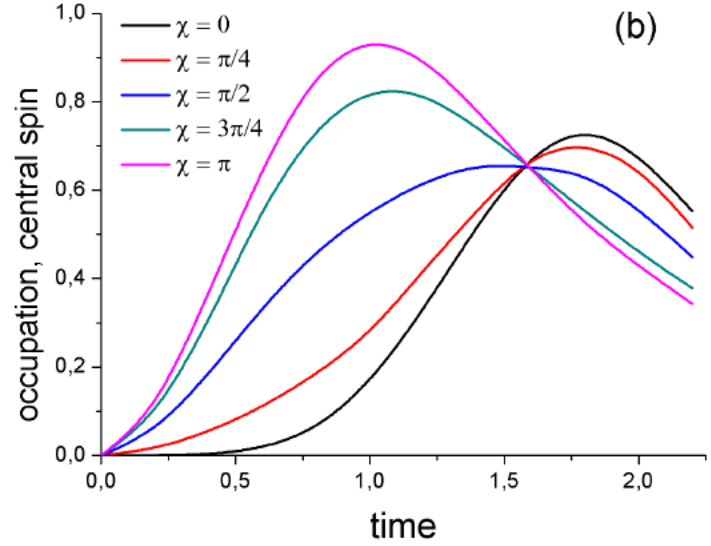
FIG. 13: Quantum circuit for the evolution of the system starting from the initial state of three-particle entangled state of the bath and unexcited central spin.



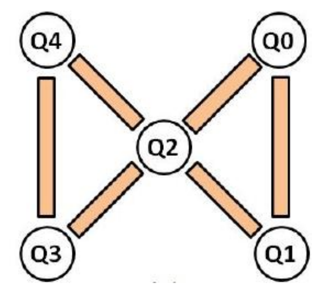
Three-particle entangled state: Population of central particle

experiment *theory*





$$\Psi(0) = |\downarrow\rangle \otimes \frac{1}{\sqrt{6}}\left(|\downarrow\downarrow\uparrow\rangle - 2e^{i\chi}|\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\rangle\right)$$



- Dark and bright states: quantum superpositions of two-particle entangled states
- Entanglement in the bath and quantum interference effects block excitation transfer to the center
- Randomization of errors.

Utility for the studies of far-from-equilibrium dynamics

Nonequilibrium quantum relaxation in closed many-body systems. Current experimental platform and setup: quenches in trapped cold-atom gases. Mapping on spin models. Digital quantum simulation: the same quantum chip can be used for simulations of different models and initial conditions.

Central issues:

1. Whether the system relaxes to a stationary state ("thermalization")? What are its characteristics?
2. Dynamical *evolution* of order, correlations, entanglement.

- Depends on the integrability of the model
- Depends on the initial state

4. Phase estimation algorithm

Phase estimation algorithm

- Hamiltonian eigenstates $|\phi_j\rangle$

Free evolution

If the initial state is one of the Hamiltonian eigenstates

$$|\psi(t=0)\rangle = \phi_n$$

Free evolution is reduced to the dynamics of the phase

$$|\psi(t)\rangle = \exp(-iE_n t)|\psi(t=0)\rangle$$

How can the phase be determined?

- Global characteristics of the whole system of qubits, not the local one
- Ancilla qubits are needed. Data qubits and measurement qubits.

Toy model

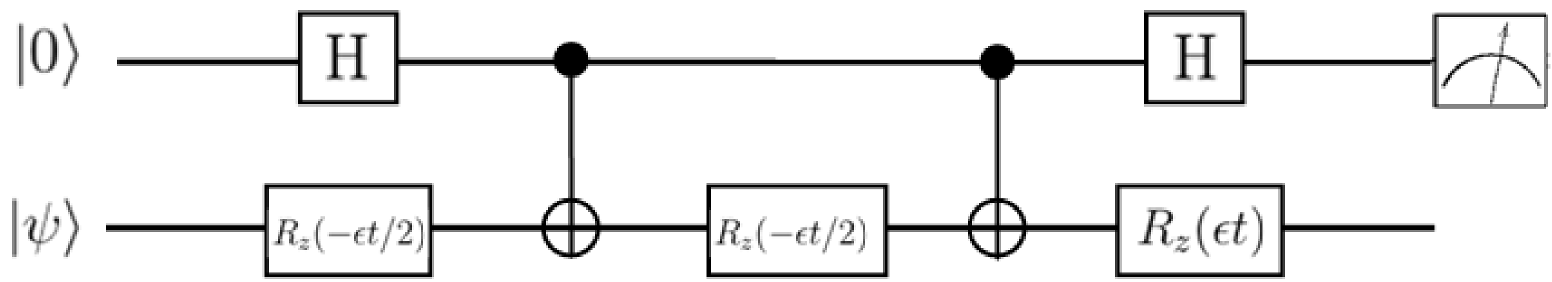
$H = \epsilon\sigma_z$ Hamiltonian of a single spin

$e^{-it\epsilon\sigma_z}$ Evolution operator $-\boxed{R_z(\tau)}-$

$$e^{-it\epsilon\sigma_z}|0\rangle = e^{it\epsilon/2}|0\rangle \qquad e^{-it\epsilon\sigma_z}|1\rangle = e^{-it\epsilon/2}|1\rangle$$

In principle, if you fix time, you might be able to determine ϵ

Quantum circuit. Controlled rotation



Let us consider the probability of measuring ancilla qubit in the state $|0\rangle$ provided that $|\psi\rangle = |1\rangle$

ancilla

data

$$\frac{1}{2}(|0\rangle(1+e^{i\epsilon t/2})+|1\rangle(1-e^{i\epsilon t/2}))\otimes|1\rangle$$

Probability to get |0> at ancilla qubit

$$P_0=\frac{1}{4}(1+e^{i\epsilon t/2})(1+e^{-i\epsilon t/2})=\frac{1}{2}(1+\cos\frac{\epsilon t}{2})=\cos^2\frac{\epsilon t}{4}$$

Statistical error after *N* measurements

$$1/\sqrt{N}$$

Number of measurements required to extract *m* binary digits of a phase

$$N\sim 2^{2m}$$

Exponentially large number! – Bottleneck!

Kitaev's iteration algorithm

Probability to get |0> at ancilla qubit

$$P_0 = \frac{1}{4}(1+e^{i\epsilon t/2})(1+e^{-i\epsilon t/2}) = \frac{1}{2}(1+\cos\frac{\epsilon t}{2}) = \cos^2\frac{\epsilon t}{4}$$

Introduce more convenient notation

$$\frac{\epsilon t}{4} = \pi\phi \qquad\qquad P_0 = \cos^2 \pi\phi$$

- Binary form of the phase

$$\phi = 0.\phi_1\phi_2\phi_3\ldots$$

- Imagine that the expansion stops somewhere

$$\phi = 0.\phi_1\phi_2\phi_3 = \frac{\phi_1}{2} + \frac{\phi_2}{4} + \frac{\phi_3}{8}$$

$$\cos^2 2^1\pi\phi = \cos^2\left(\frac{\pi\phi_2}{2} + \frac{\pi\phi_3}{4}\right) \qquad \cos^2 2^2\pi\phi = \cos^2\left(\frac{\pi\phi_3}{2}\right)$$

$$\cos^2 2^2 \pi \phi = \cos^2 \left(\frac{\pi \phi_3}{2} \right)$$

$$\phi_3 = 0 \quad \Rightarrow \quad \cos^2 \left(\frac{\pi \phi_3}{2} \right) = 1$$

$$\phi_3 = 1 \quad \Rightarrow \quad \cos^2 \left(\frac{\pi \phi_3}{2} \right) = 0$$

- Probability to obtain 0 is either 0 or 1 (no intermediate values).
- Last digit can be measured deterministically just from a single measurement of ancilla qubit

- Step 1. Consider the evolution on the time interval 4*t*

$$\cos^2 2^2\pi\phi = \cos^2\left(\frac{\pi\phi_3}{2}\right) \Rightarrow \text{Deterministically extract } \phi_3$$

- Step 2. Consider the evolution on the time interval 2*t.* Add additional rotation on angle $\frac{\pi\phi_3}{4}$

$$\cos^2(2^1\pi\phi - \pi\phi_3/4) = \cos^2\left(\frac{\pi\phi_2}{2}\right) \Rightarrow \text{Deterministically extract } \phi_2$$

- Step 3. Consider the evolution on the time interval *t.* Add additional rotation on angle $\frac{\pi\phi_2}{4} + \frac{\pi\phi_3}{8}$

$$\cos^2(\pi\phi - \pi\phi_2/4 - \pi\phi_3/8) = \cos^2\left(\frac{\pi\phi_1}{2}\right) \Rightarrow \text{Deterministically extract } \phi_1$$

More realistic situation

- 1. **If the binary expansion of the phase does not stop**

$$\phi = 0.\phi_1\phi_2\phi_3\dots$$

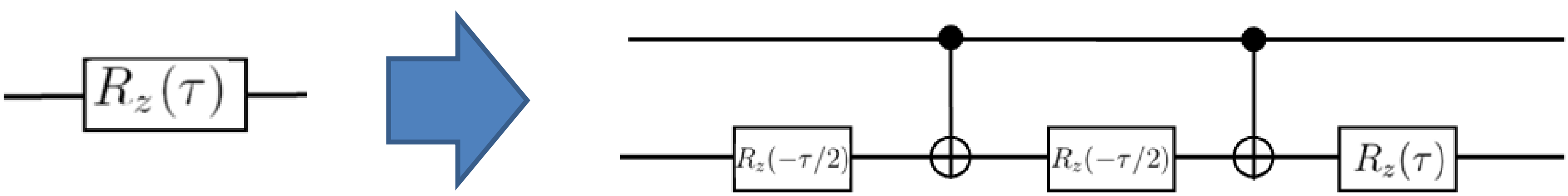
The algorithm is not deterministic anymore. Repetitive measurements of each digit. Estimate.

- 2. **If the initial state is not an exact eigenstate**. PEA still works provided an overlap between the true ground state and the initial state is > 0.5.

Repetitive measurements of each digit. Since 0 or 1 only, good overlap yields correct result. Many measurements.

General rule

- For more realistic Hamiltonians. All rotations to be replaced by controlled rotations.



- Ancilla qubit is strongly affected by CNOT errors (many CNOTs are applied to the ancilla).

Quantum simulation of the unitary evolution

I. Correspondence between the degrees of freedom of a modeled system and qubits of the chip depending on the connectivity topology of the chip and the model.

II. Preparation of the initial state in real quantum device.

III. Simulation of unitary (free) evolution in real quantum device using evolution operator representation and Trotterization technique.

IV. Possible determination of ground state energy using phase estimation algorithms.

- We acknowledge use of the IBM Quantum Experience for this lecture.
- The viewpoints expressed are those of the author and do not reflect the official policy or position of IBM or the IBM Quantum Experience team.