Pasqal Defining the quantum reality

Q-KHAI Quantum Simulation

Part 2:
- 중성원자 양자 시뮬레이션
- Pasqal Pulser & 양자 시뮬레이션 실습

Woojun Lee, Ph. D.
Technical Business Developer, Pasqal
Aug. 3, 2025

Contents

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Part 1 (3, Mon) 1:30 pm

- 양자컴퓨팅 소개
- 중성원자 양자컴퓨터
- Pasqal 소프트웨어 스택
- Pulser Studio 실습

Part 2 (3, Mon) 2:30 pm

- 양자 시뮬레이션 (Spin sytems, AFM states, Direct quantum simulation)
- 실습 (Pulser, 양자시뮬레이션)

Part 3 (4, Tue) 9 am

- MIS, QUBO theory, use cases, sdk
- QEK theory, use cases, sdk
- 실습 (QUBO, QEK)

Pasqal Defining the quantum reality

양자 시뮬레이션

양자컴퓨터 - 자연 자체를 모방하는 계산 기계

Pasqal

International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

about what the computer was, we can say: Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws. Or we can turn the other way and say: Let the computer still be the same kind that we thought of before—a logical, universal automaton; can we imitate this situation? And I'm going to separate my talk here, for it branches into two parts.

4. QUANTUM COMPUTERS—UNIVERSAL QUANTUM SIMULATORS

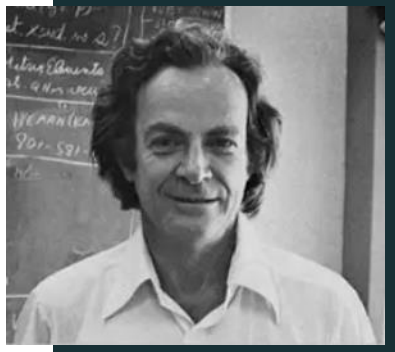
The first branch, one you might call a side-remark, is, Can you do it with a new kind of computer—a quantum computer? (I'll come back to the other branch in a moment.) Now it turns out, as far as I can tell, that you can simulate this with a quantum system, with quantum computer elements. It's not a Turing machine, but a machine of a different kind. If we disregard the continuity of space and make it discrete, and so on, as an approximation (the same way as we allowed ourselves in the classical case), it does seem to

양자컴퓨터

파인만의 주장: **자연 자체를 모방하는 계산 기계**

"만약 자연이 양자역학적으로 움직인다면,
자연을 정확히 시뮬레이션하는 컴퓨터도 양자역학을 따르지 않을까요??"

즉, **고전 컴퓨터로 양자 시스템을 시뮬레이션하는 데는** 근본적인 한계가 존재합니다. 그렇다면 컴퓨터 자체를 양자역학적 실체로 만들 수 있을까요?



(Dr. Richard P. Feynman)

양자 시뮬레이션

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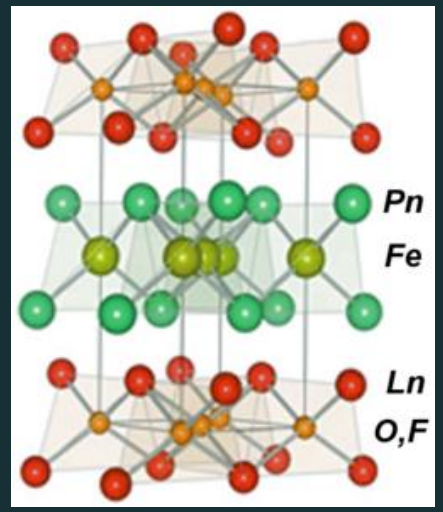
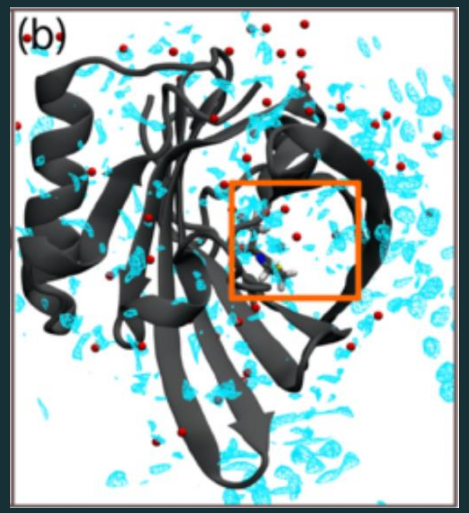
고부가 가치가 있는 많은 영역들에서 복잡한 양자 시스템의 계산이 필요하지만 직접 계산하기엔 계산량이 너무 방대





- 소재 (공정, 디스플레이, 초경량, …)
- 상온 초전도체
- 신약 개발
- 화학

계산하려는 시스템과 같은 해밀토니안 구조를 갖는 양자 시스템을 만들어서 결과를 측정

⇒ 양자 시뮬레이션

보통 어떤 계가 해밀토니안에 따라 시간 t만큼 time evolution 했을 때의 상태 $|\psi(t)\rangle$를 구하는게 목적.

양자컴퓨터의 필요성

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$$10^{60} \approx 2^{200}$$

중간 정도 복잡한 분자의 양자 상태를 정확하게 나타내기 위해 관련된 전자,
진동, 스핀 자유도를 모두 고려할 때, 필요한 상태 벡터는
$10^{60} \approx 2^{200}$ 에 근접하는 차원을 갖는 힐베르트 공간이 필요.

10^{60} 개의 숫자를 저장하려면 전 지구를 고전
데이터 센터로 채워도 충분하지 않음

양자컴퓨터를 사용하면 200개의
큐비트로 가능

6

Analog or Digital Quantum Computing/Simulation

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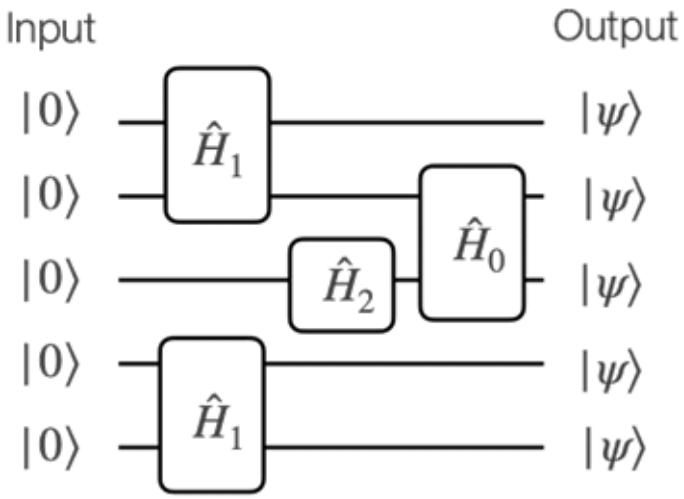
Digital Control

Programming a quantum circuit with digital quantum gates

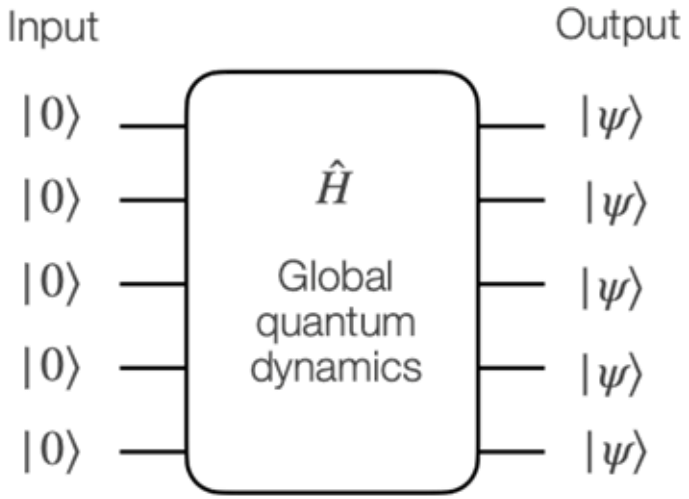
Elementary operations are discrete digital quantum gates, that can act either on individual qubits, or on several qubits at the same time.



Analog Control

Programming a Hamiltonian sequence

The Hamiltonian faithfully describes the dynamics of a physical quantum system or a reformulation of an operational case. Parameters can be tuned continuously.



Ising model

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스핀(spin): 입자들이 전하라는 전기적 단위를 가지는 것과 비슷하게 스핀이라는 자기적 단위를 가짐.

물체의 자기적 성질은 스핀들 사이, 그리고 외부 자기장과의 상호작용으로 결정되며 아래와 같이 분류

- 상자성 (paramagnetism) - 외부 자기장 방향으로 자성이 정렬
- 강자성 (ferromagnetism) - 외부 자기장이 사라져도 자성이 남아있음
- 반강자성 (ferromagnetism) - 거시적으로 자성이 없지만 스핀들이 번갈아가며 배치
- 반자성 (diamagnetism) - 외부 자기장에 반대방향으로 약한 자성

강자성
Ferromagnetic

반강자성
Antiferromagnetic

Ising model

$$H(\sigma) = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j,$$

*스핀 σ_i 는 +1 (up) 또는 -1 (down)

이웃한 두 스핀 i, j의 상호작용 에너지

외부 자기장과 스핀들의 상호작용 에너지

- $J_{ij} > 0$ 인 경우: 스핀 i, j가 같은 방향일 때 $J_{ij}\sigma_i\sigma_j < 0$ 이므로 안정적 ⇨ Ferromagnetic
- $J_{ij} < 0$ 인 경우: 스핀 i, j가 다른 방향일 때 $J_{ij}\sigma_i\sigma_j < 0$ 이므로 안정적 ⇨ Antiferromagnetic

Digital quantum simulation

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시뮬레이션 할 H의 time evolution을 양자 게이트들로 구현.

$$H = -J\sum_{i=0}^{N-2} Z_i Z_{i+1} - h\sum_{i=0}^{N-1} X_i, \qquad \text{(Ising model)}$$

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

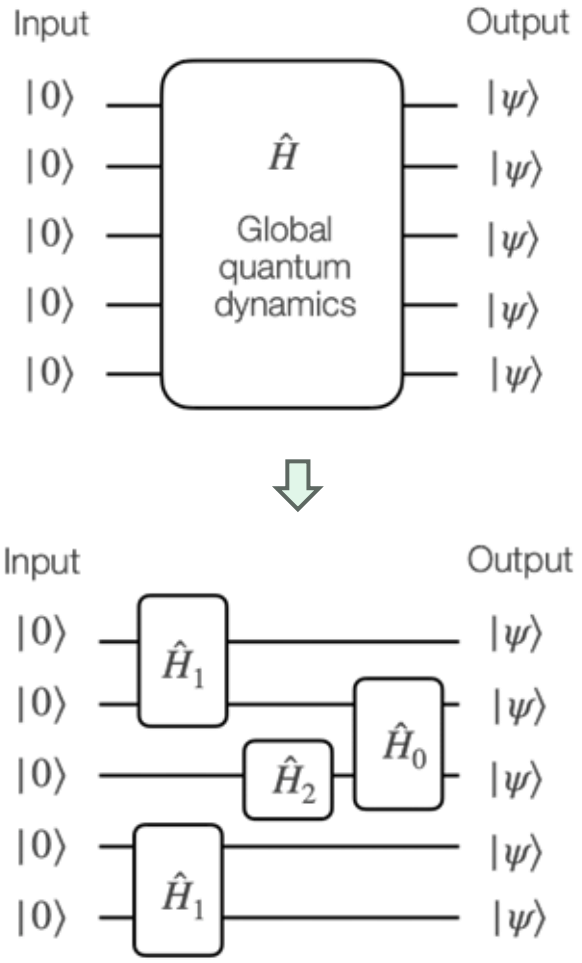
X-회전 게이트와 Z-회전 게이트를 순차적으로 걸면 될 것 같다.
하지만 H가 행렬일 때는 일반적으로

$$e^{-i(H_1+H_2)t} = e^{-iH_1 t}e^{-iH_2 t}$$

가 성립하지 않음. 단순히 X를 걸고 Z를 거는 걸로는 안 됨.
대신, 작은 시간 스텝 $\Delta t = T/r$을 잡고,

$$e^{-i\sum_j H_j} \approx \left(\prod_j e^{-iH_j \Delta t}\right)^r$$

와 같이 X와 Z의 작은 회전 번갈아가며 r번 걸어주면 근사적으로 같은 operation을 얻을 수 있음. ⇒ "Trotterization"



Review: Hamiltonian and time evolution

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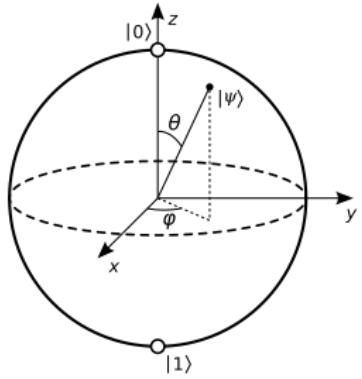
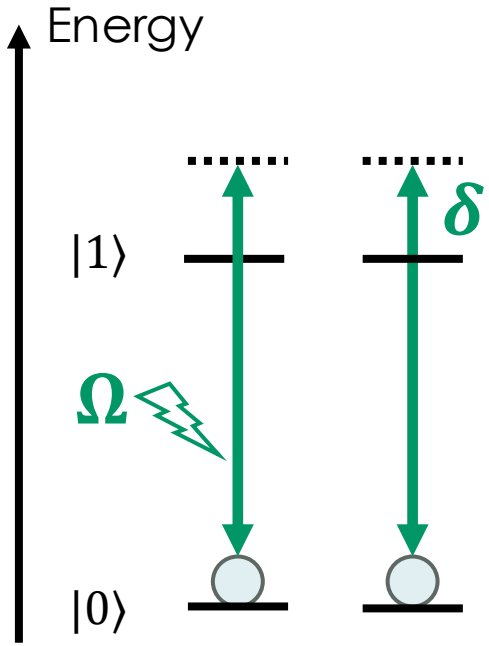


Neutral atom system Hamiltonian



$$\hat{\mathcal{H}} = \hbar \sum_{i=1}^{N} \left(\frac{\Omega}{2} \hat{\sigma}_i^x - \delta\, \hat{n}_i \right) + \sum_{i<j} \frac{C_6}{|\mathbf{r}_i - \mathbf{r}_j|^6} \hat{n}_i \hat{n}_j$$

X-rotation | Z-rotation | Interaction

Ω: Rabi frequency (~ laser amplitude)

$\hat{n}_i$: 0=ground, 1=excited

δ: Detuning (~ laser frequency offset)

Analog quantum computing

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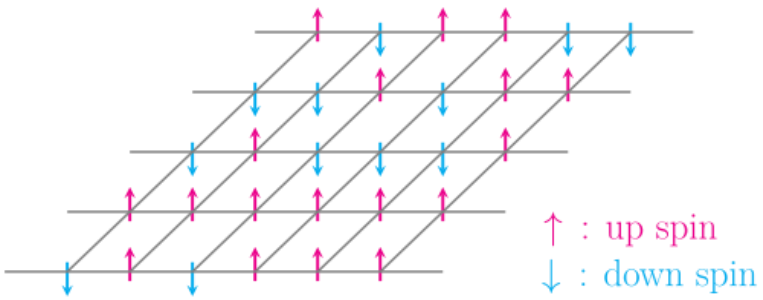


e.g. Ising model /
Antiferromagnetic state

Transverse field

Ising couplings: $J_{ij} \propto 1/R_{ij}^6$

$$\mathcal{H}(t) = \sum_i \left(\frac{\hbar\Omega(t)}{2}\sigma_i^x - \hbar\delta(t)\hat{n}_i + \sum_{j<i} \frac{C_6}{(R_{ij})^6}\hat{n}_i\hat{n}_j \right)$$

$$\hat{n}_i = \frac{1+\sigma_i^z}{2}$$

Quantum Simulation

Permits the simulation of quantum many-body systems far beyond the limits of classical computers, allowing, for example, the:

- Observation of out-of-equilibrium dynamics
- Adiabatic preparation of ground states

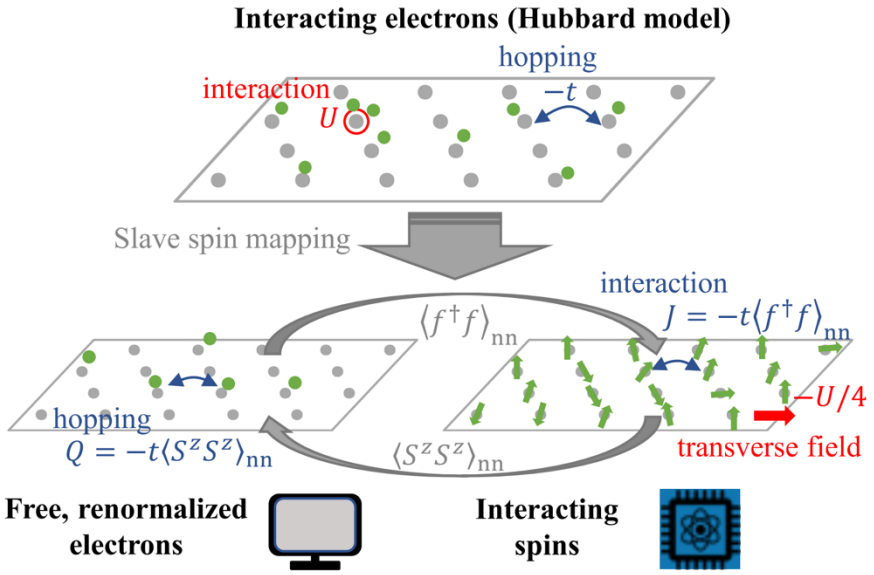
Quantum-classical simulation of fermionic spin system

Pasqal

Hubbard physics with Rydberg atoms: using a quantum spin simulator to simulate strong fermionic correlations

Antoine Michel,[1,2,*] Loïc Henriet,[3] Christophe Domain,[1] Antoine Browaeys,[2] and Thomas Ayral[4]

[1] *Electricité de France, EDF Recherche et Développement, Département Matériaux et Mécanique des Composants, Les Renardières, F-77250 Moret sur Loing, France*
[2] *Université Paris-Saclay, Institut d'Optique Graduate School, CNRS, Laboratoire Charles Fabry, F-91127 Palaiseau Cedex, France*
[3] *PASQAL, 7 rue Léonard de Vinci, F-91300 Massy, France*
[4] *Eviden Quantum Laboratory, Les Clayes-sous-Bois, France*



The electrons are under

- Fermionic interaction: hopping to next sites with a probability
- Ising interaction

둘 다 고려해서 정확히 계산하는 것은 매우 어려움.
특히 Ising interaction의 계산량이 매우 많음.

Ising interaction 계산만 분리해서 양자컴퓨터로 하는 방법을 제안하고 numerical하게 확인.

Quantum-classical simulation of fermionic spin system

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원래 해밀토니안

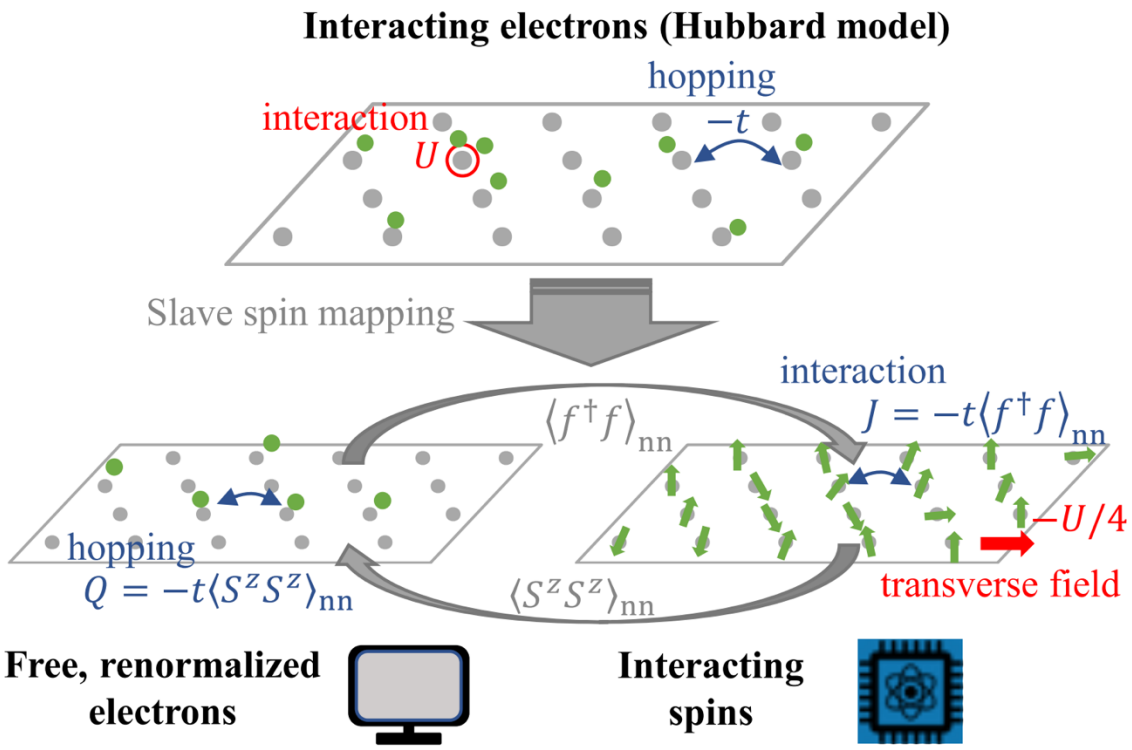
$$H_{\text{Hubbard}} = \sum_{i,j,\sigma} t_{ij} d^{\dagger}_{i\sigma} d_{j\sigma} + \frac{U}{2} \sum_{i} (n^{d}_{i} - 1)^2$$

Mean field approximation을 적용해
Fermionic hamiltonian과 Ising hamiltonian을 분리.

$$H_{\text{f}} = \sum_{i,j,\sigma} Q_{ij} f^{\dagger}_{i,\sigma} f_{j,\sigma} \quad \text{(Fermionic Hamiltonian)}$$

$$H_{\text{s}} = \sum_{i,j} J_{ij} S^{z}_{i} S^{z}_{j} + \frac{U}{4} \sum_{i} S^{x}_{i} \quad \text{(Ising Hamiltonian)}$$

with $Q_{ij} = t_{ij} \langle S^{z}_{i} S^{z}_{j} \rangle$ and $J_{ij} = \sum_{\sigma} t_{ij} \langle f^{\dagger}_{i,\sigma} f_{j,\sigma} \rangle$



그리고 고전컴퓨터로 H_f를, 양자컴퓨터로 H_s를 계산.

Quantum simulation: 256-qubit real material simulation

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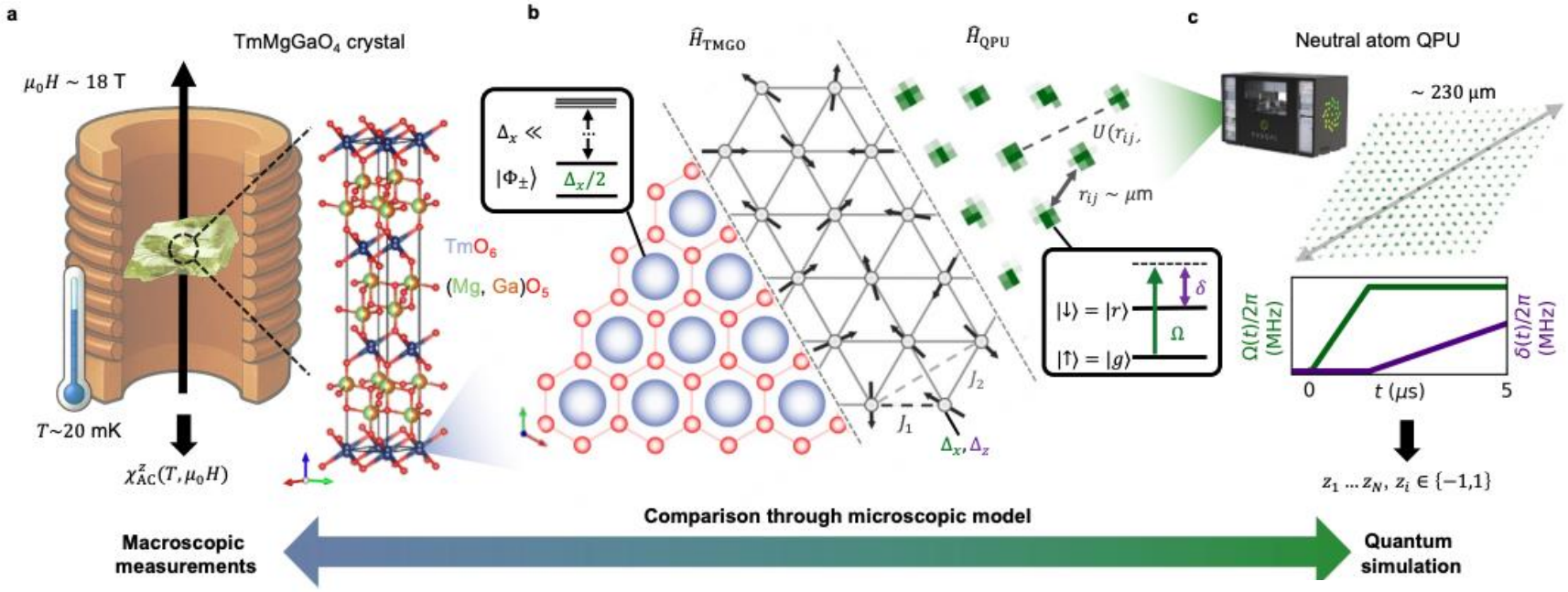
Direct quantum simulation of magnetic material: Theory ↔ Experiment ↔ QPU



- Magnetic material $TmMgGaO_4$
- 2d triangular spin lattice → frustration
- Phase transition by external B-field

$$\frac{\hat{H}_{\mathrm{TMGO}}}{\hbar} = J_1 \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z + \sum_{i=1}^{N} (\Delta_x \hat{\sigma}_i^x - \Delta_z \hat{\sigma}_i^z)$$

$$\hat{H}_{\mathrm{QPU}} = \sum_{i<j} U_{ij} \hat{n}_i \hat{n}_j + \frac{\hbar\Omega(t)}{2} \sum_i \hat{\sigma}_i^x - \hbar\delta(t) \sum_i \hat{n}_i$$

$$\hat{H}_{\mathrm{QPU}} \approx \alpha_{\mathrm{QPU}} \hat{H}_{\mathrm{TMGO}} \text{ with } \alpha_{\mathrm{QPU}} \approx 1.5 \times 10^{-5}$$

Quantum simulation: 256-qubit real material simulation

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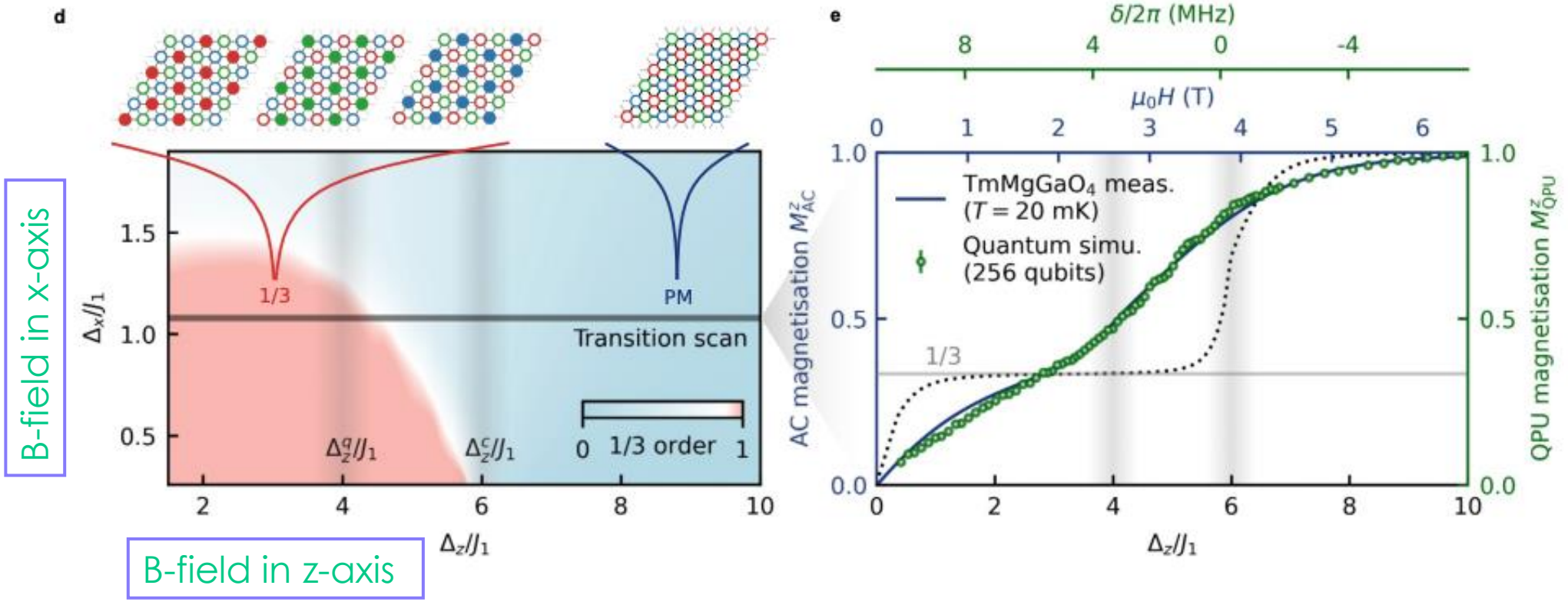
Phase transition by external B-fields in x & z axis



"QPU result well matches experimental measurement!"

256-qubit quantum simulation with real material

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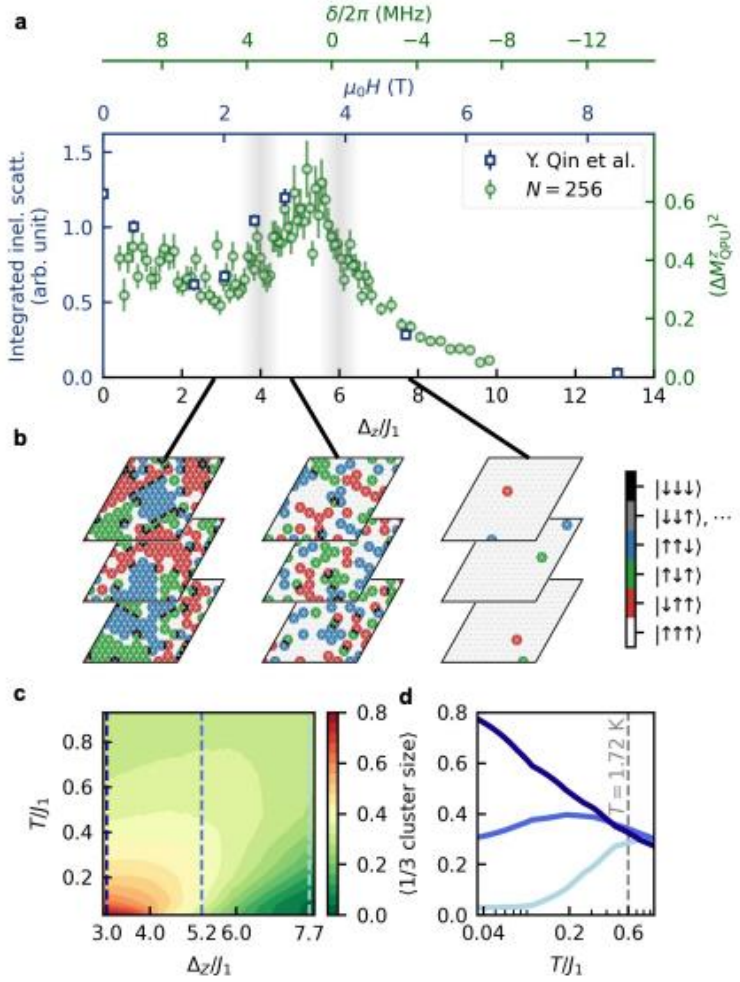
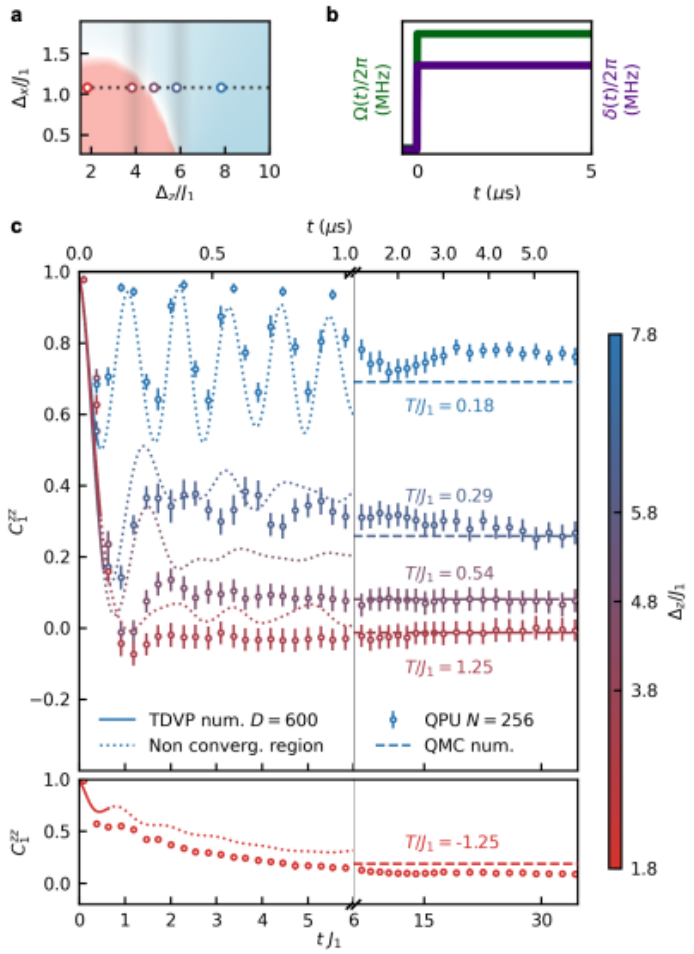
Quantum fluctuation & 1/3 order vs. B_z



Post-quench dynamics



Pulser studio: Antiferromagetic state

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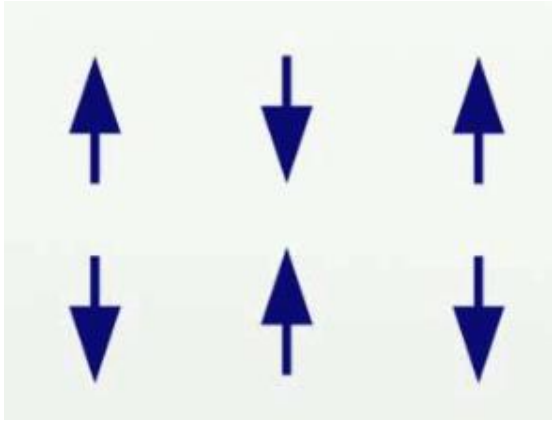

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Pasqal 클라우드

Cloud User Portal

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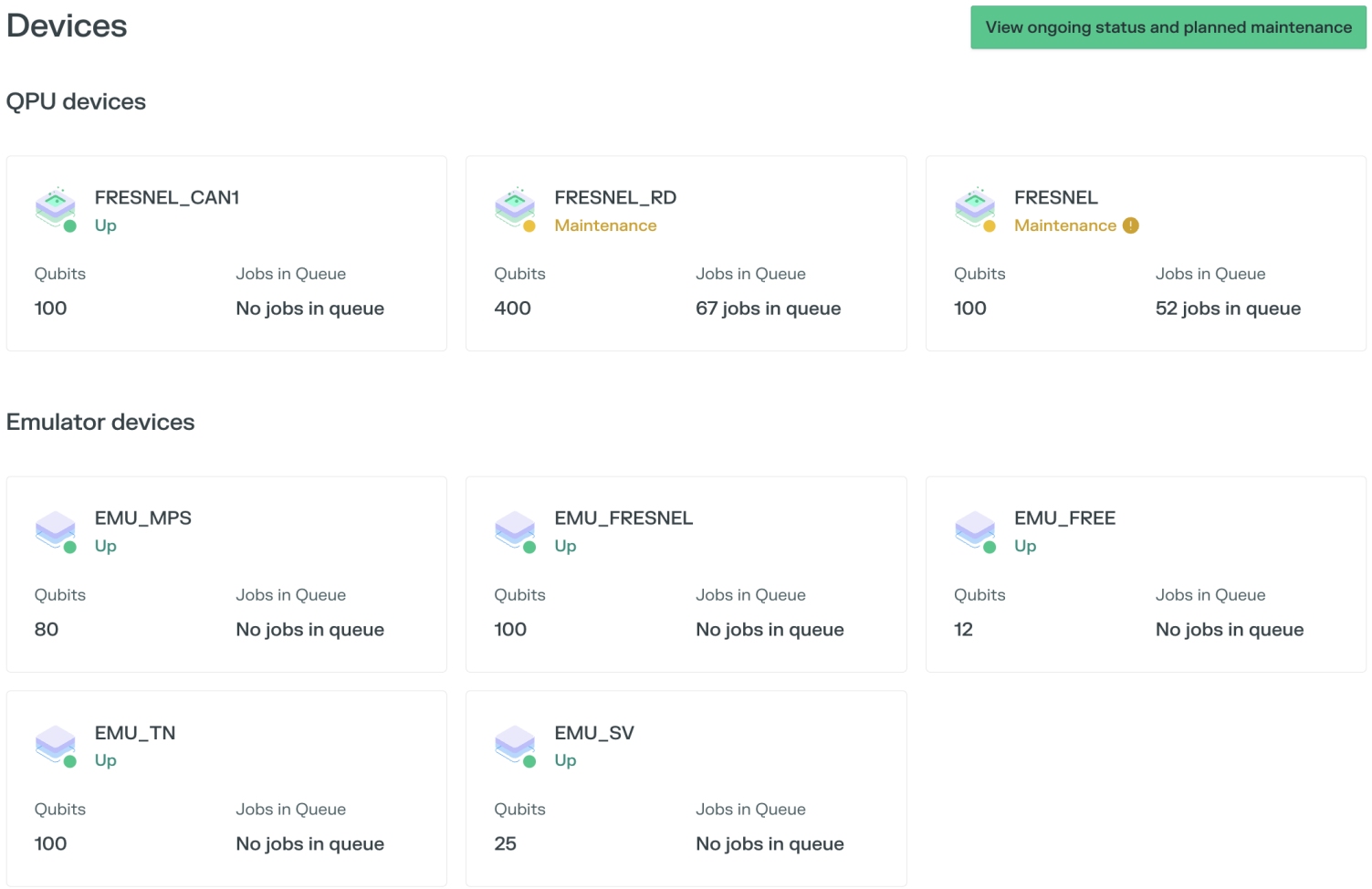
portal.pasqal.cloud

- Dashboard
- Devices
- Batches/Jobs



Pasqal Cloud Offers

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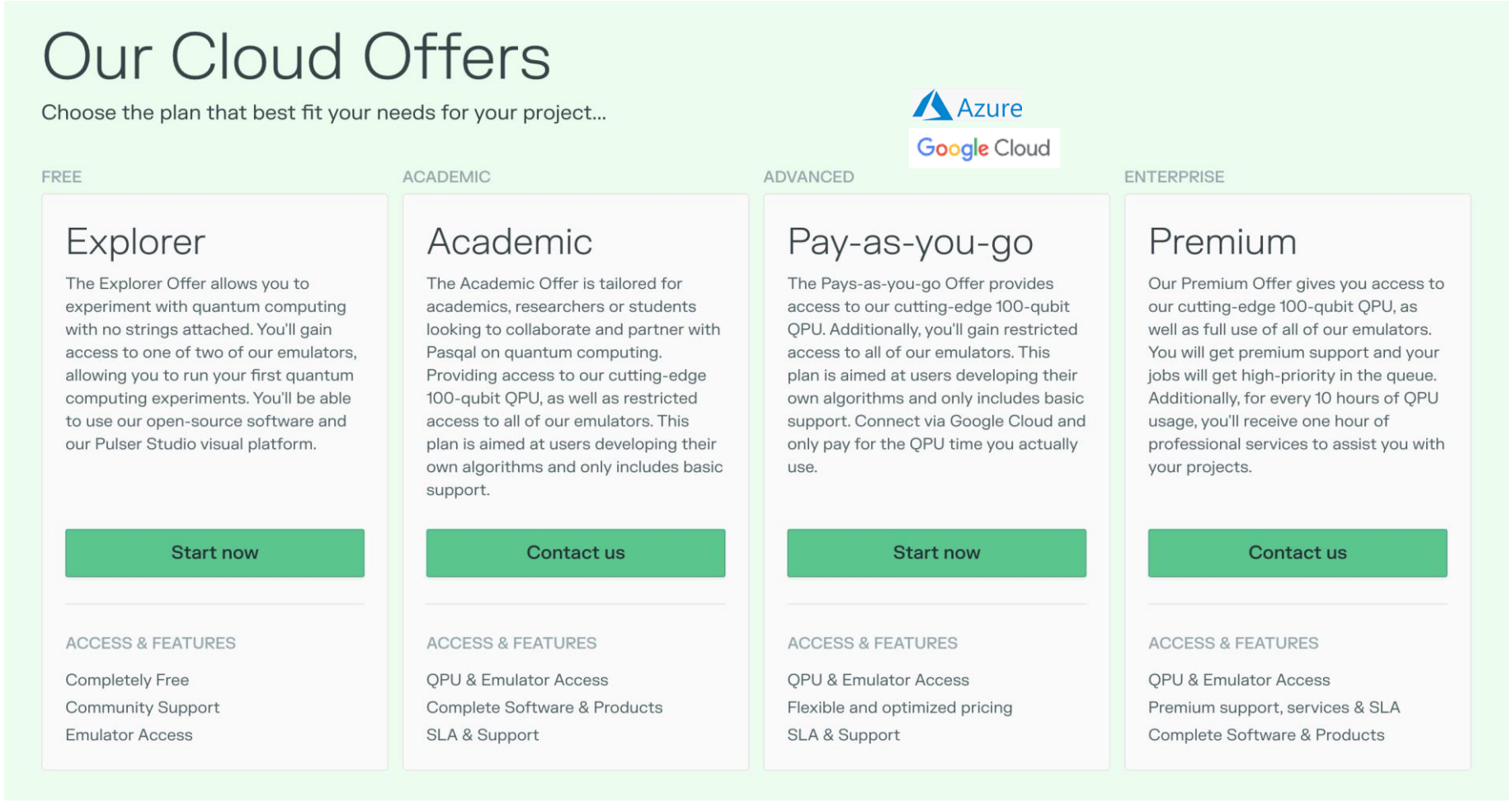

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실습: Antiferromagnetism simulation with Pulser

Hands-on: Antiferromagnetic state

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Adiabatic preparation of an Anti-Ferromagnetic State

Let's now program the Ising Hamiltonian such that a set of 9 atoms initially in the ground state $|ggggggggg\rangle$ are prepared in an antiferromagnetic state $|rgrgrgrgr\rangle$.

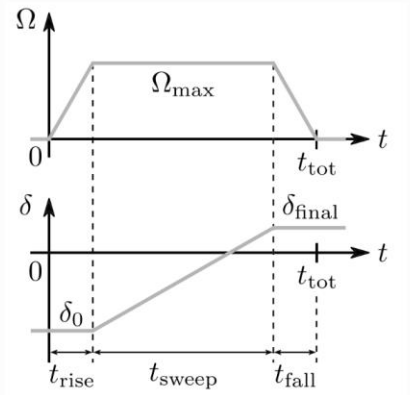
To reach the desired antiferromagentic state, we can take advantage of the adiabatic theorem. The idea is to use a time-dependent Hamiltonian that changes slowly so that the system stays in its ground state. Therefore, we must choose a final Hamiltonian that has the antiferromagnetic state as its ground state.

This final Hamiltonian should simultaneously favor having the largest number of atoms in the $|r\rangle$ state (by having $\delta > 0$) and discourage nearest neighbors from being both in $|r\rangle$ (via the interaction Hamiltonian). When these contributions are appropriately balanced, we get an Hamiltonian with $|rgrgrgrgr\rangle$ as its ground state.

Let's follow the protocol from this paper, where we define the parameters with respect to the interaction strength between nearest neighbours, U (see Table 1 of the paper):

$$
\begin{aligned}
U &= 2\pi\ rad/\mu s \\
\Omega_{max} &= 2U \\
\delta_0 &= -6U \\
\delta_f &= 2U \\
t_{rise} = 252\ ns,\ t_{fall} &= 500\ ns \\
t_{sweep} &= \frac{\delta_f - \delta_0 [rad \cdot \mu s^{-1}]}{2\pi \cdot 10\ [rad \cdot \mu s^{-2}]}
\end{aligned}
$$

and define $\Omega(t)$ and $\delta(t)$ over time as (see Figure 1 (b)):



Any questions?

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