Quantum computing for nuclear physics

Part 2: Applications to nuclear physics

REYES Mentoring Program
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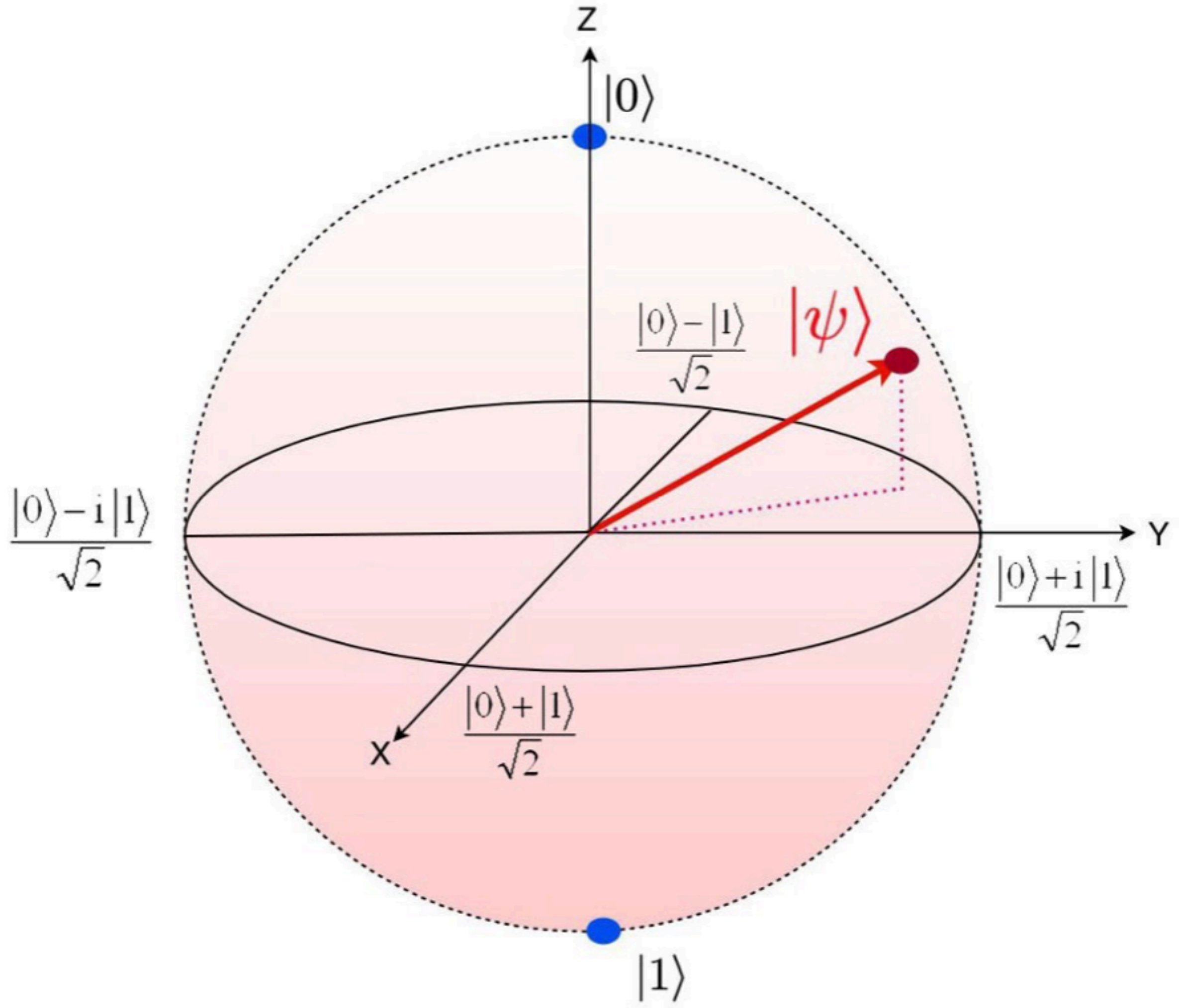
Recap

Quantum bit (qubit): $|\psi\rangle = a_0|0\rangle + a_1|1\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$



When we measure the state $|\psi\rangle$, we obtain either:

- State $|0\rangle$, with a probability $|a_0|^2$
- State $|1\rangle$, with a probability $|a_1|^2$

For N qubits, there are 2^N amplitudes

e.g. $|\psi\rangle = a_1|000\rangle + a_2|001\rangle + a_3|010\rangle + a_4|011\rangle + a_5|100\rangle + a_6|101\rangle + a_7|110\rangle + a_8|111\rangle$

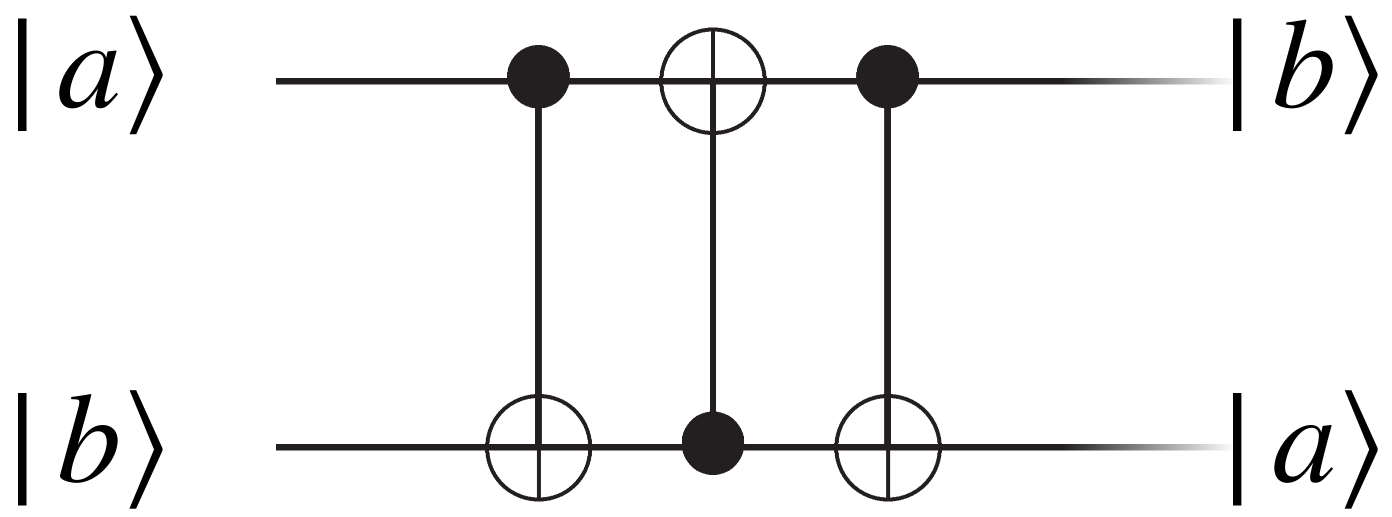
A quantum operation modifies all of these 2^N amplitudes simultaneously!

$$|a\rangle = \sum_{i=1}^{2^N} a_i|\psi_i\rangle \rightarrow |b\rangle = \sum_{i=1}^{2^N} b_i|\psi_i\rangle$$

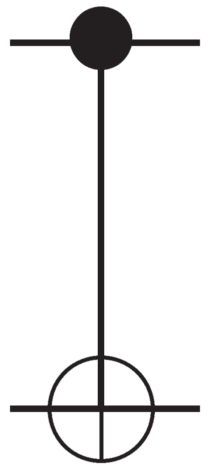
Quantum circuits

Nothing more than (clever) unitary matrix multiplications!

Example: SWAP circuit



where



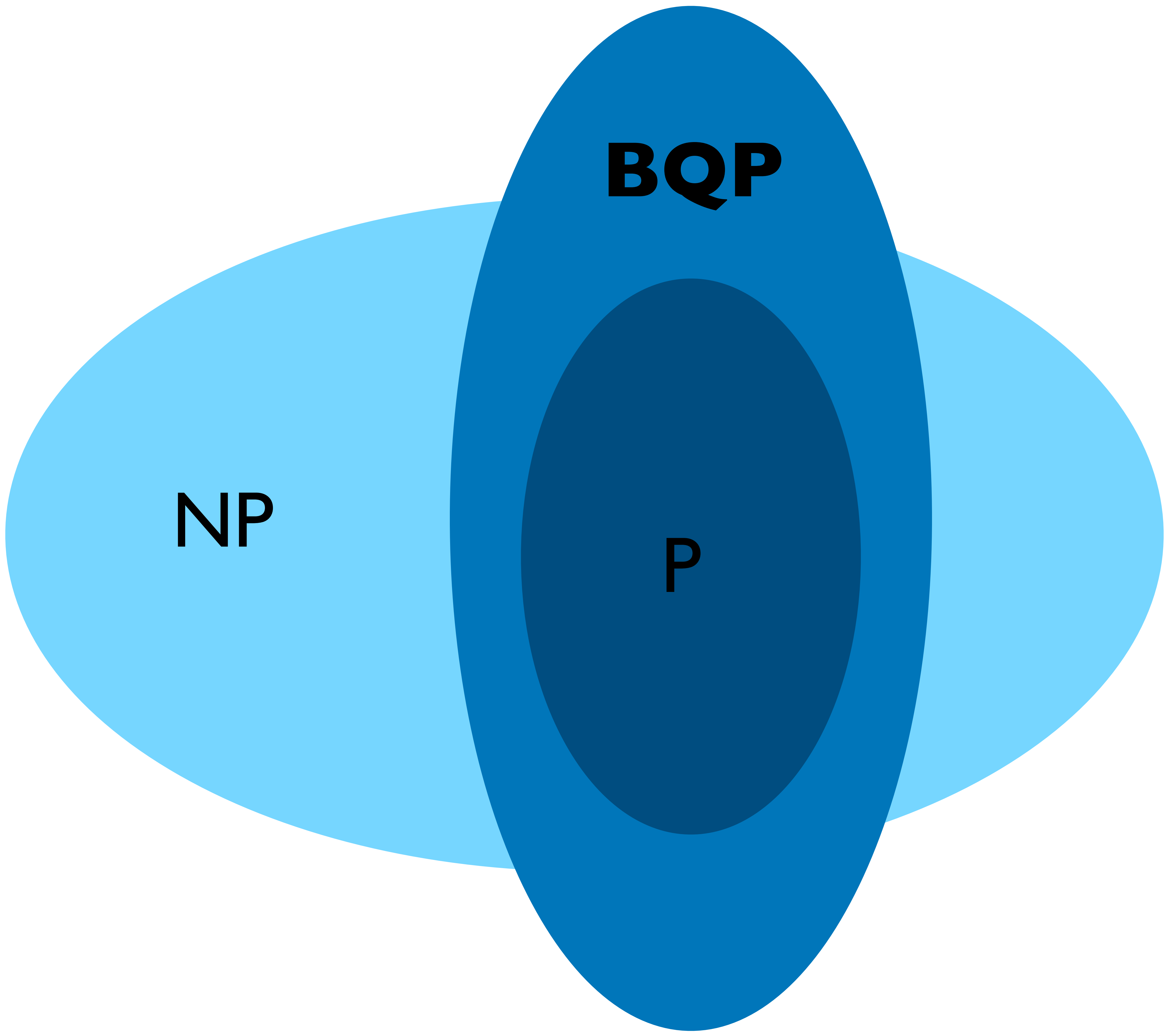
$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

CNOT gate

$$SWAP\left(|a\rangle \otimes |b\rangle\right) = CNOT_{0,1} \times CNOT_{1,0} \times CNOT_{0,1} \times \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \otimes \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix} = \begin{pmatrix} b_0 a_0 \\ b_0 a_1 \\ b_1 a_0 \\ b_1 a_1 \end{pmatrix} = |b\rangle \otimes |a\rangle$$

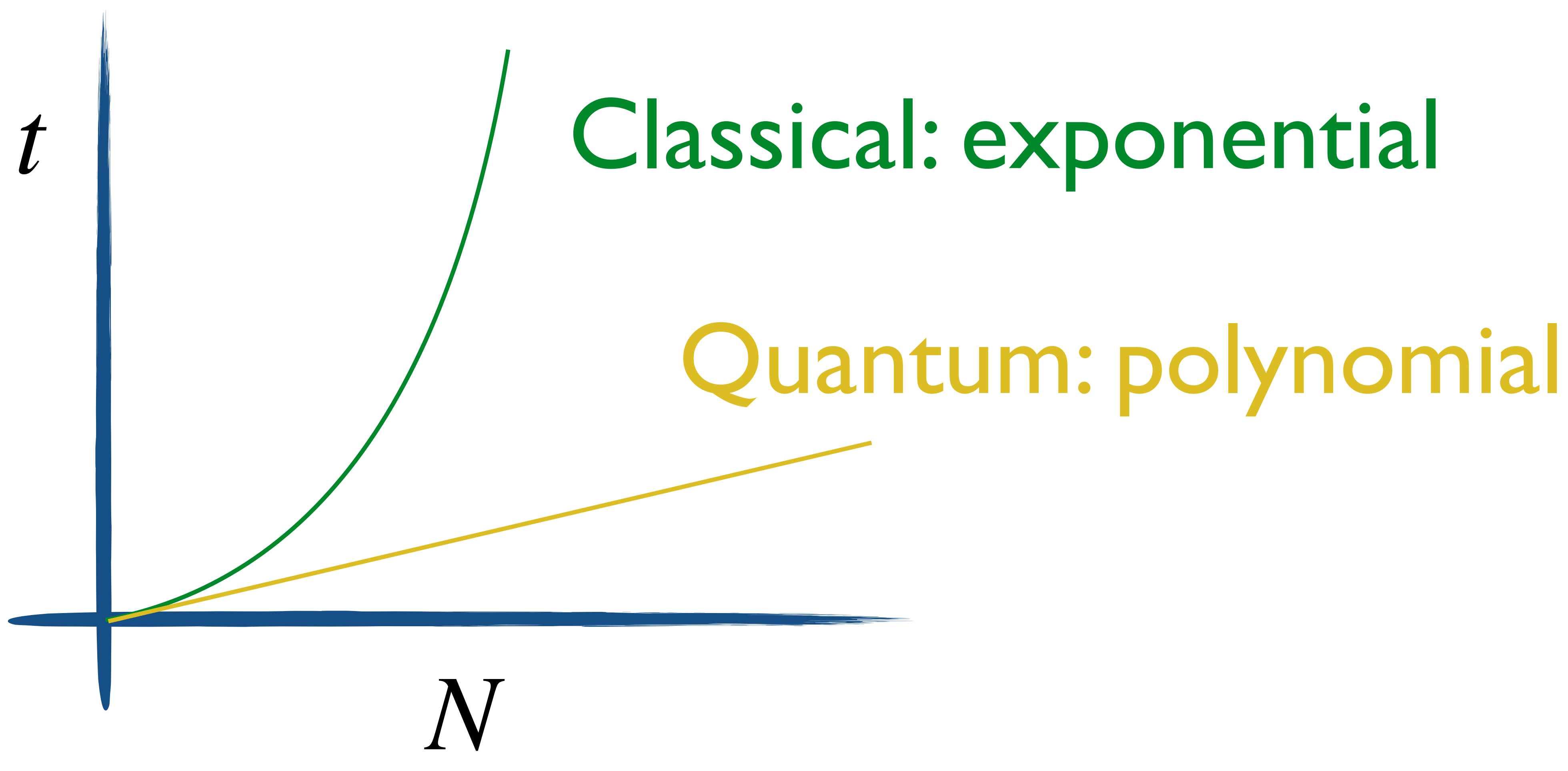
QC can solve *some* classically hard problems



P: Polynomial-time solution on classical computer

NP: Polynomial-time verification on classical computer

BQP: Polynomial-time solution on quantum computer



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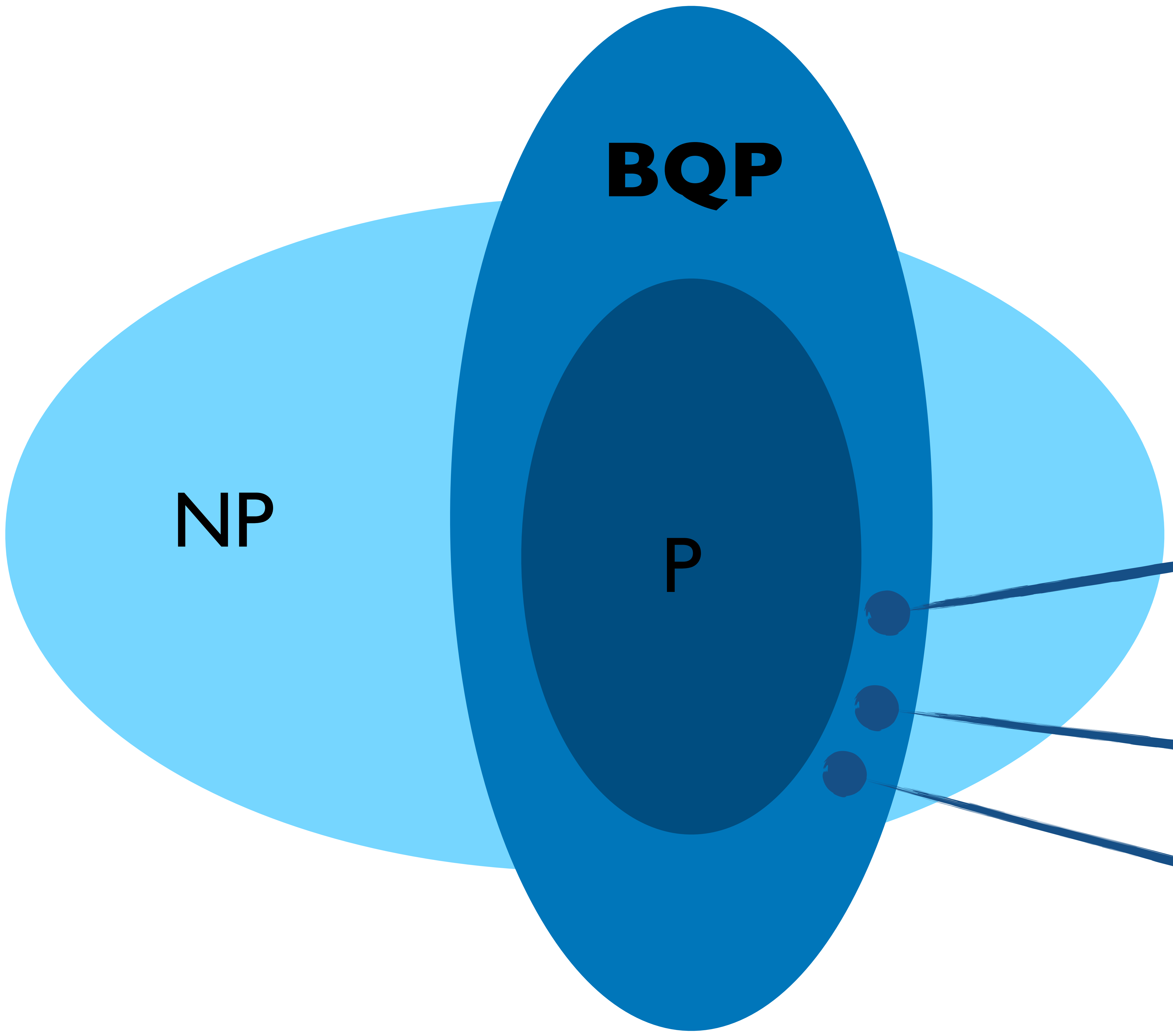


Dynamics of many-body non-relativistic quantum system

Feynman (1982), Lloyd (1996)

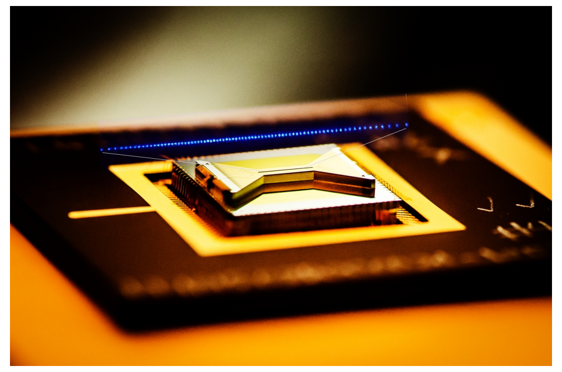
Scattering in scalar field theory

Jordan, Lee, Preskill (2012-2018)

QCD?

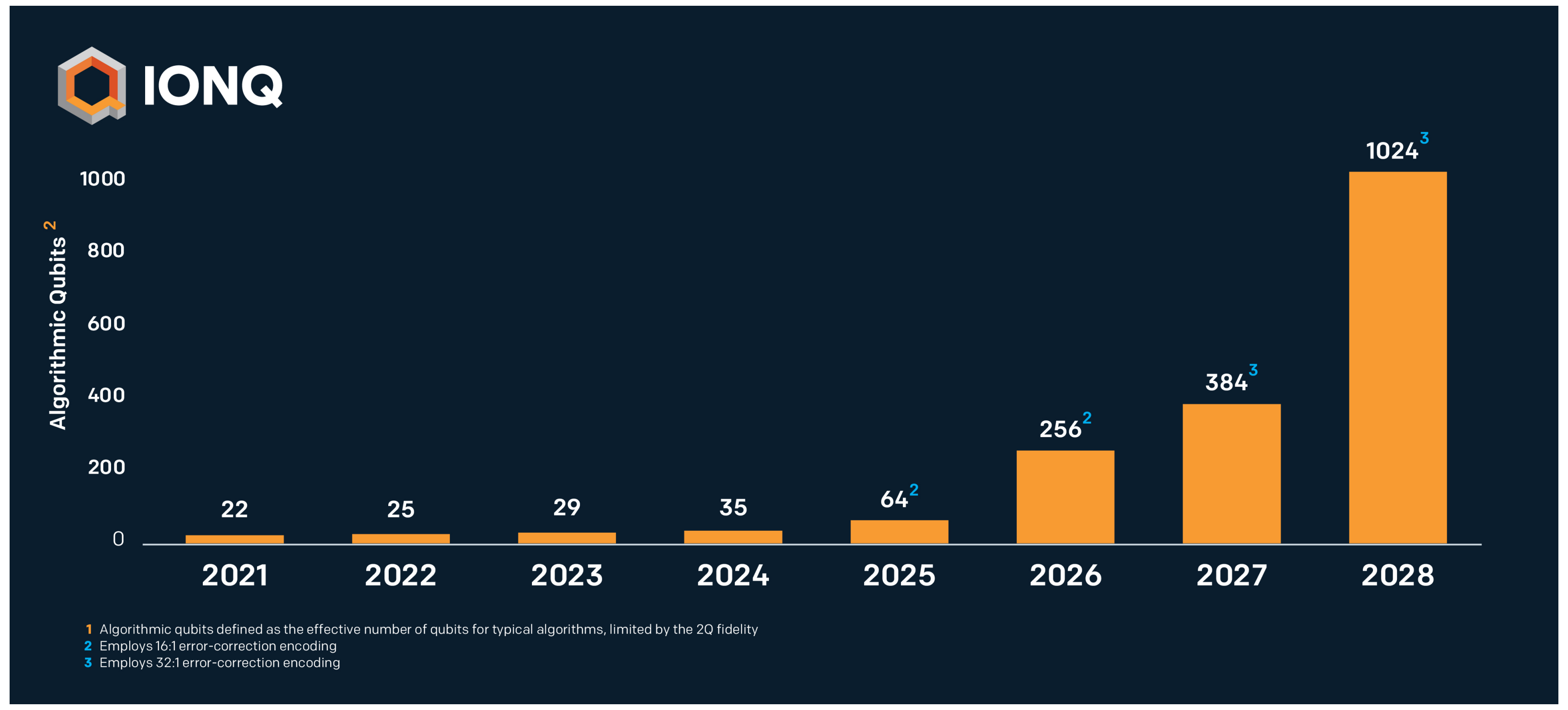
Preskill (2018), Klco, Savage (2018), Muschik et al. (2016), Davoudi et al. (2019), …

Current quantum devices



Few qubits

Current devices are limited to $\mathcal{O}(10) - \mathcal{O}(100)$ qubits

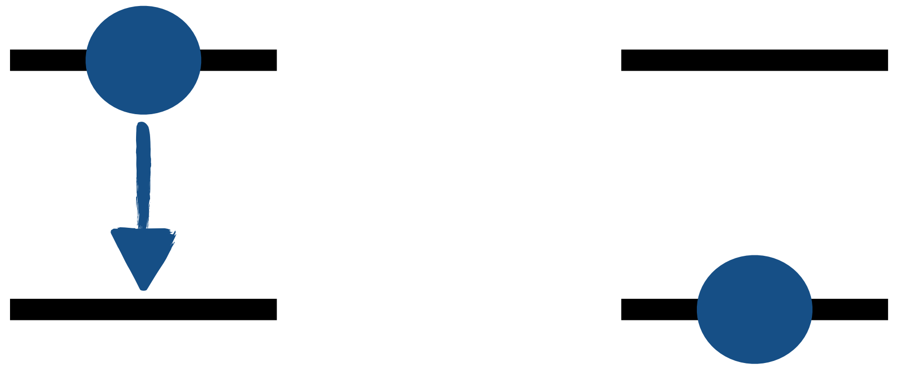


Need more qubits to achieve quantum advantage

Decoherence

The quantum state of a qubit is stable only for a limited time

T_1: decay time $|1\rangle \rightarrow |0\rangle$



T_2: dephasing time

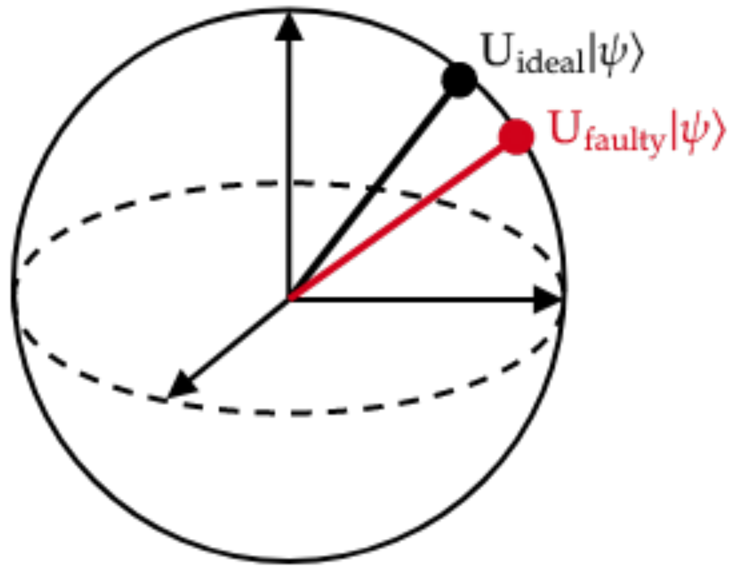
$$|1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

Need longer coherence times to increase the "gate depth" of circuits

Gate noise

Single- and two-qubit gate operations are imperfect

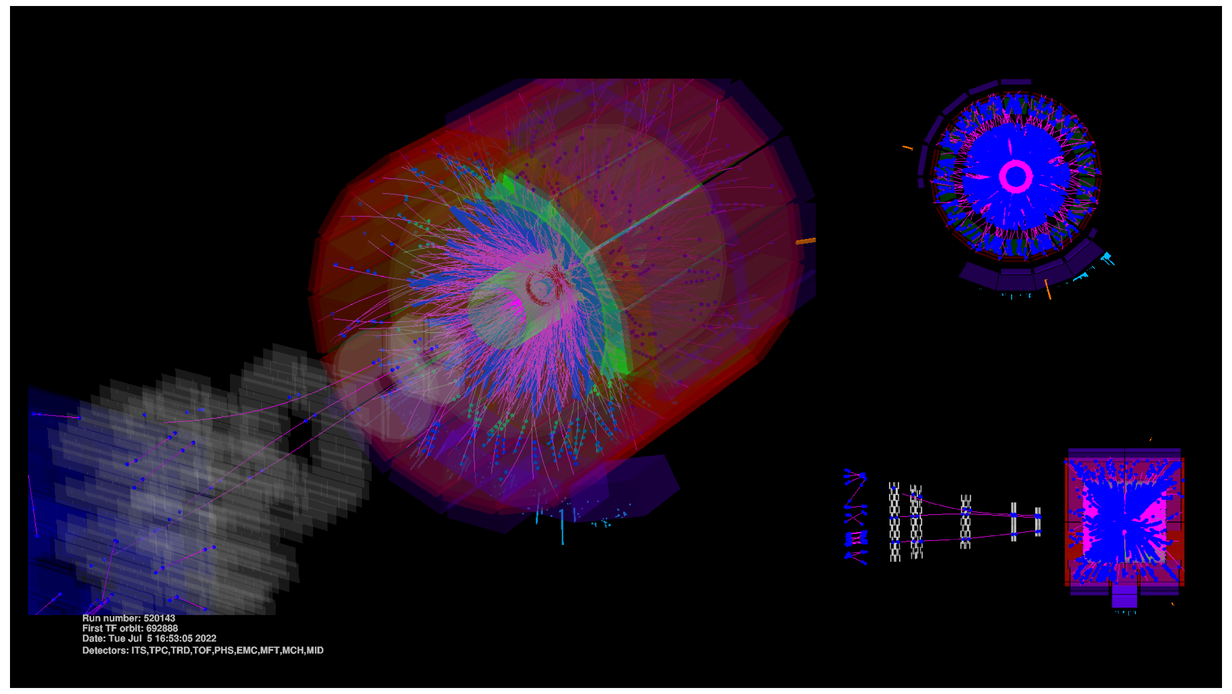
$$U_{\text{faulty}} = A\ U_{\text{ideal}}$$

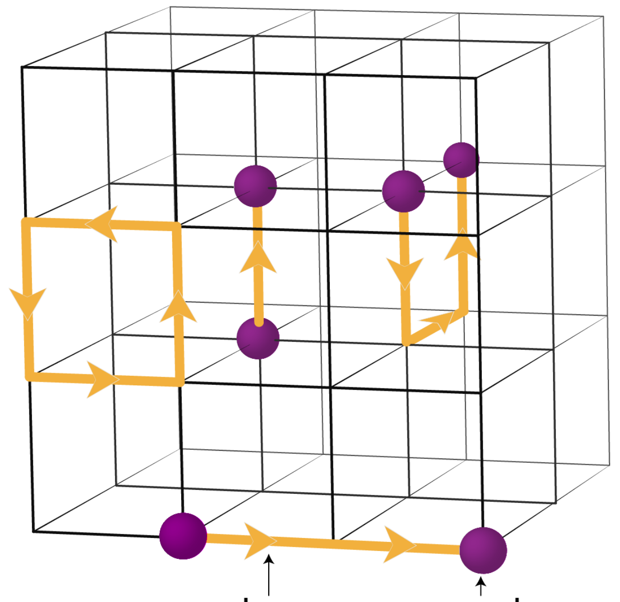


Need smaller gate noise to perform quantum error correction

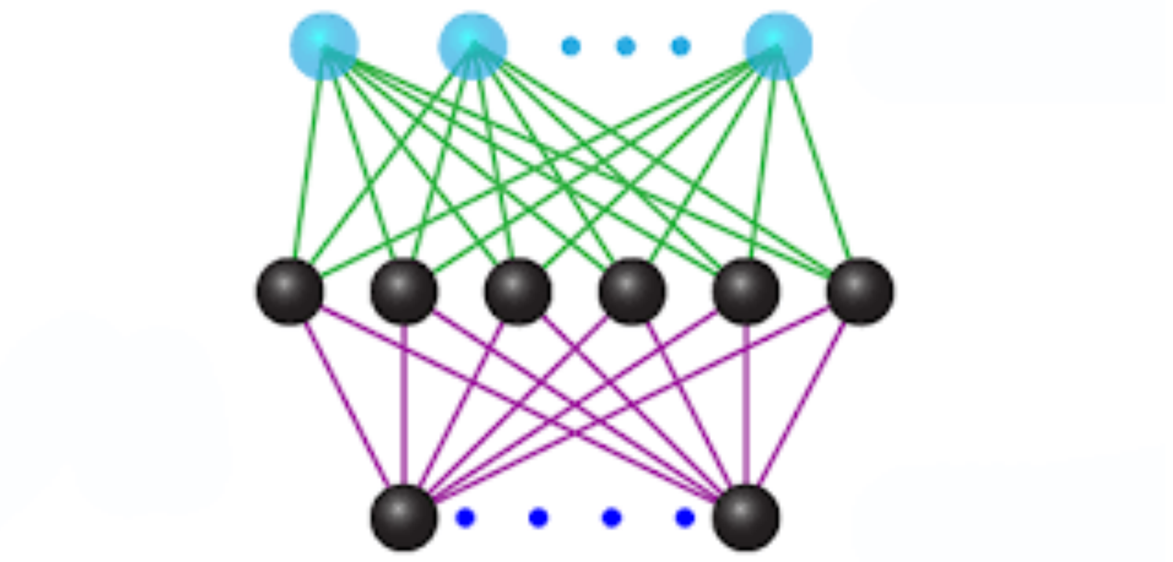
Future applications of quantum computers

Simulation of quantum field theory





Quantum machine learning



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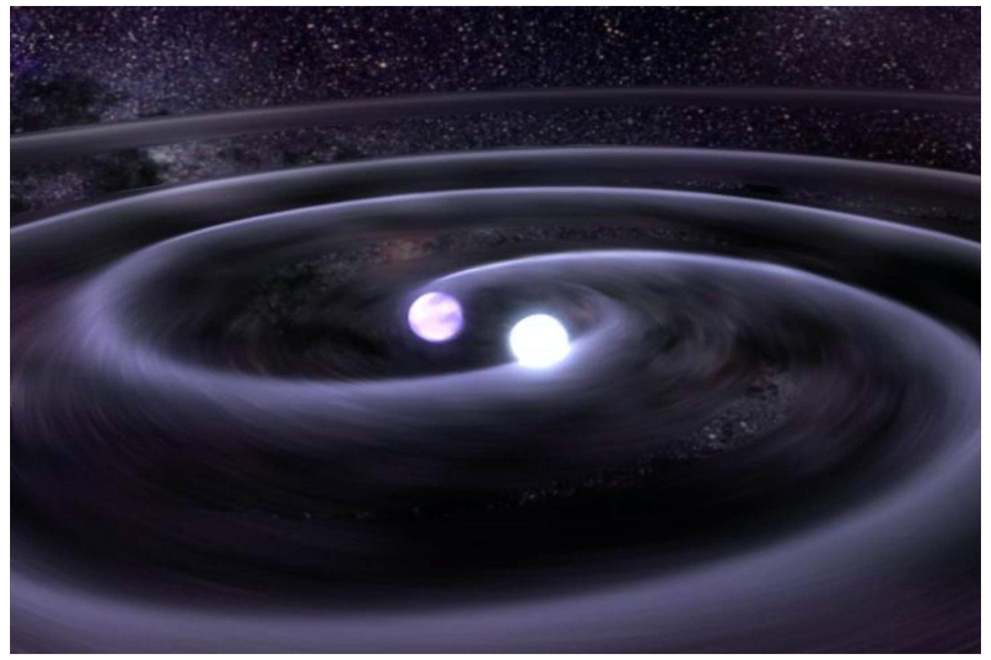
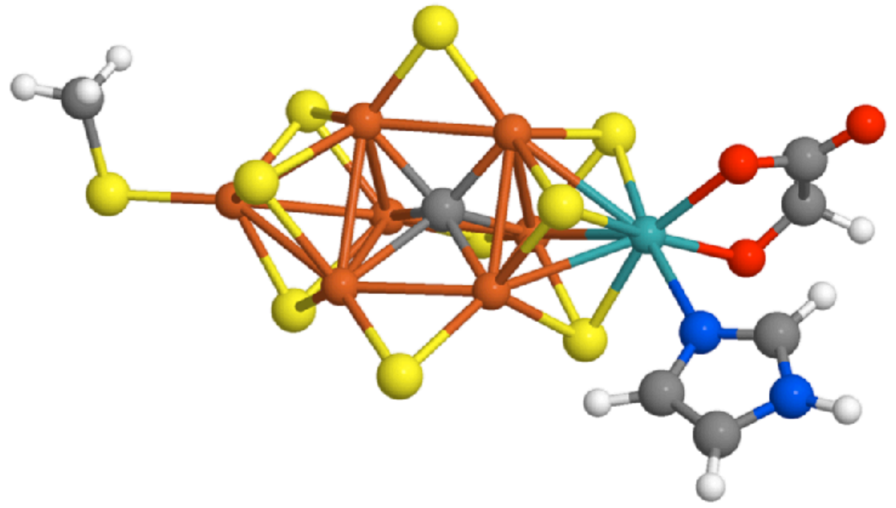
Dense nuclear matter



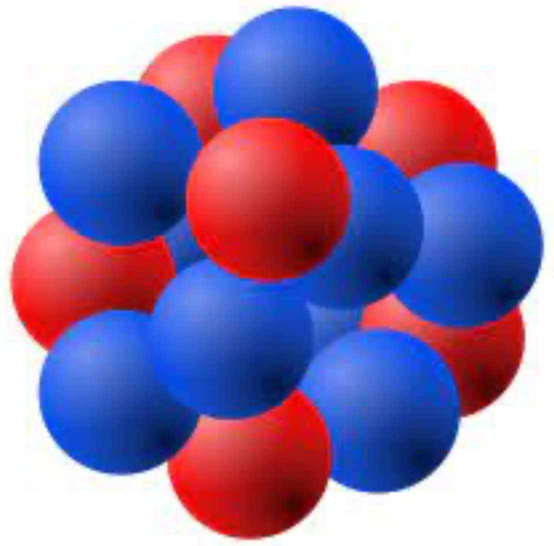
Molecular dynamics



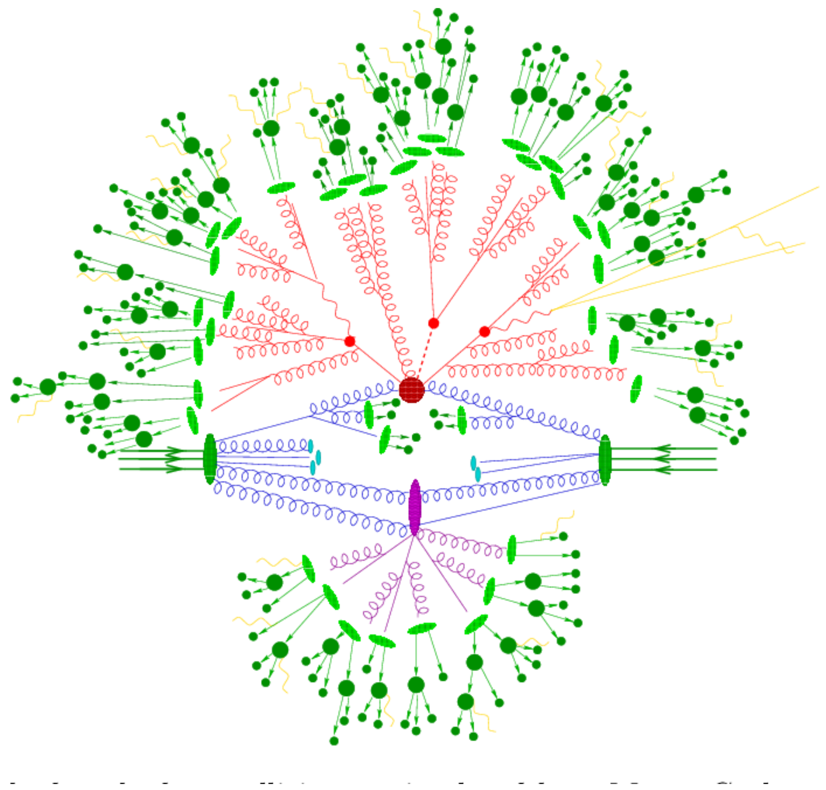
Cryptography

Outline

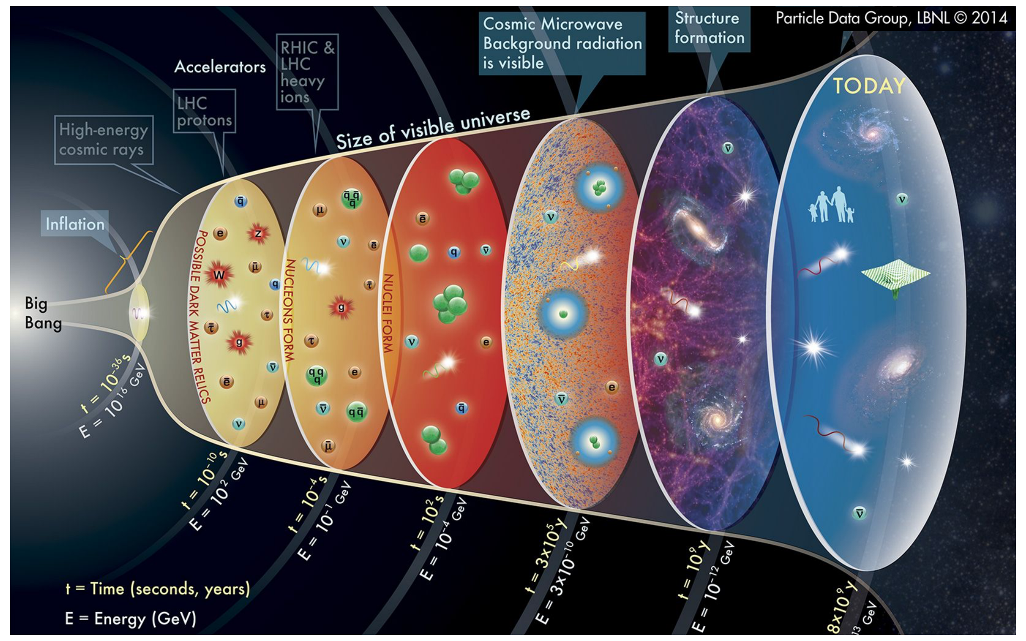
1. Many-body nuclear structure



2. Real-time dynamics of scattering and hadronization



3. High-temperature/density QCD



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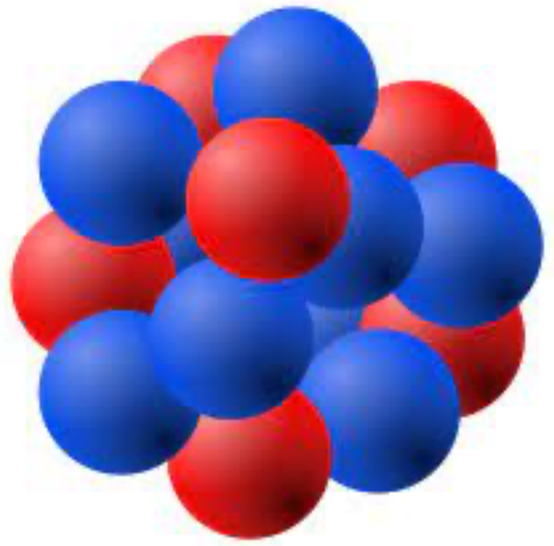
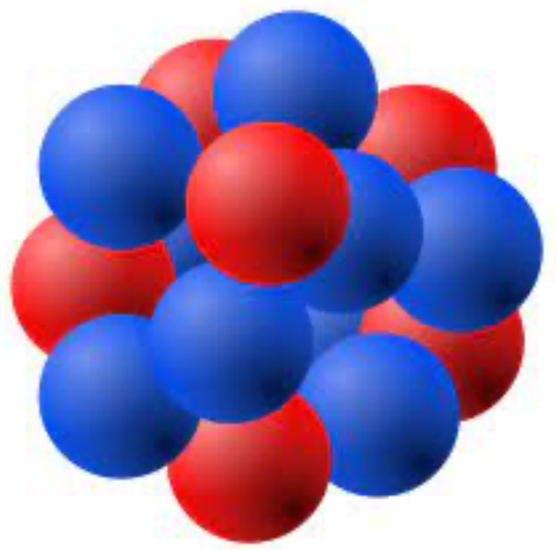


2. Real-time dynamics of scattering and hadronization

3. High-temperature/density QCD

Many-body nuclear physics

Nucleus of A nucleons can be described by a **Hamiltonian**

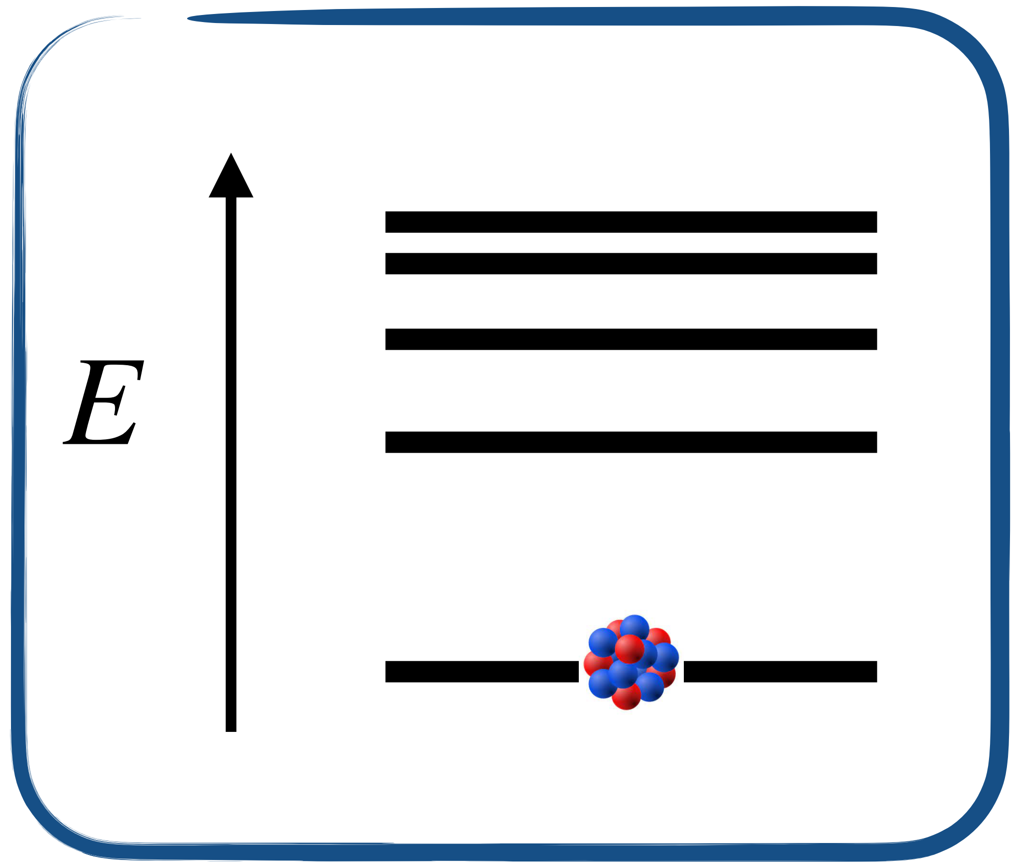


$$H = T + V$$

Kinetic energy — Potential energy

H encodes the ground state and excited state energies of the nucleus

$$H|\psi_0\rangle = E_0|\psi_0\rangle$$
$$H|\psi_1\rangle = E_1|\psi_1\rangle$$
$$\dots$$



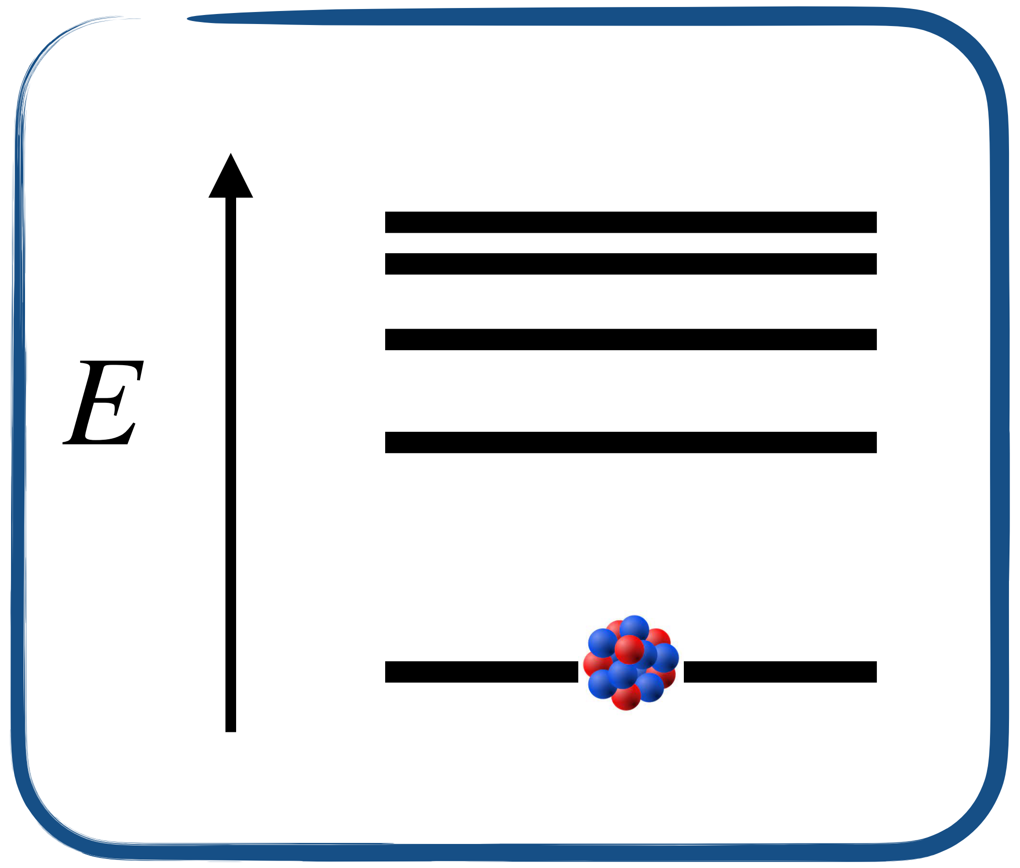
Goal: describe the quantum properties of large nuclei, such as the ground state energy

Variational principle

The expectation value of the Hamiltonian is always greater than or equal to its smallest eigenvalue:

$$E_{\text{trial}} = \langle \psi_{\text{trial}} | H | \psi_{\text{trial}} \rangle \geq E_0$$

where E_0 is the ground state energy of the system



We can use this to approximate the ground state energy:

1. Parameterize the wavefunction: $|\psi(\theta)\rangle$
2. Guess an initial set of parameters: $|\psi_{\text{trial}}\rangle = |\psi(\theta_{\text{trial}})\rangle$
3. Compute the energy of that wavefunction: $E_{\text{trial}} = \langle \psi_{\text{trial}} | H | \psi_{\text{trial}} \rangle$
4. Update our guess for the trial wavefunction parameters, and repeat!

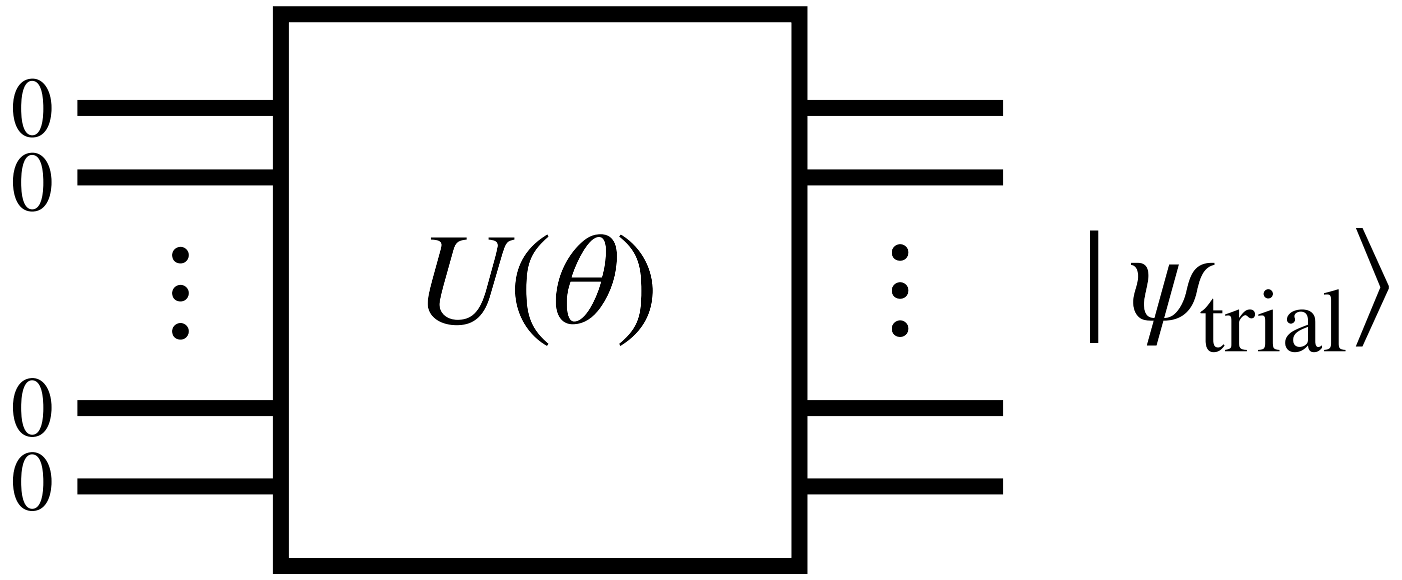
Variational Quantum Eigensolver

We can implement this in a **hybrid quantum-classical algorithm**

Quantum computer

Classical computer

Choose parameters θ_{trial} in a quantum circuit $U(\theta)$



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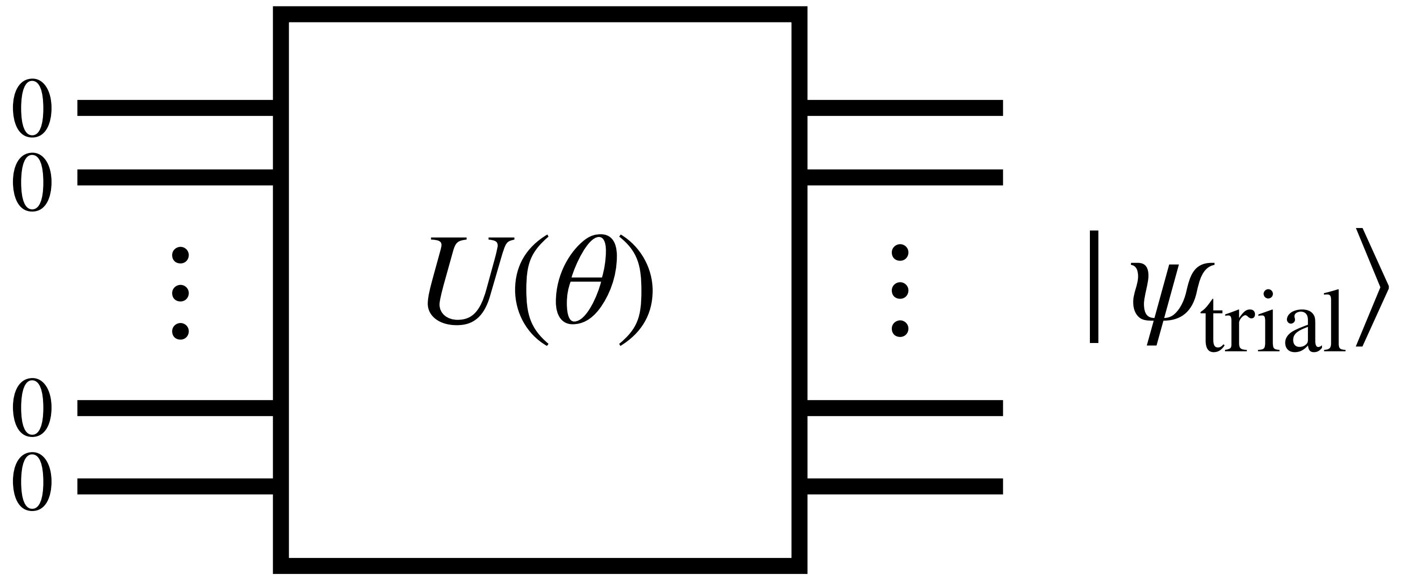
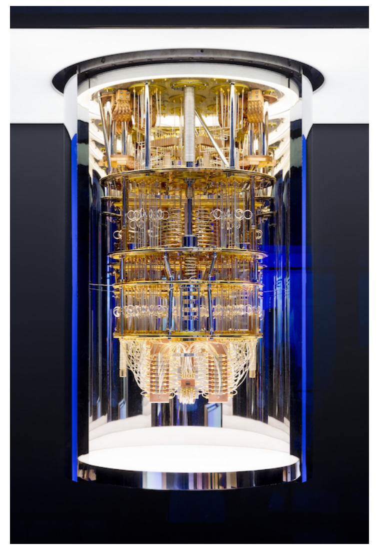
Choose parameters θ_{trial} in a quantum circuit $U(\theta)$

Initialize the trial wavefunction:
$$|\psi_{\text{trial}}\rangle = U(\theta)\,|0\cdots0\rangle$$





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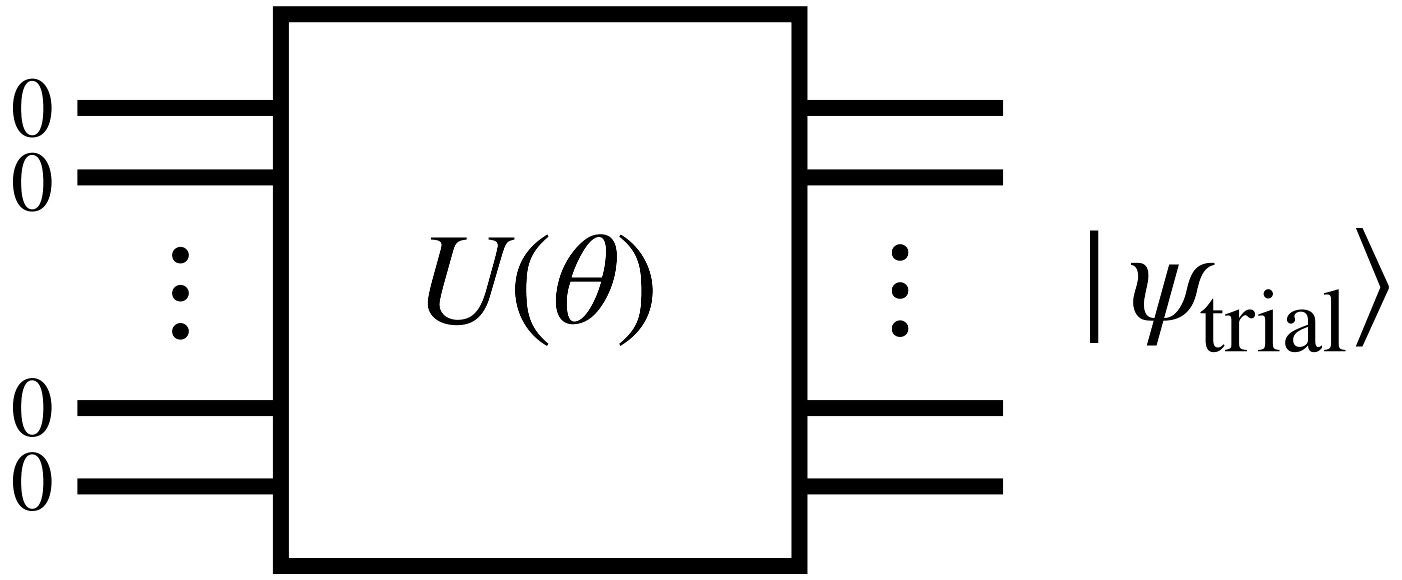
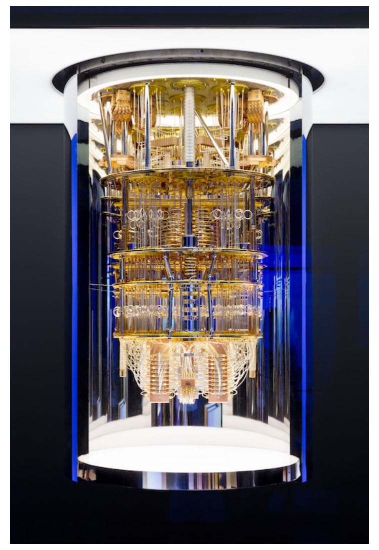


Measure the energy: $E_{\text{trial}} = \langle\psi_{\text{trial}}|H|\psi_{\text{trial}}\rangle$



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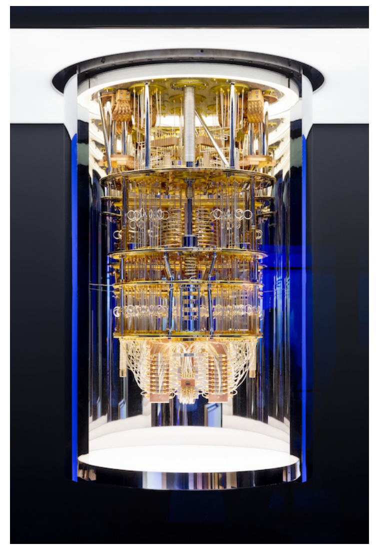
Compare E_{trial} to E_{min}

Classical optimizer (e.g. SPSA)



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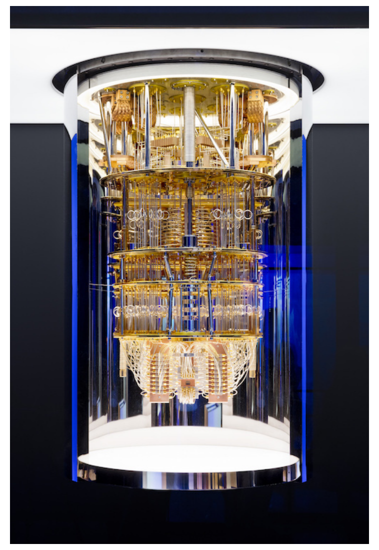


Note: Eigenvalues can also be found by the Quantum Phase Estimation algorithm

VQE for deuteron ground state energy

Hamiltonian obtained from **effective field theory**

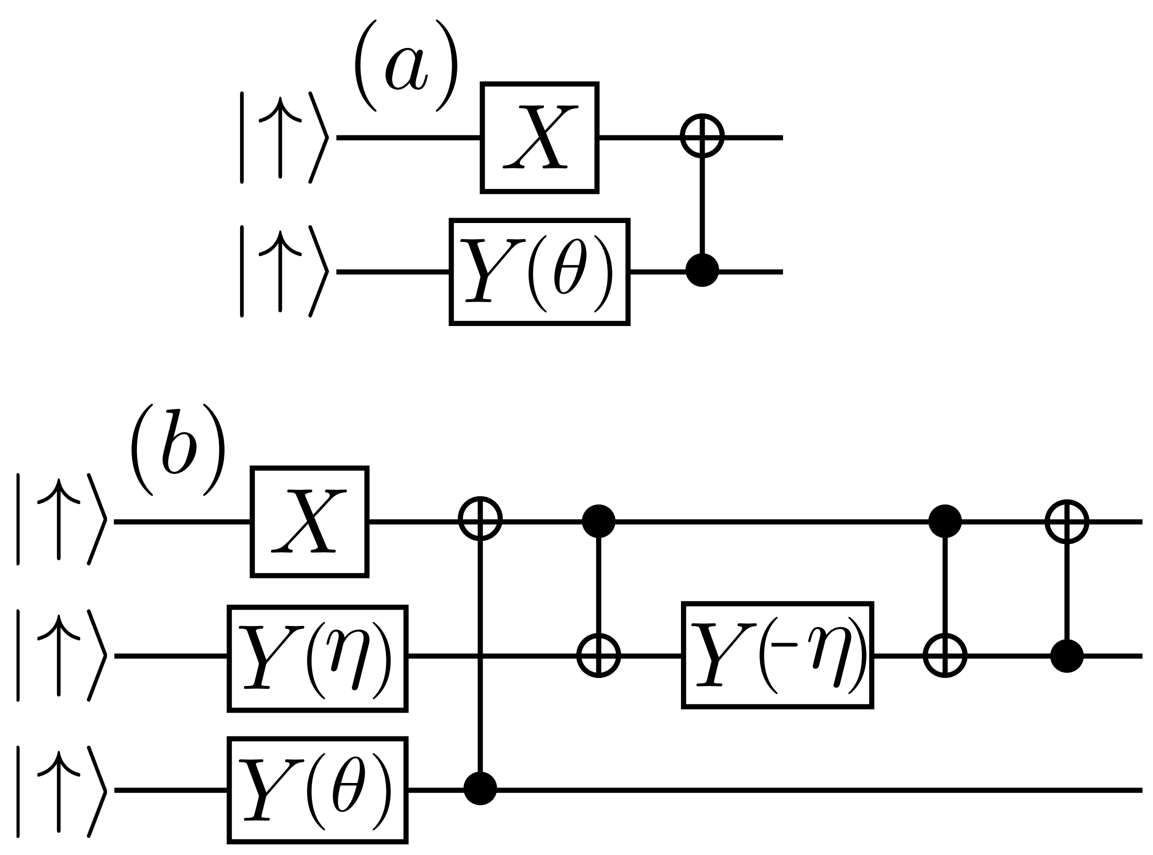
$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n$$

Mapping to qubits

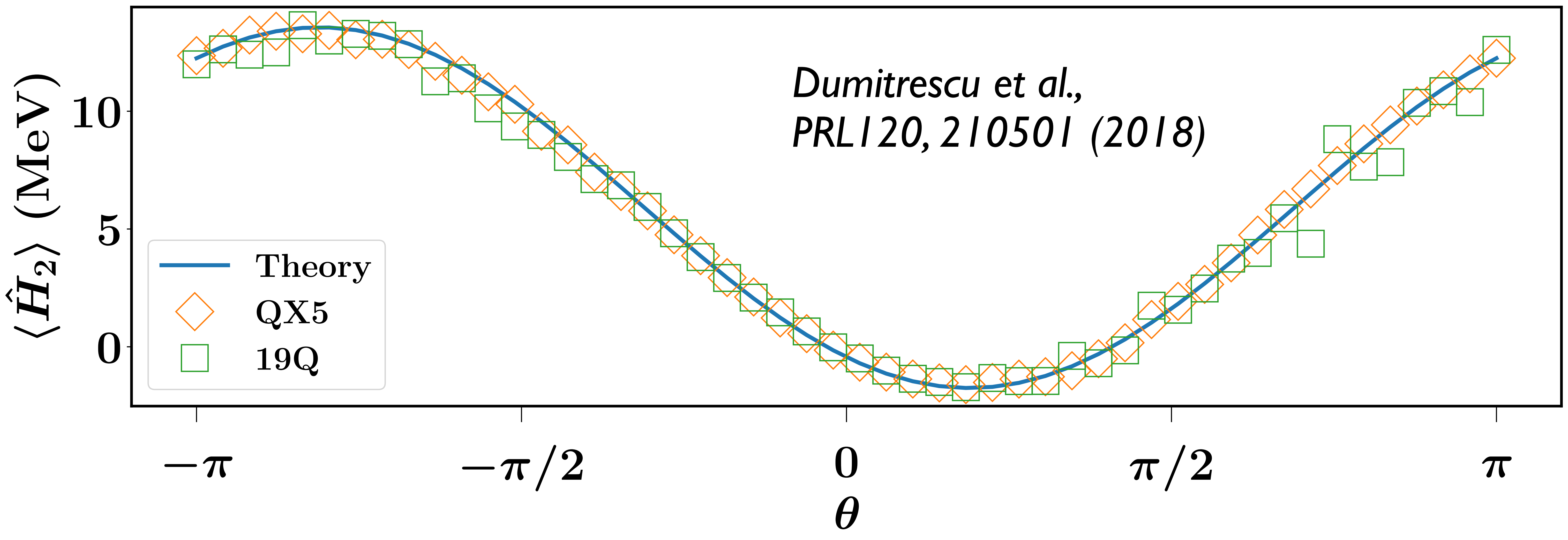
e.g.

$$a_n \to \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n + iY_n)$$

Quantum circuit



Results



Outline

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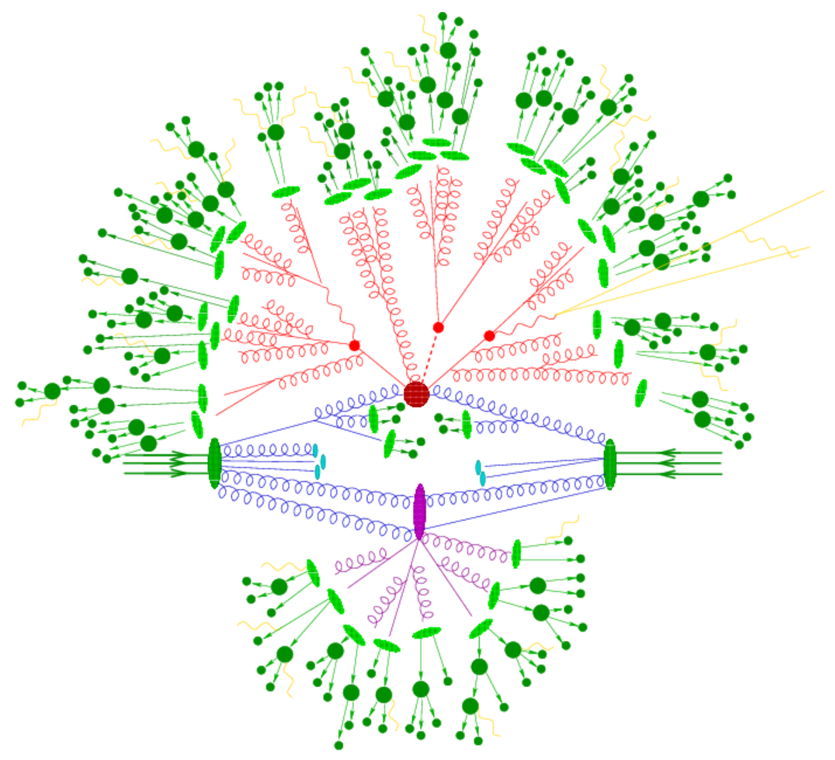
2. Real-time dynamics of scattering and hadronization



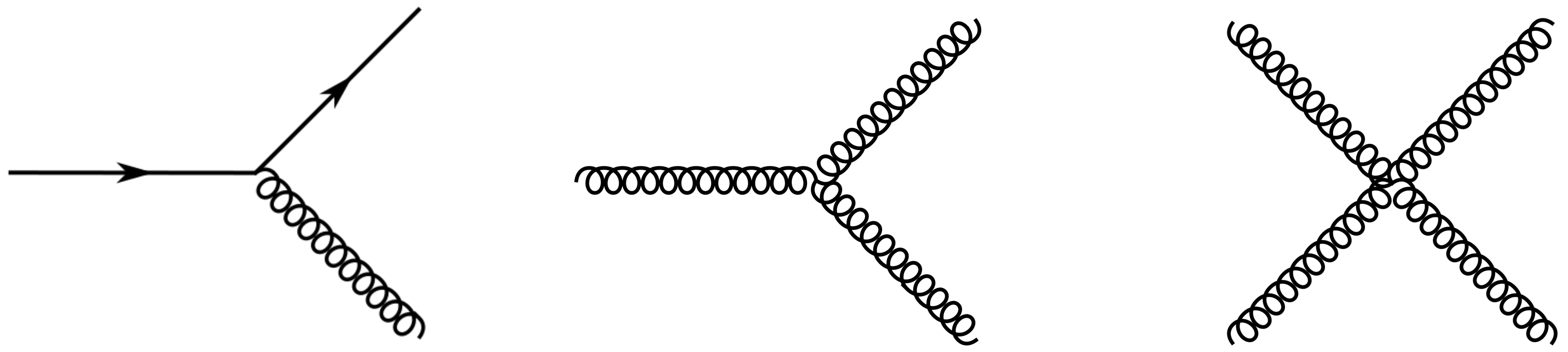
3. High-temperature/density QCD

Solving the equations of QCD

$$\mathscr{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \sum_{j=1}^{6} \bar{q}_j \left(i\gamma^\mu D_\mu - m_j \right) q_j$$

Perturbative QCD

For $\alpha_s \ll 1$, compute scattering amplitudes with Feynman diagrams

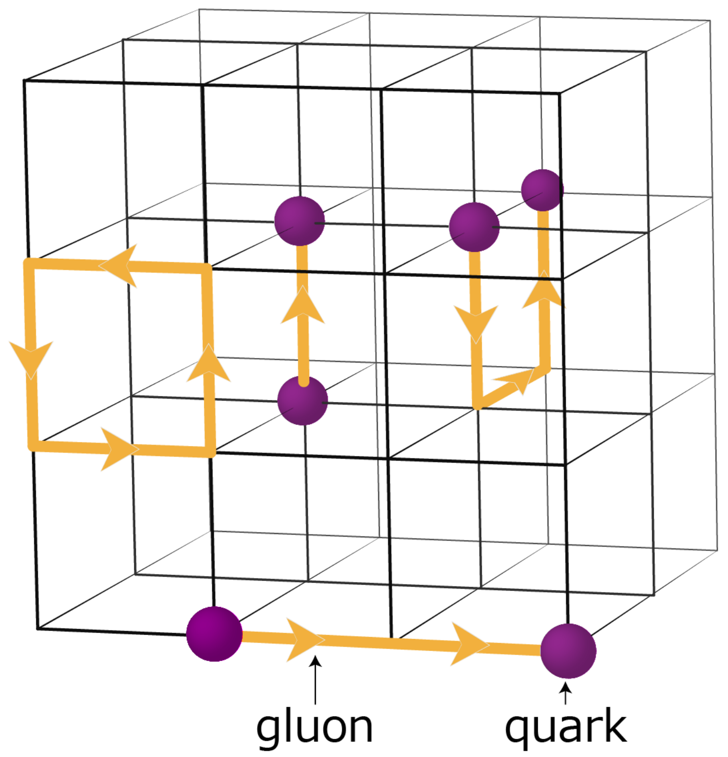


$$\sigma = \sigma^{(0)} + \alpha_s \sigma^{(1)} + \alpha_s^2 \sigma^{(2)} + \ldots$$

...but no strong coupling!

Lattice QCD

For low-density systems, compute static quantities with lattice regularization

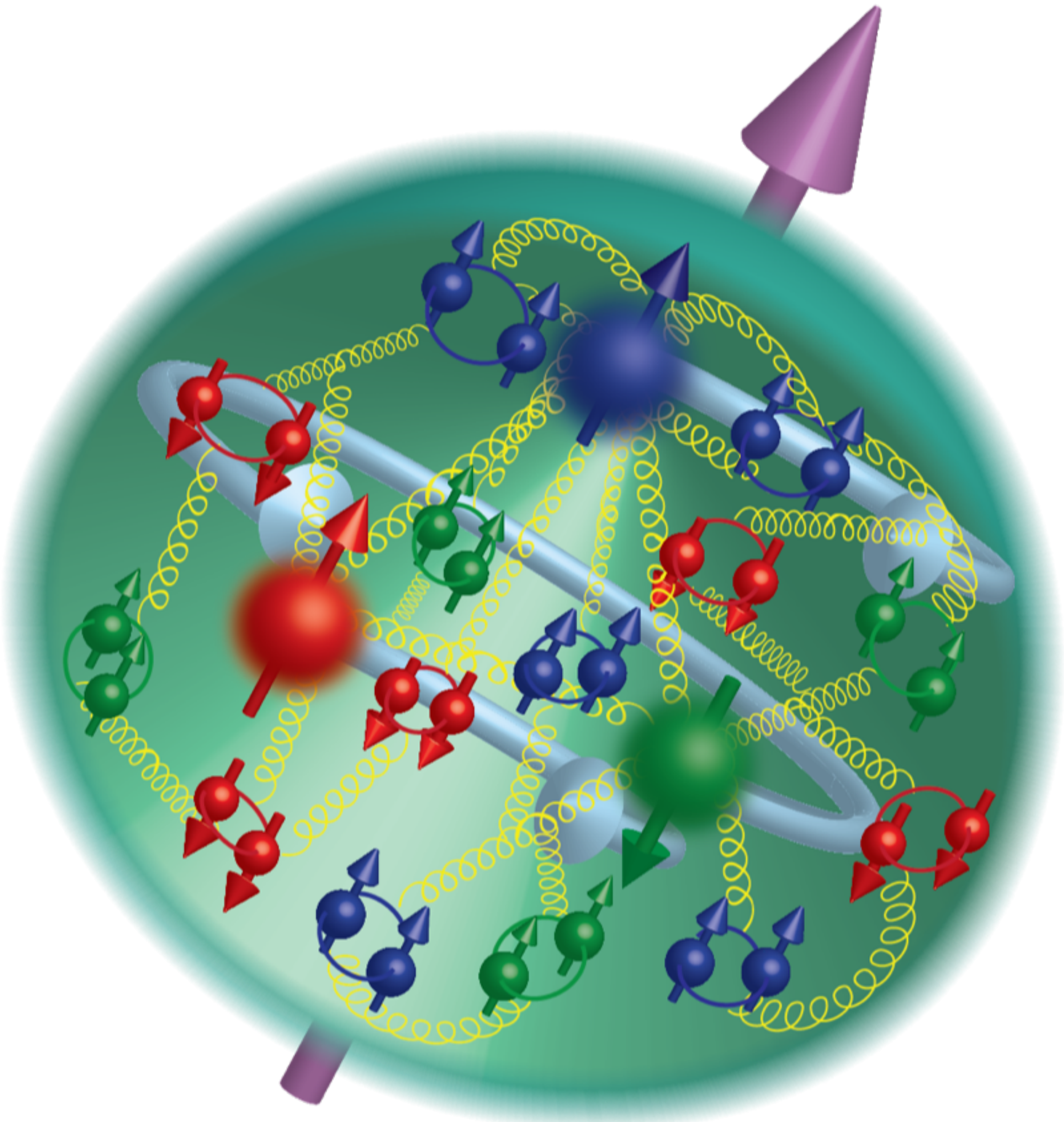


- Hadron spectra
- Deconfinement transition
- Chiral symmetry restoration

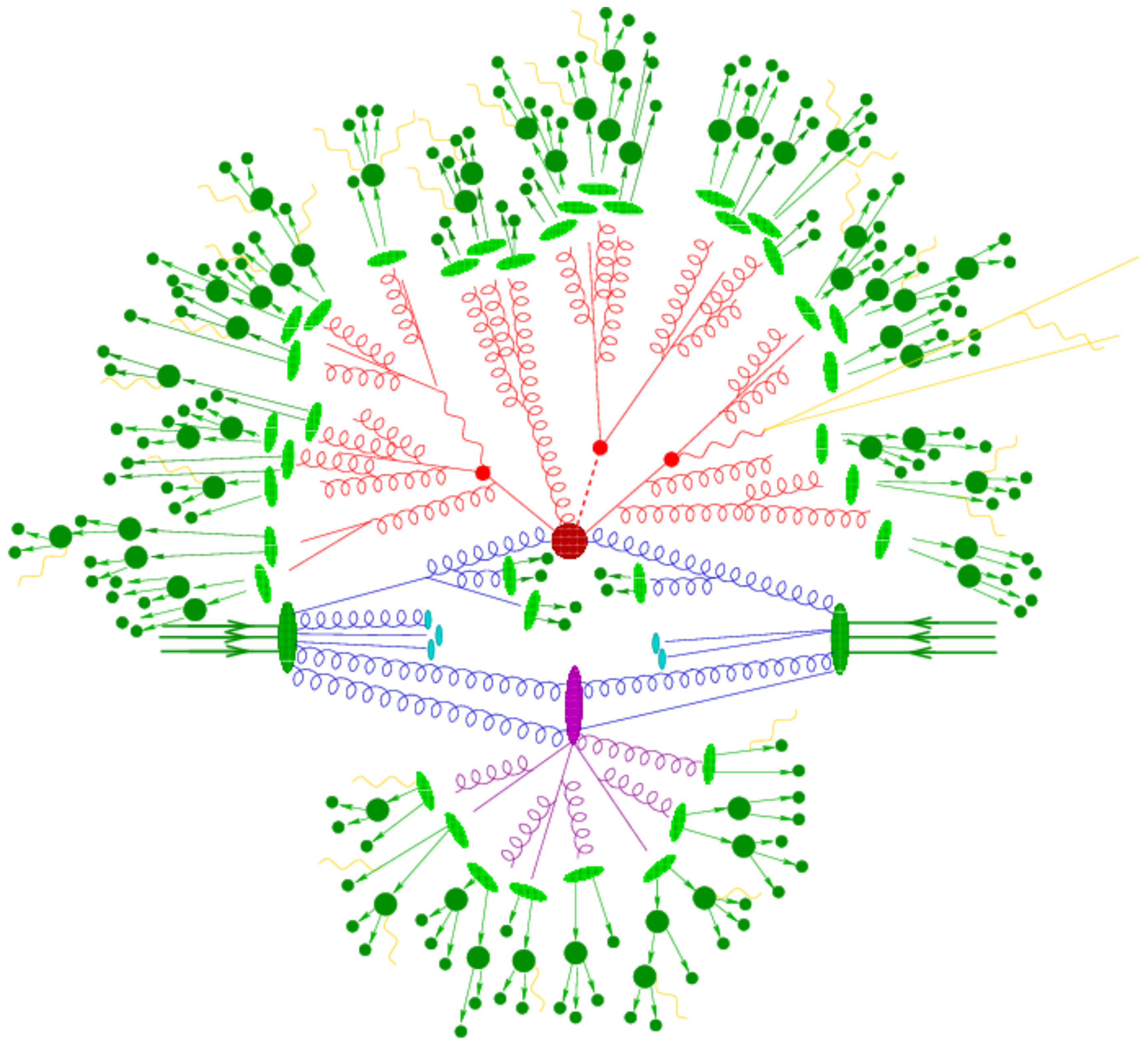
...but no dynamics!

Real-time dynamics

What are the *dynamics* that confine quarks and gluons into hadrons?



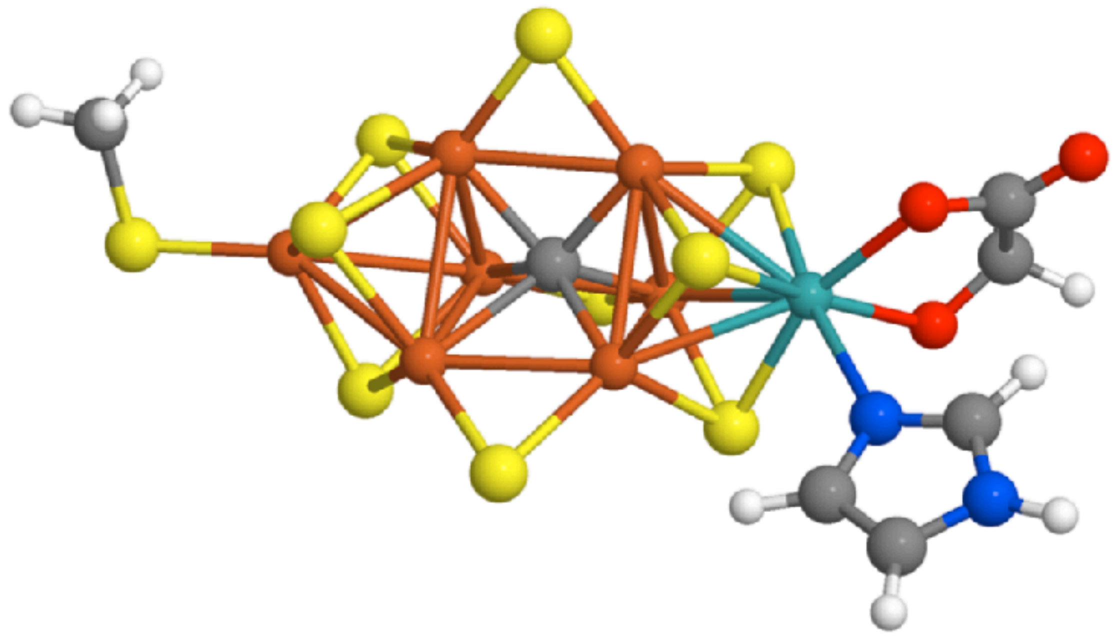
How does a high-energy quark or gluon fragment into a jet?



Quantum simulation

Feynman `81
Lloyd `96

A quantum computer can naturally simulate a quantum system described by a Hamiltonian H



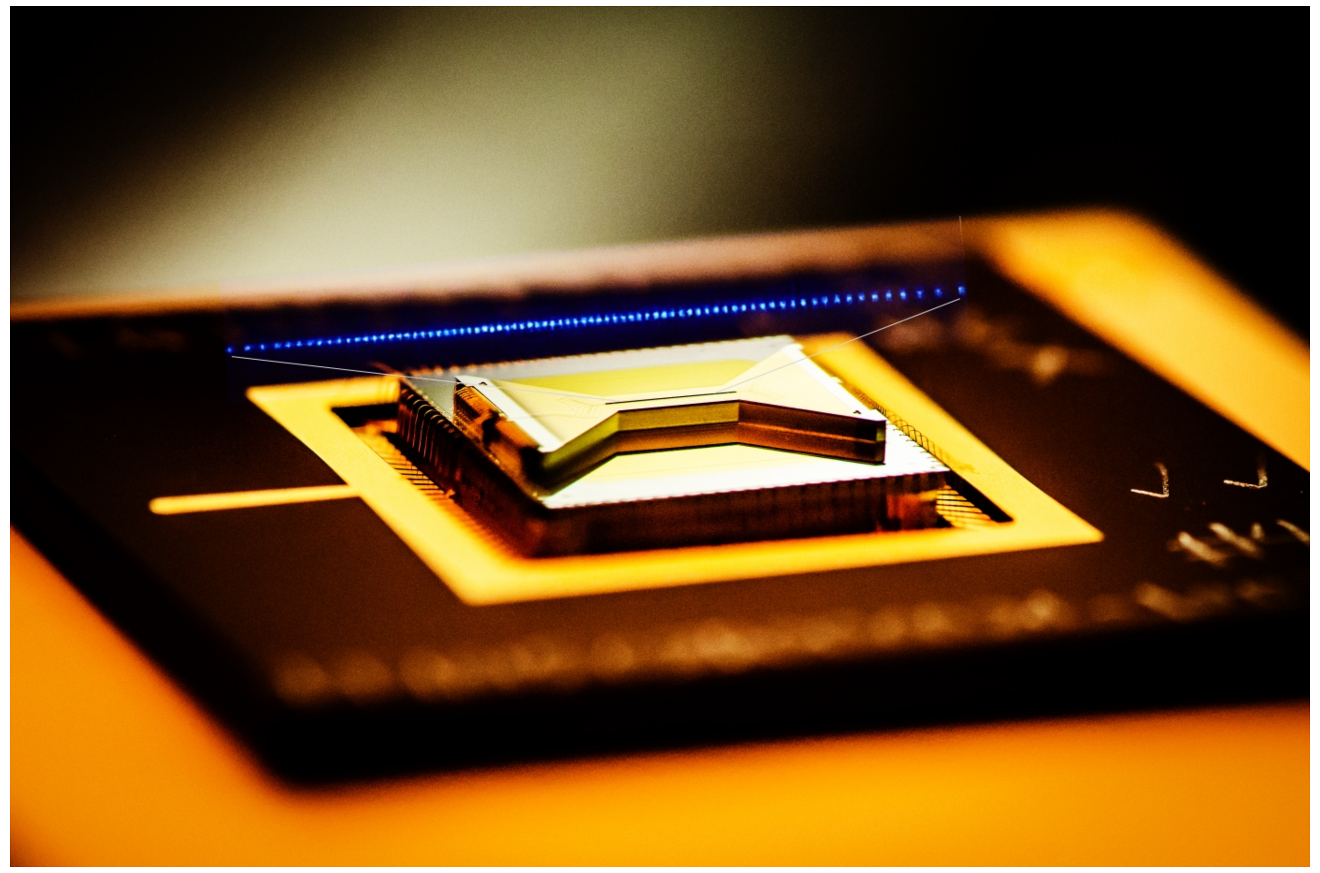
(1) Initial state preparation

$$|0\cdots0\rangle \rightarrow |\psi(0)\rangle$$

(2) Time evolution

$$|\psi(0)\rangle \; \text{—} \boxed{U_H(t)} \text{—} \; |\psi(t)\rangle$$

$$\text{where} \quad U_H = e^{-iHt/\hbar}$$

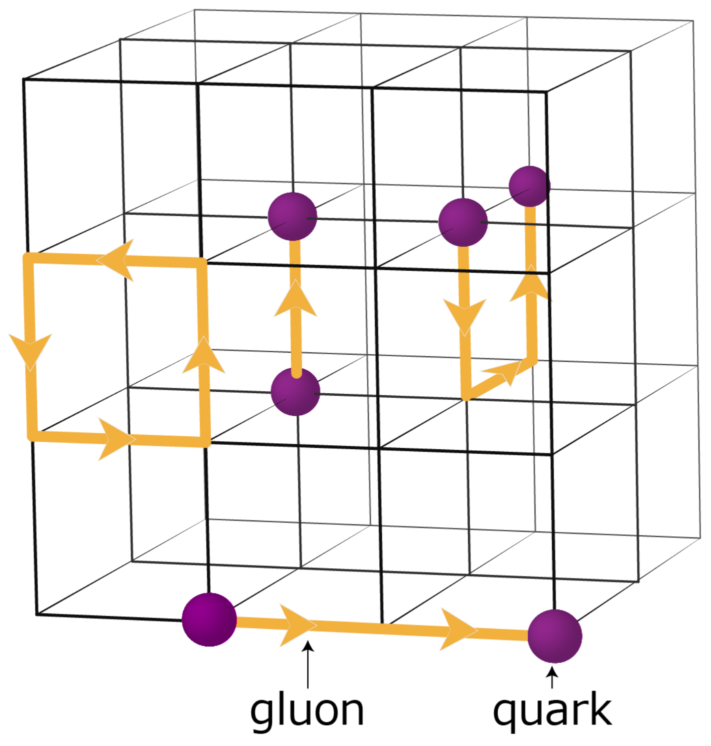


IONQ

(3) Measurement

Simulating quantum field theories

There is an extra complication if we want to simulate QCD: it is a *quantum field theory* — the particle number is not fixed



→ This requires us to simulate fields at all points in spacetime: lattice QCD

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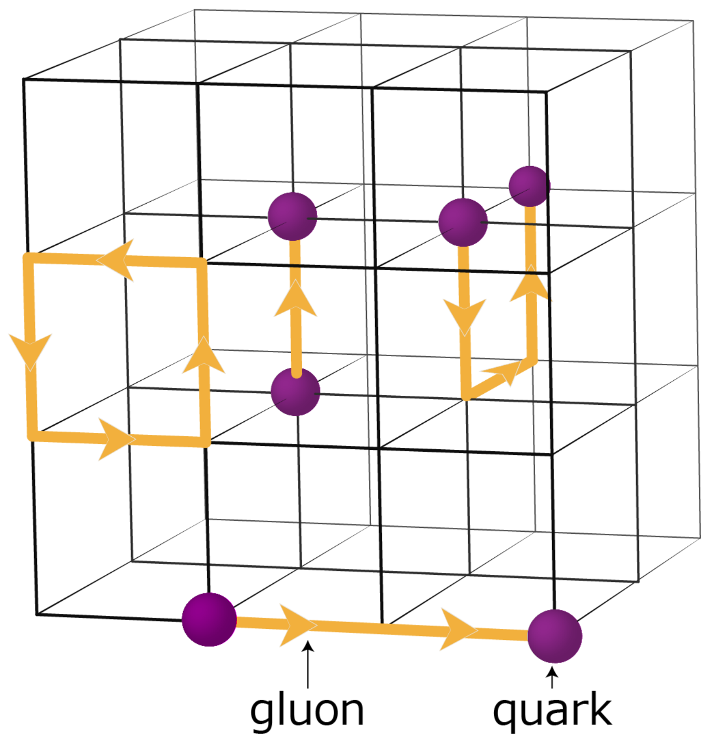


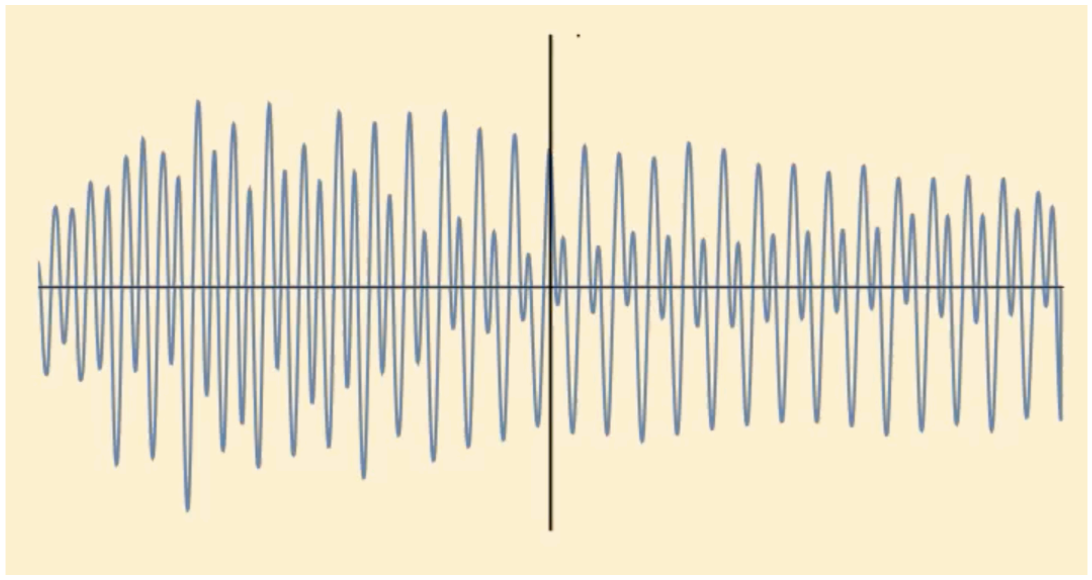
→ This requires us to simulate fields at all points in spacetime: lattice QCD

However, traditional Lattice QCD cannot simulate dynamics due to infamous sign problem

Integrals of form: $\int e^{i\mathscr{L}t}$

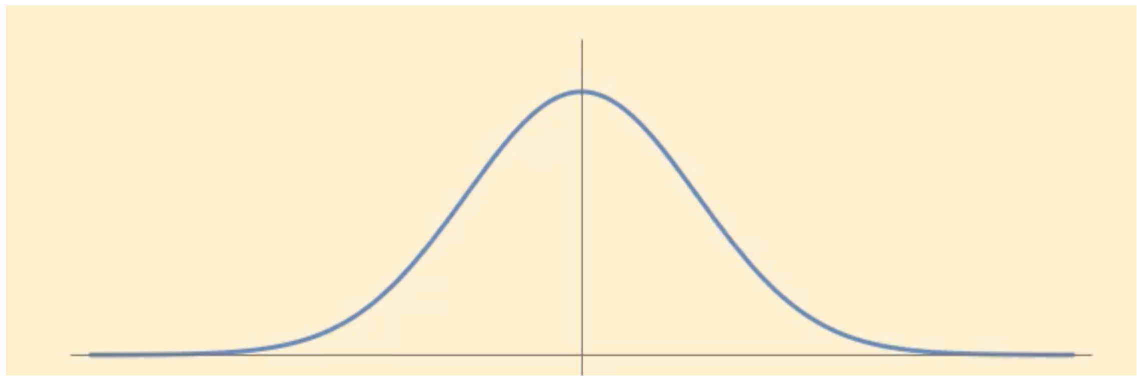
Traditional lattice QCD uses imaginary time, not real time

Real time



Imaginary time

$t \rightarrow it$

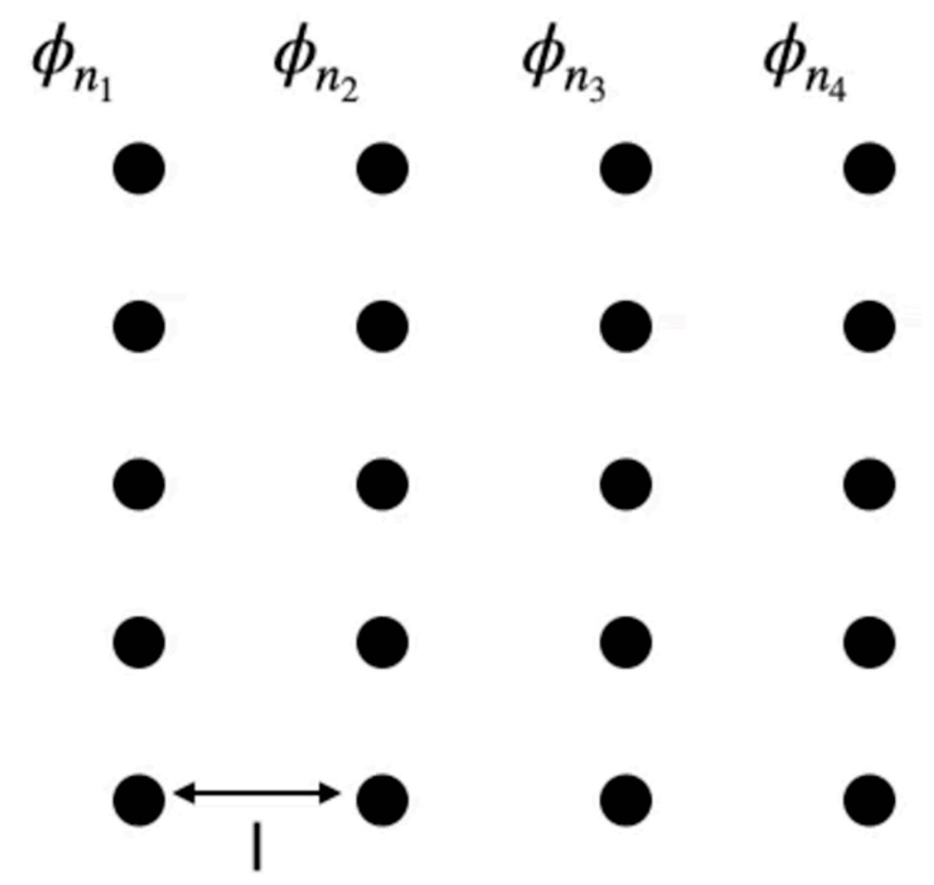


Quantum simulation of real-time dynamics

Hamiltonian formulation of field theories

- Discretize space, keep time continuous
- Digitize fields

Kogut, Susskind `75



The matrix H will be huge…but we can use quantum simulation!

$$|\psi(0)\rangle \; — \boxed{U_H(t)} — \; |\psi(t)\rangle$$

where $U_H = e^{-iHt/\hbar}$

Bauer, Nachman, Freytsis (2021)

Hilbert space has dimension

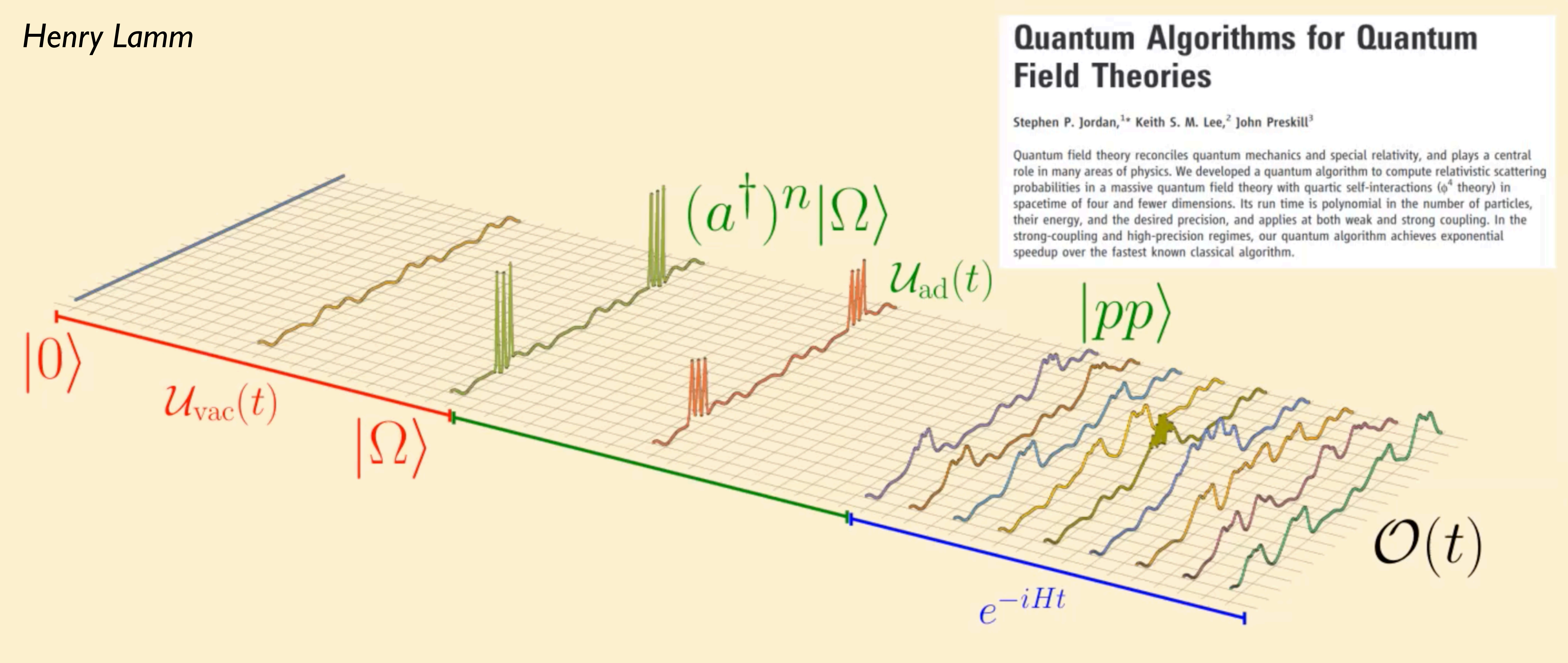
$(n_\phi)^{N^d}$

n_ϕ : # of digitized field values
N : # of lattice points per dim
d : # of dimensions

Example 1: Scattering in scalar field theories

Can be simulated efficiently using quantum computers!

Jordan, Lee, Preskill (2014)

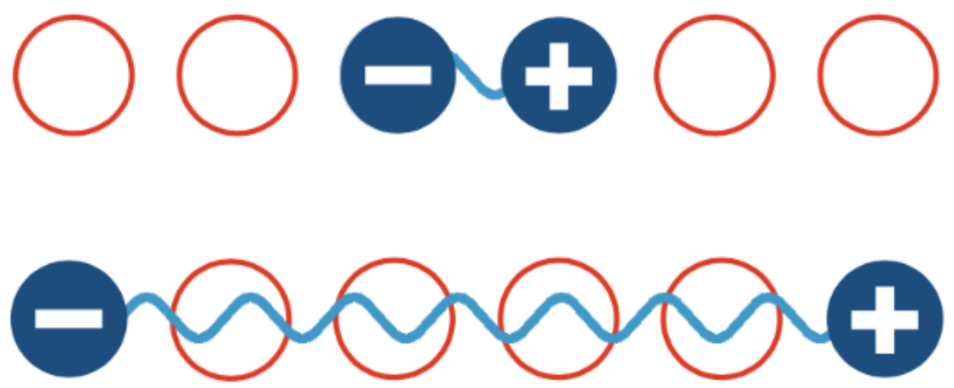


Example 2: Hadronization

Magnifico, Dalmonte, Facchi, Pascazio, Pepe, Ercolessi (2020)

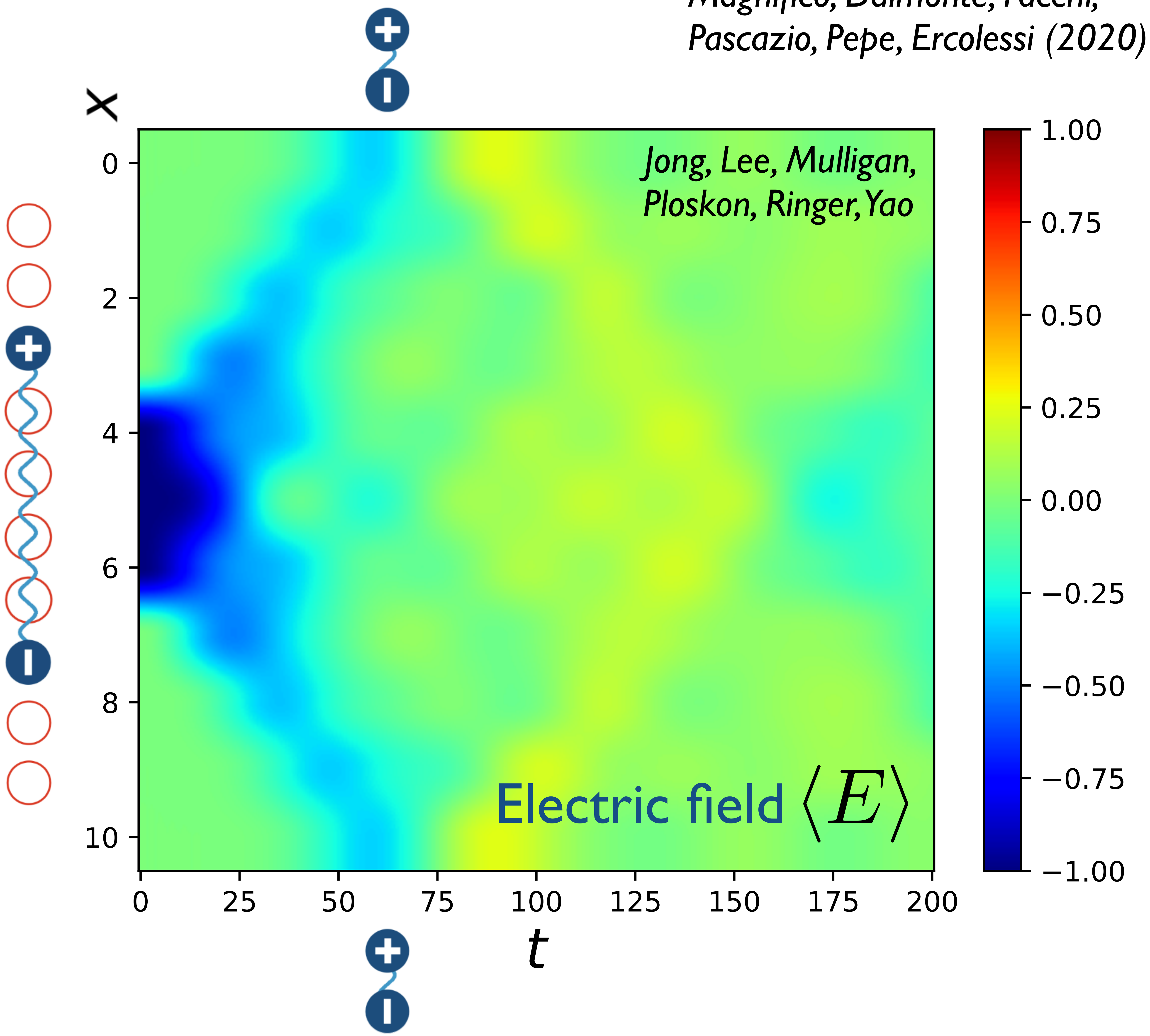
Schwinger model: QED in 1+1D

- Confinement
- Chiral symmetry breaking



Real-time picture of string breaking mechanism

Long-term goal: QCD hadronization



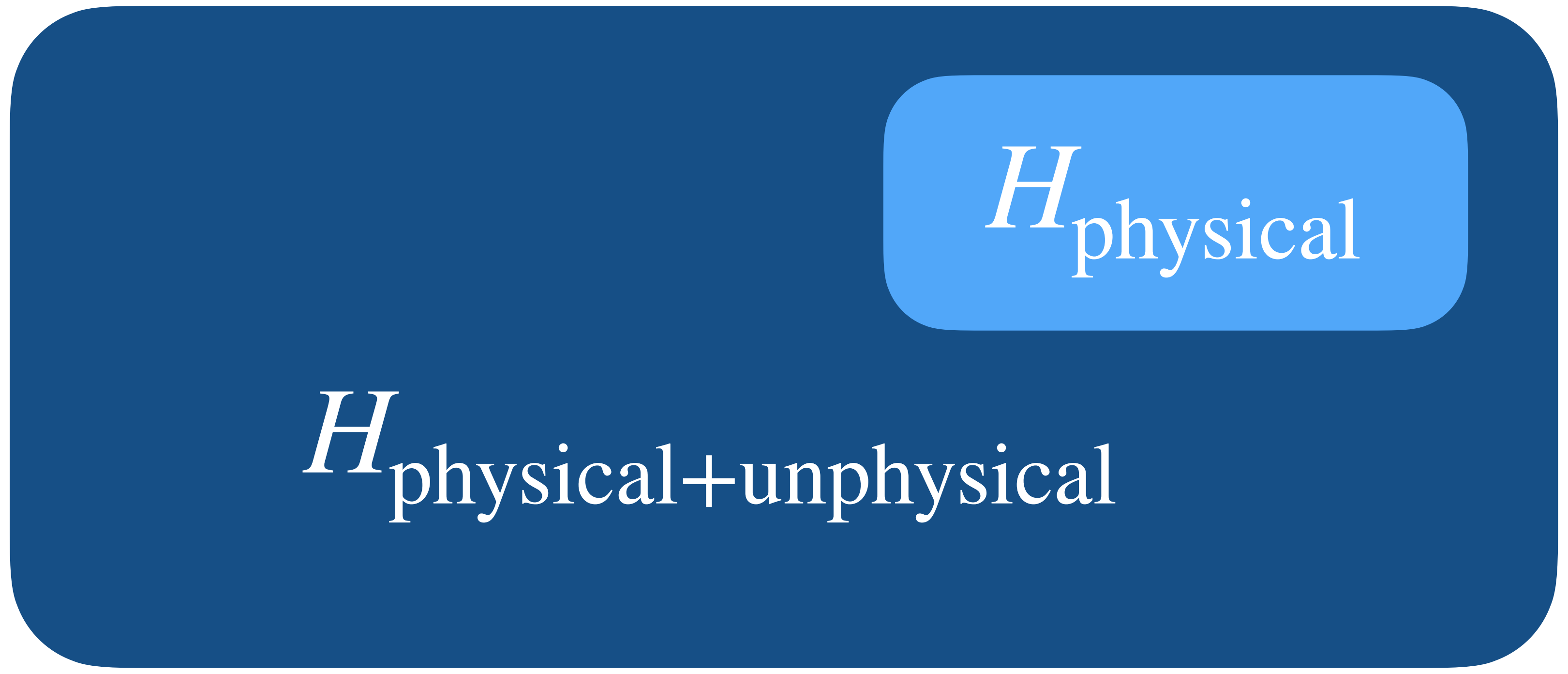
The path towards QCD

Quantum computers have opened the prospect to simulate real-time dynamics of QCD

- We do not yet know whether it is possible!
- Fundamental question: *Can any system realized in nature be computed efficiently by a quantum computer?*

But there are several major challenges

- Is it possible to efficiently encode H_{QCD} into quantum gates?
- How to enforce gauge invariance?
- …



Many ongoing efforts:

- Formulate how to efficiently digitize QCD
- Simulate simpler QFTs in order to gain insights about QCD

Klco et al. (2021)
Bauer et al. (2021)
Shaw et al. (2020)
Raychowdhury, Stryker (2020)
Alexandru et al. (2019)
Davoudi et al. (2019)
Klco, Savage (2018)
Muschik et al. (2016)
…

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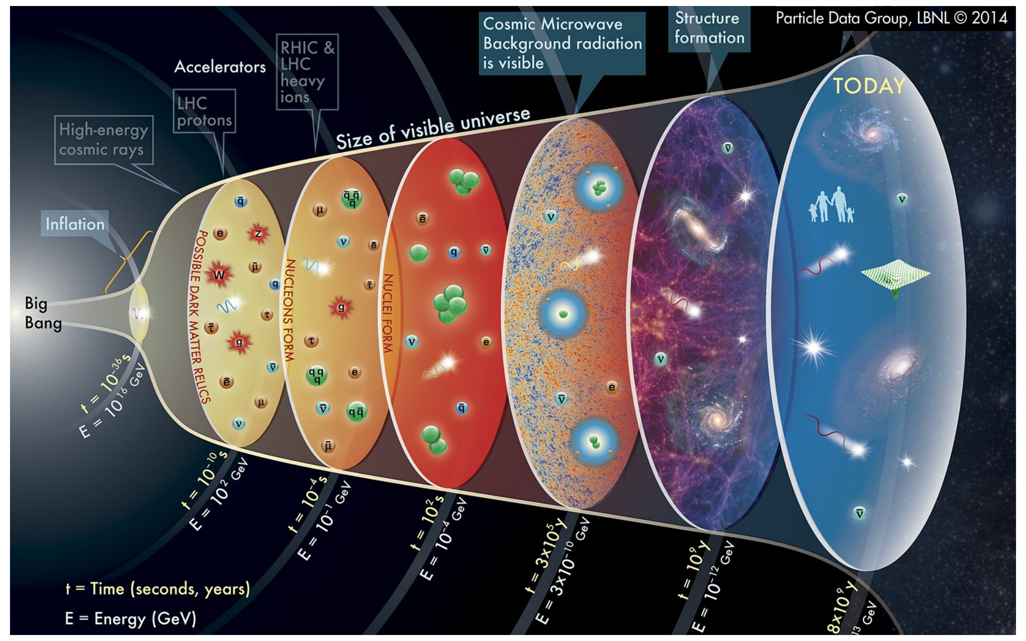
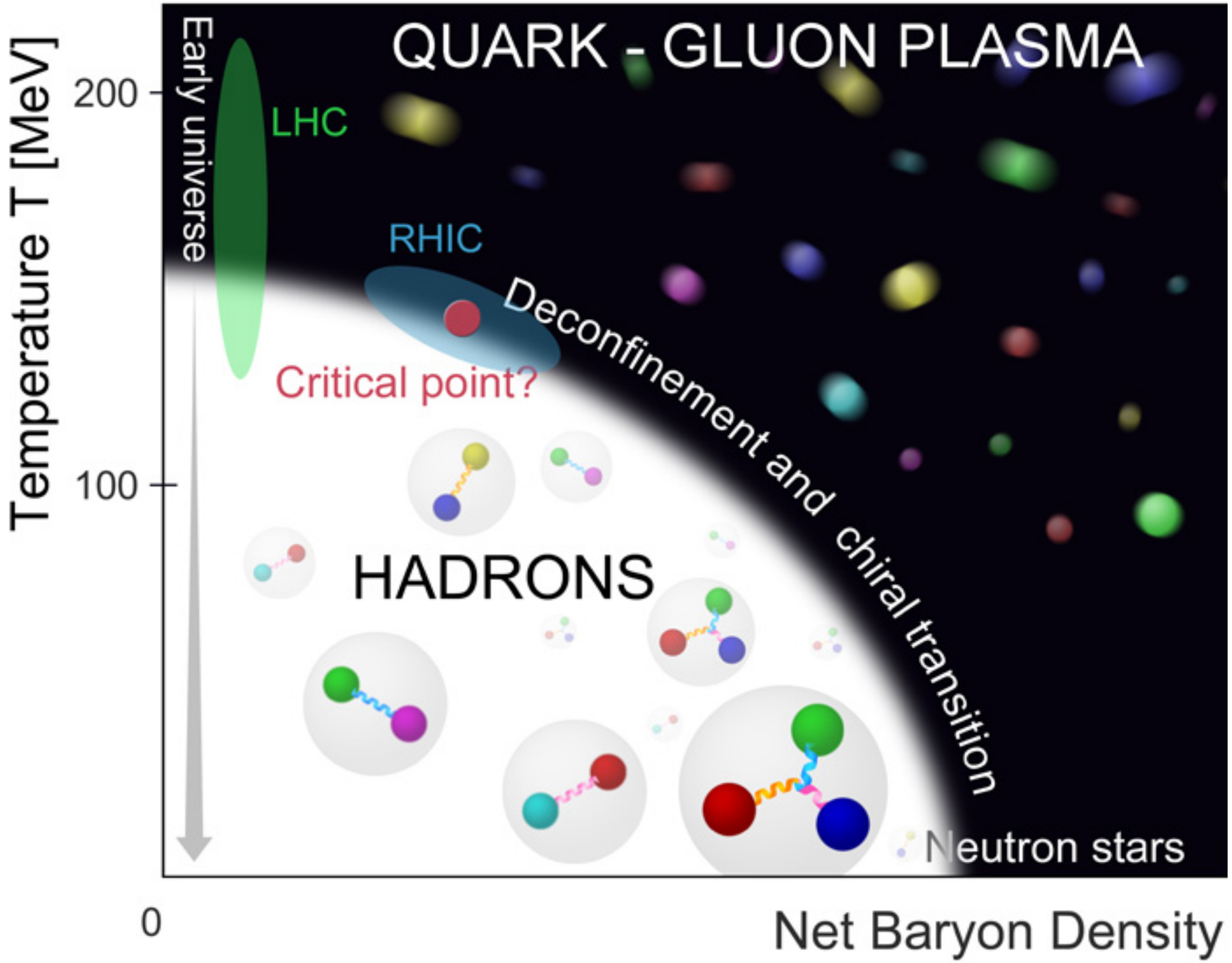
2. Real-time dynamics of scattering and hadronization

3. High-temperature/density QCD

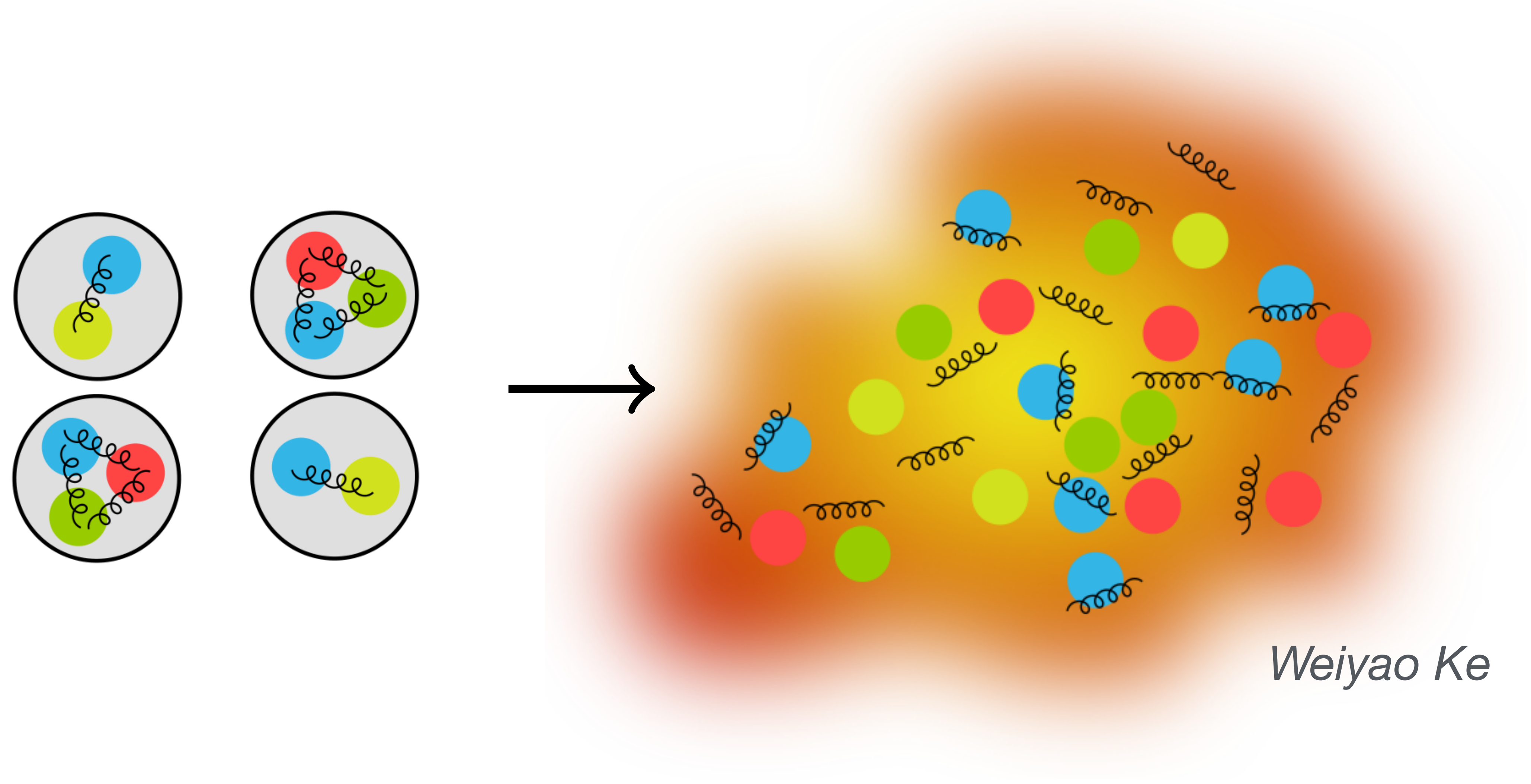


The landscape of QCD matter

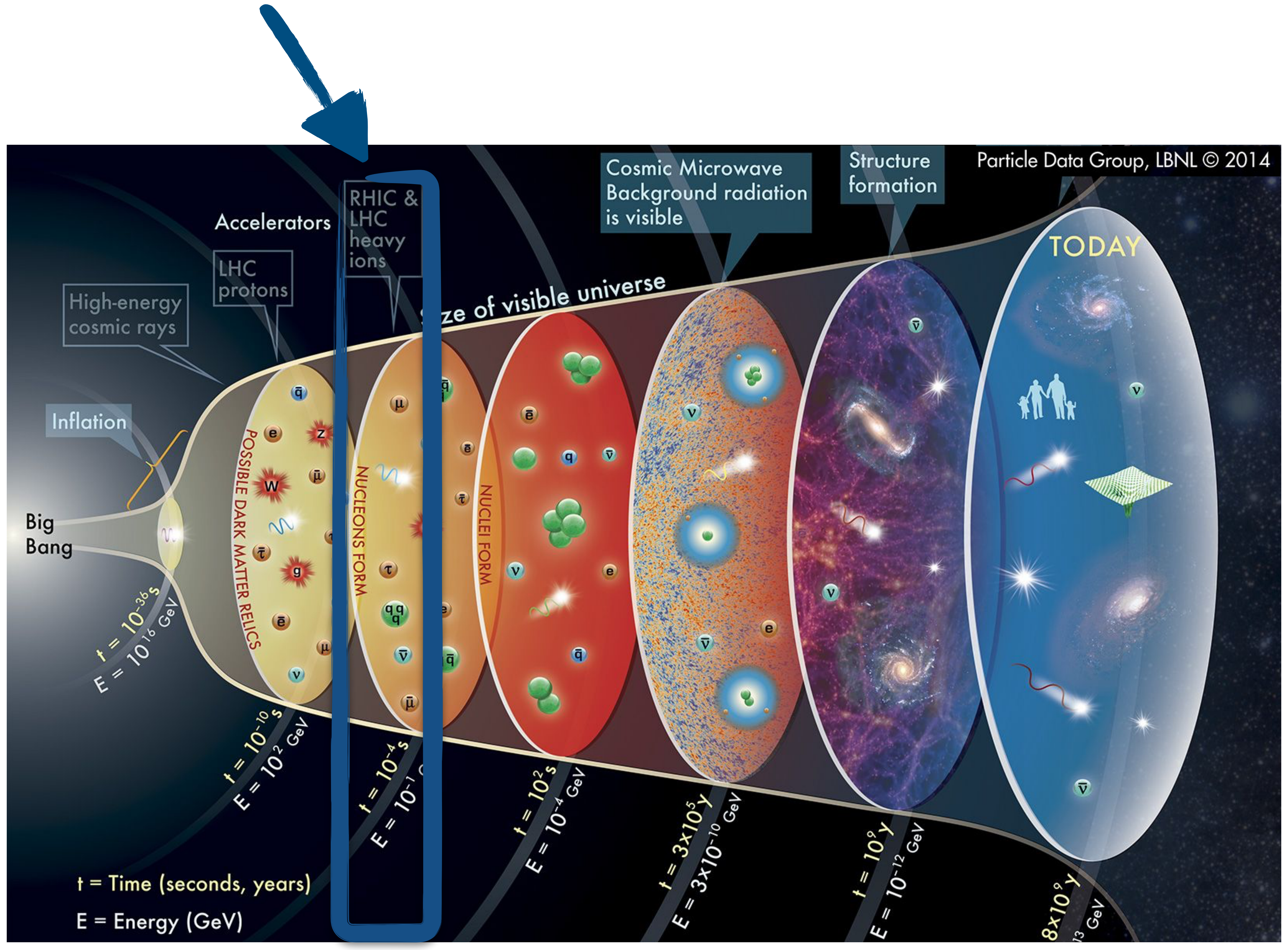


The quark-gluon plasma

If we heat nuclear matter to $T \approx 150$ MeV, quarks and gluons become deconfined into a **quark-gluon plasma**



This phase of matter filled the universe for most of the first few microseconds after the Big Bang



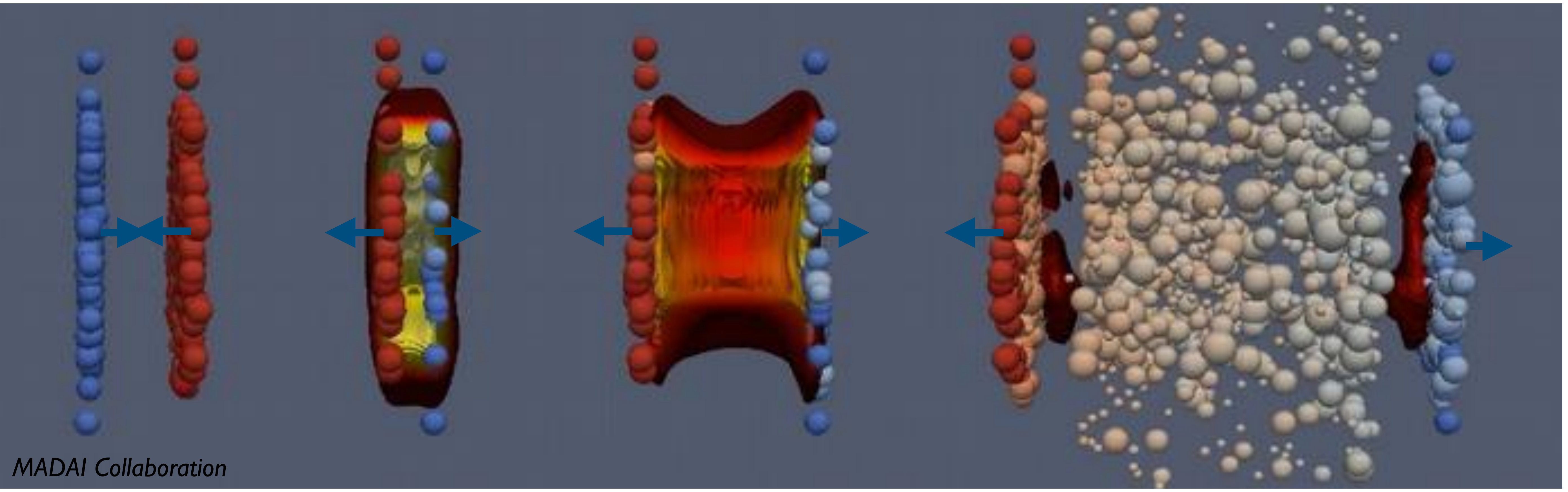
Heavy-ion collisions

We collide nuclei together at the

Large Hadron Collider (LHC)

Relativistic Heavy Ion Collider (RHIC)

to produce droplets of hot, dense quark-gluon plasma

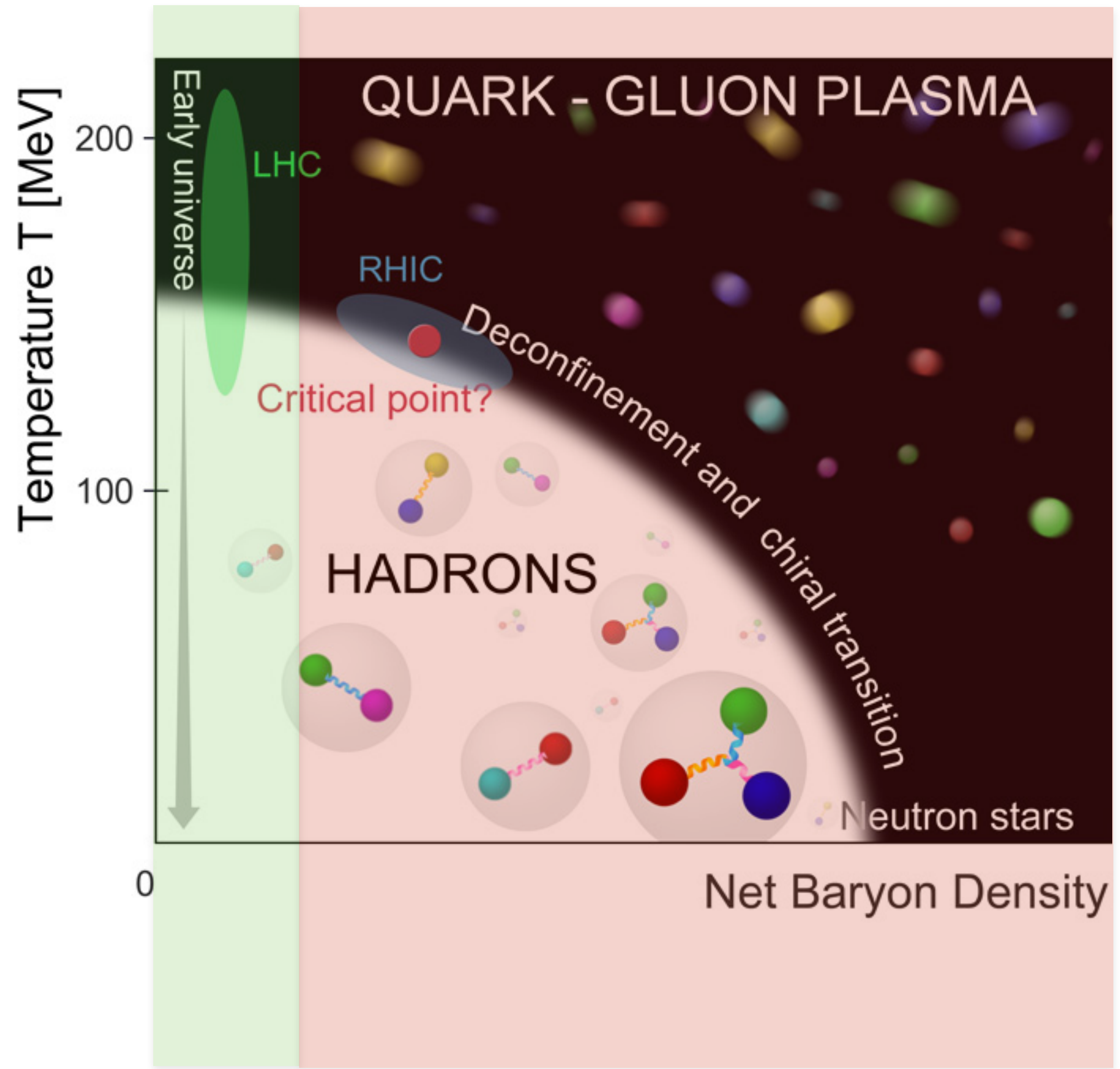


Soft collisions transform kinetic energy of nuclei into region of large energy density

$T \approx$ 150-500 MeV $\quad t \sim \mathcal{O}\left(10 \text{ fm}/c\right)$

Potential applications for quantum computing

High density QCD: Lattice QCD can only calculate static quantities at **low density**



calculable

not calculable: sign problem

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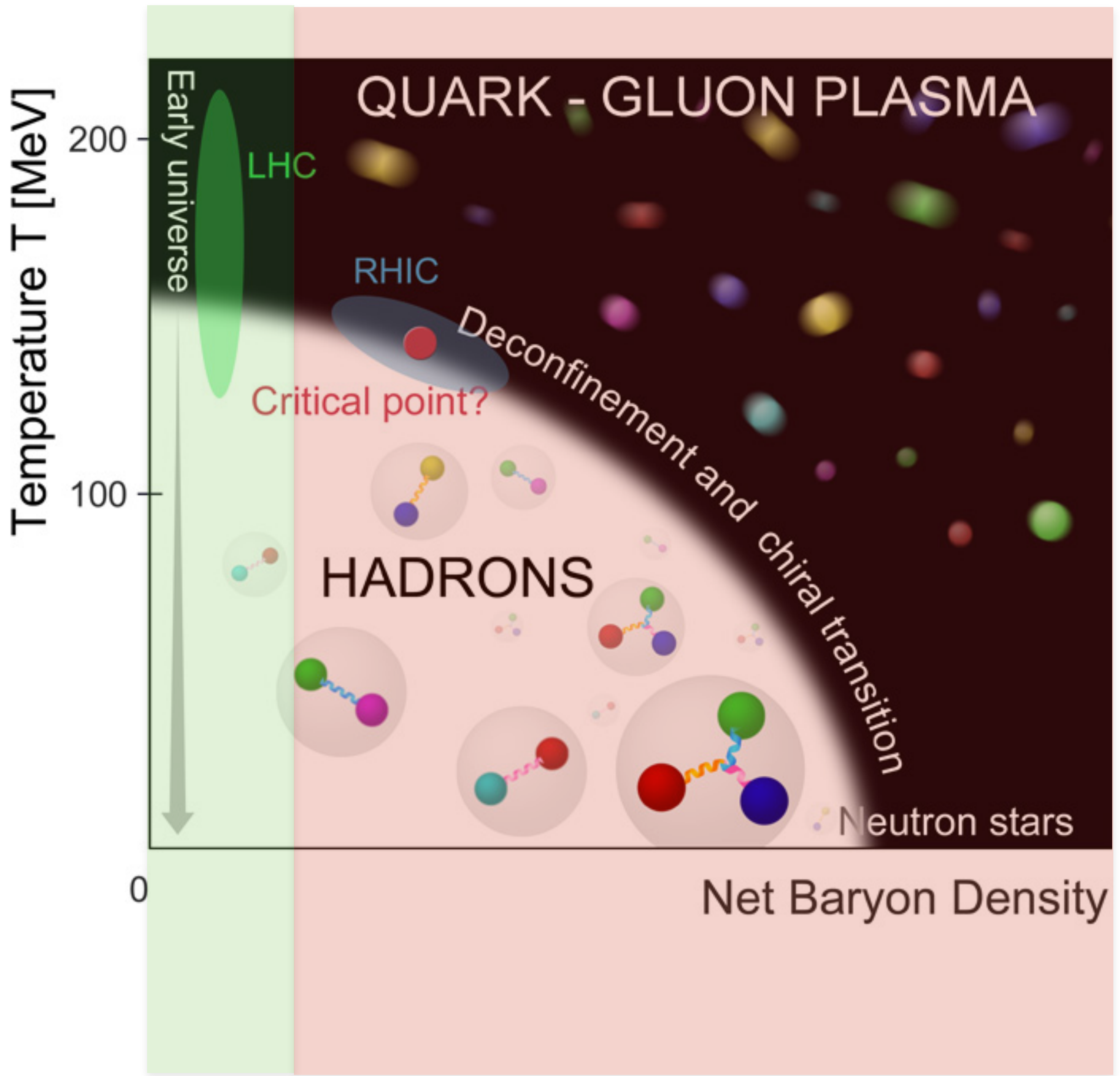
High density QCD: Lattice QCD can only calculate static quantities at **low density**



calculable

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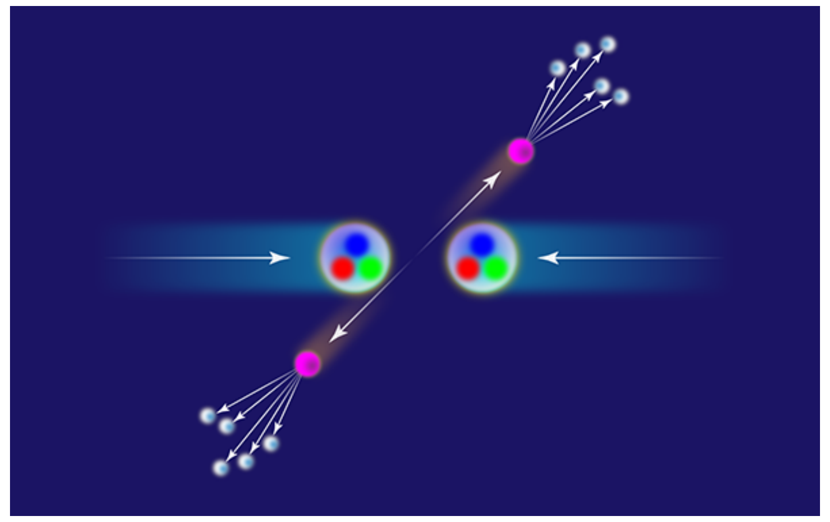
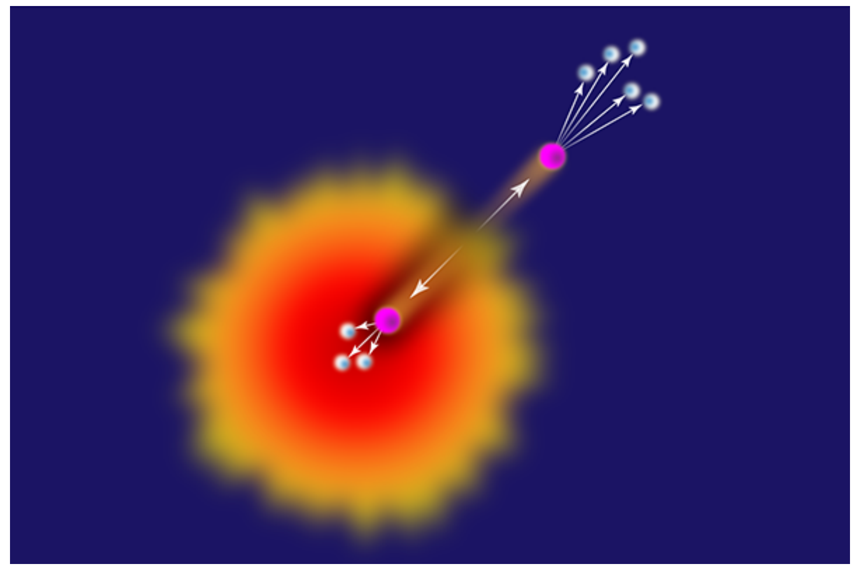
Real-time dynamics of probes evolving through the quark-gluon plasma

In vacuum: perturbative QCD

- No sense of "time evolution"



In medium: must combine probe evolution with hydrodynamic evolution of the QGP

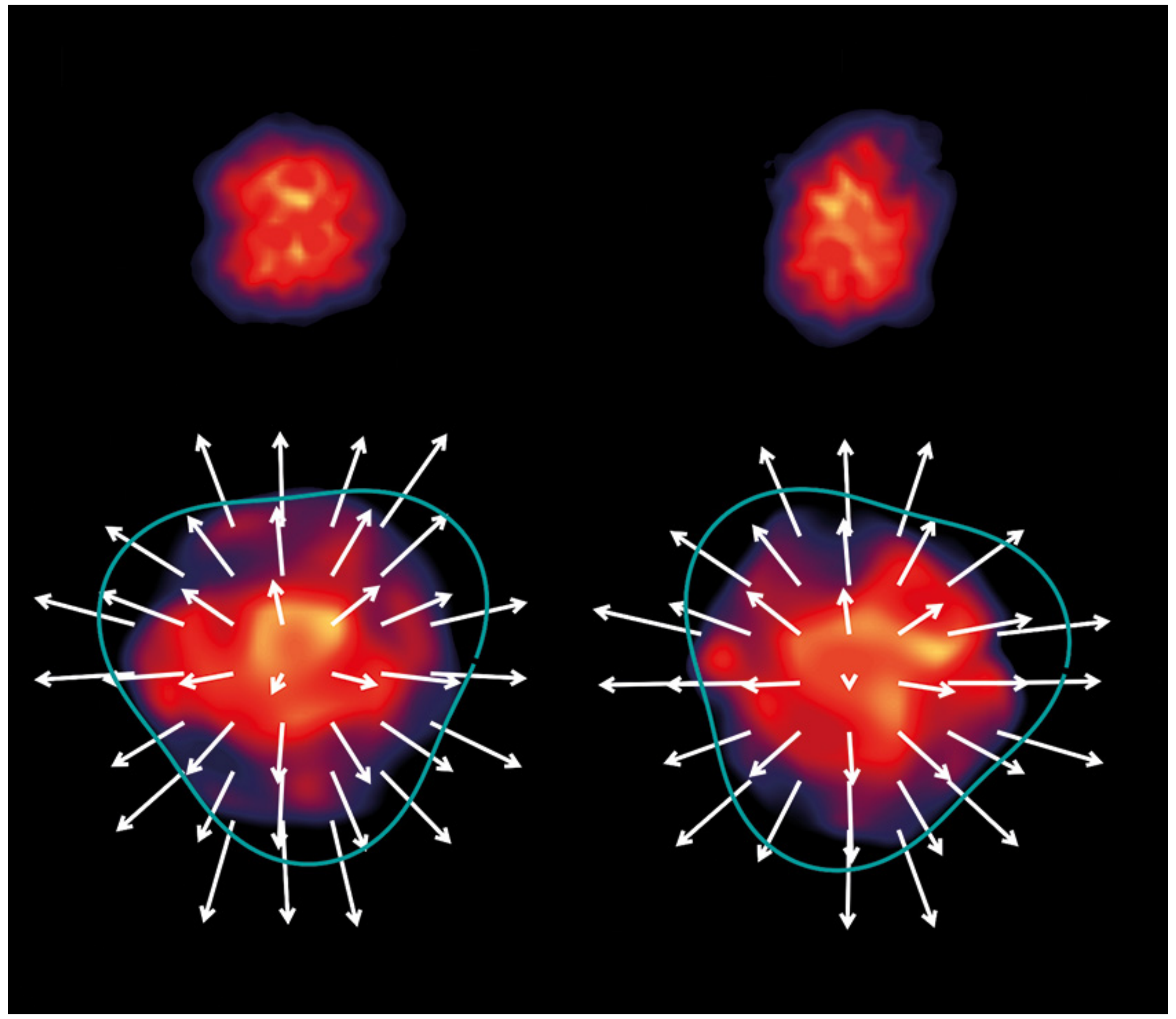


Example 1: Transport coefficients

Cohen, Lamm, Lawrence, Yamauchi (2021)

The quark-gluon plasma can be characterized by various transport coefficients:

- Shear viscosity
- Bulk viscosity
- Transverse diffusion
- …



Can be computed from energy-momentum tensor:

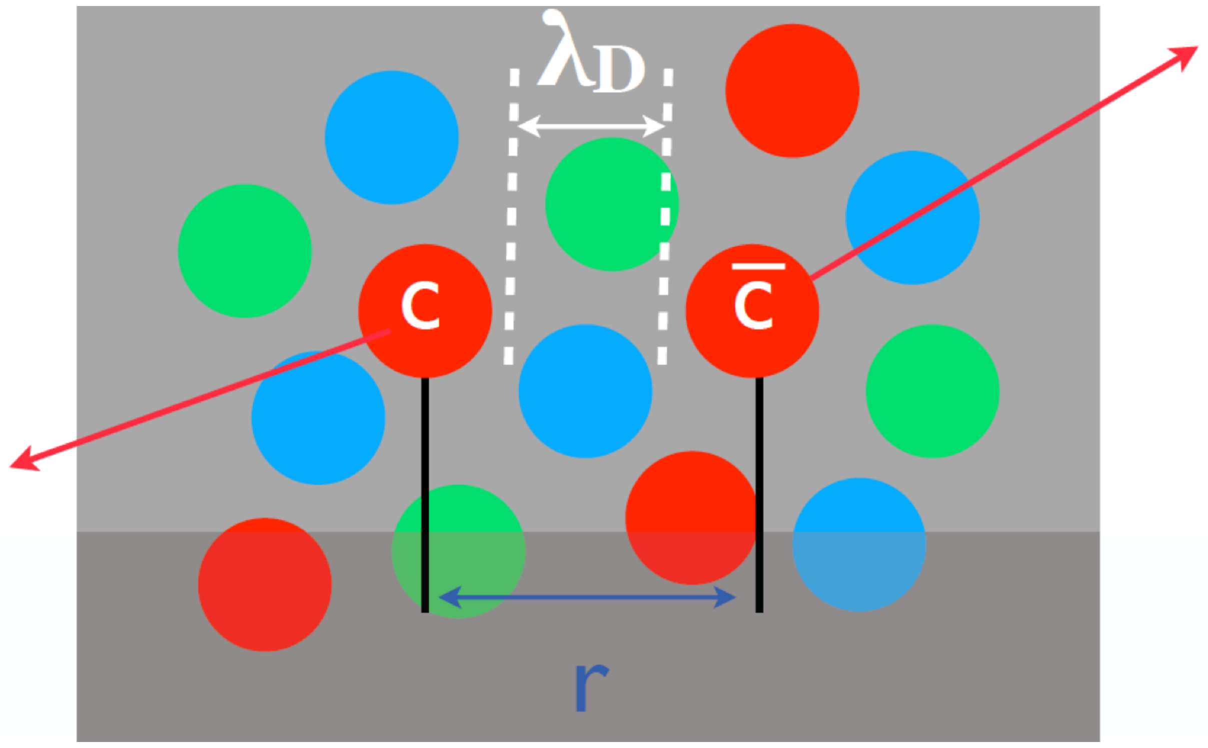
$$T_{\mu\nu} = \frac{1}{4} g_{\mu\nu} \mathrm{Tr}\left[F_{\alpha\beta}F^{\alpha\beta}\right] - \mathrm{Tr}\left[F_{\mu\alpha}F^{\alpha}_{\nu}\right]$$

Modest qubit requirement: $\approx 10^4$ qubits for gluonic theory

→ More tractable than full simulation of quark-gluon plasma

Example 2: Probing the quark-gluon plasma

Simulate the rate of heavy quark bound pairs (quarkonium) that are "melted" by the quark-gluon plasma)

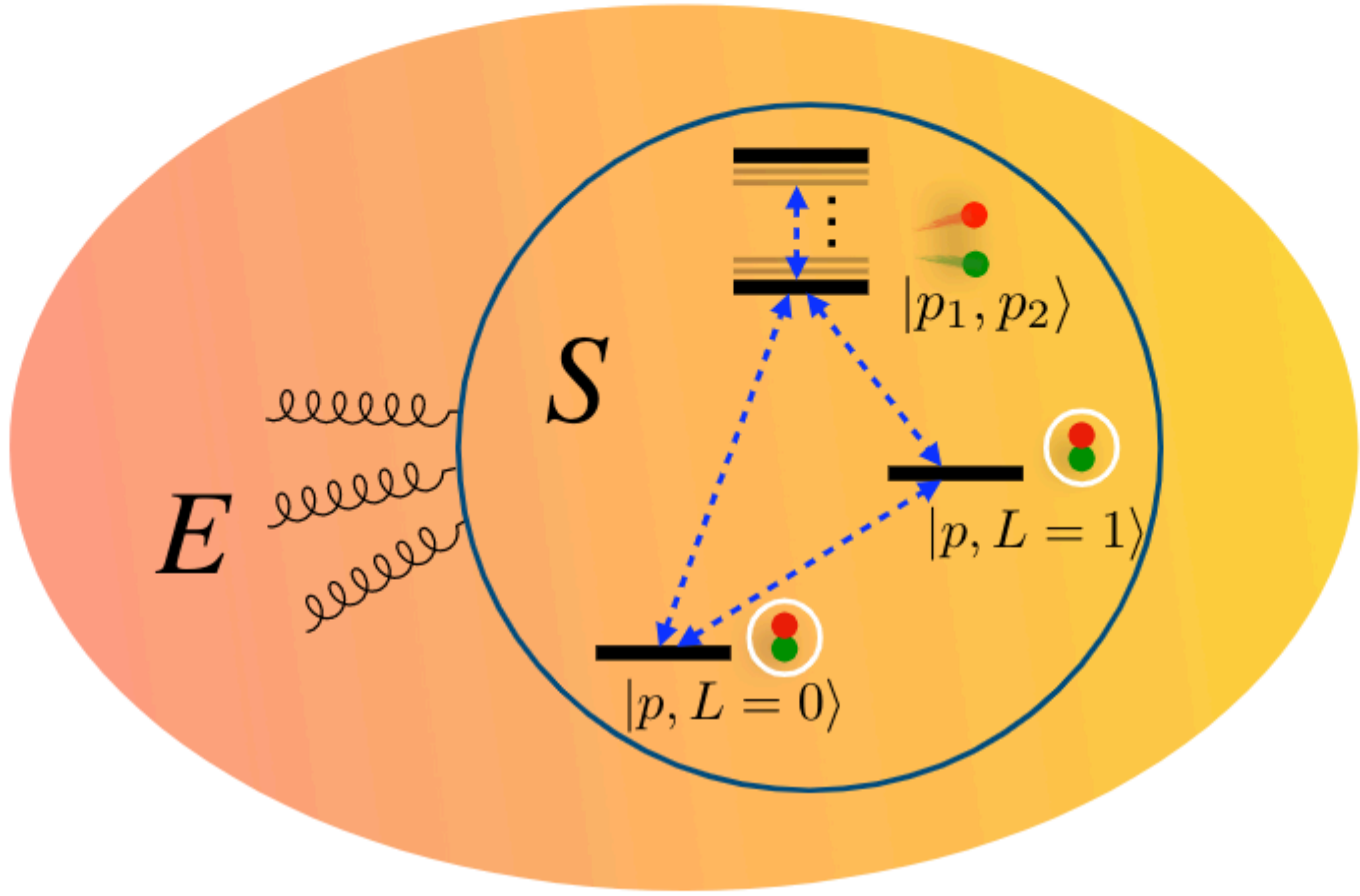


Open quantum system formalism

Subsystem - Probe — Jet, heavy quarks, …

Environment - Nuclear matter

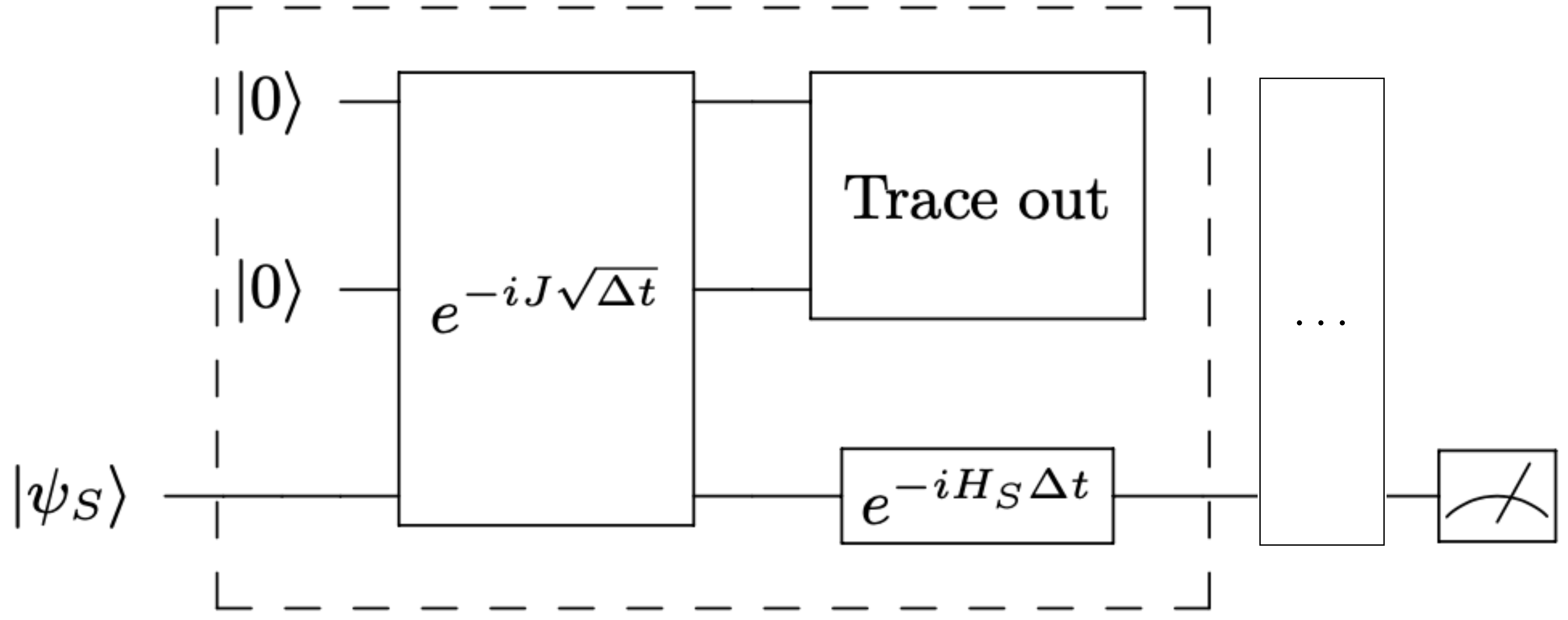
$$H(t) = H_S(t) + H_E(t) + H_I(t)$$



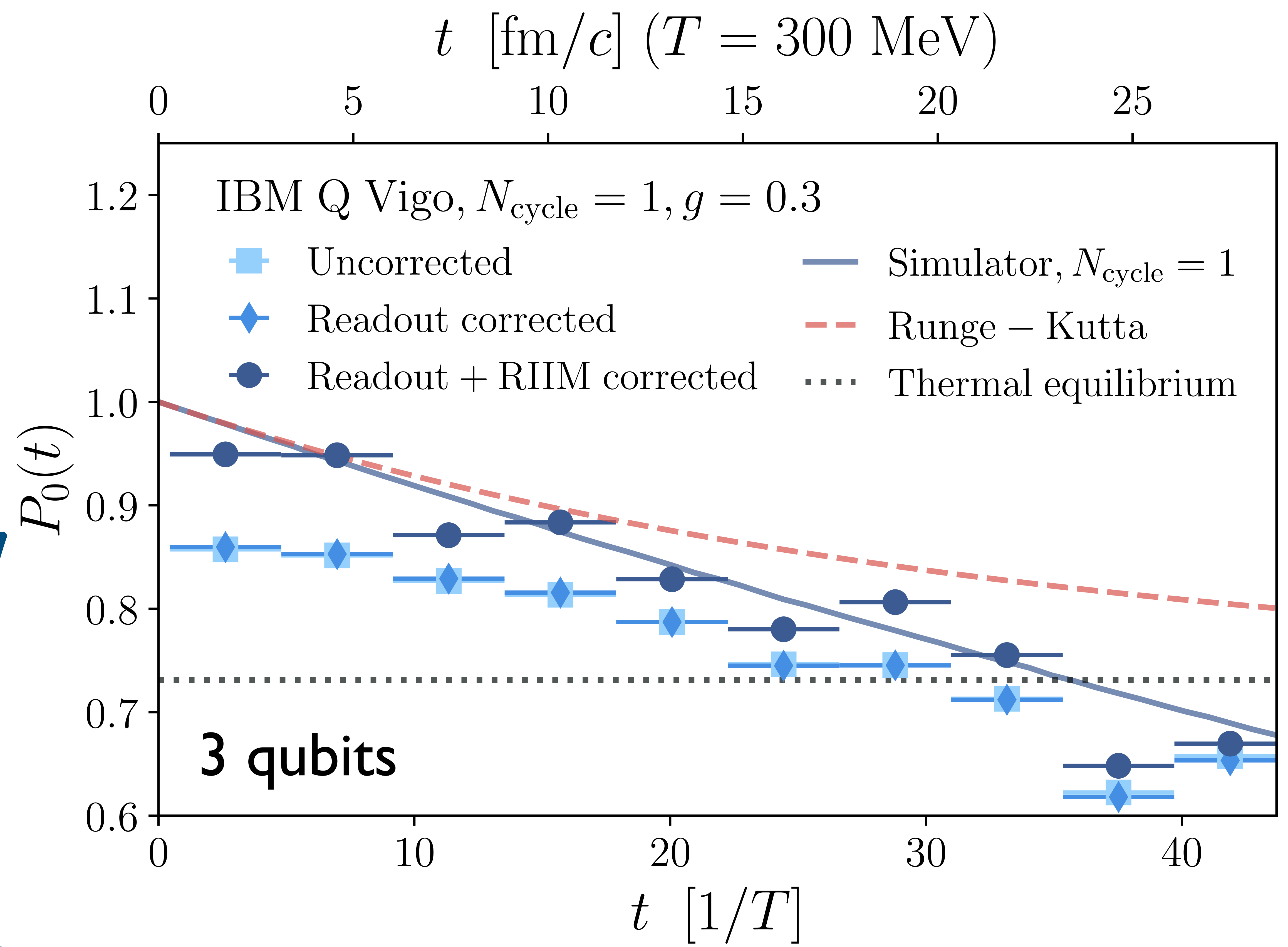
Example 2: Probing the quark-gluon plasma

Simulate the rate of heavy quark bound pairs (quarkonium) that are "melted" by the quark-gluon plasma)

Jong, Metcalf, Mulligan, Ploskon, Ringer, Yao
PRD 104, 051501 (2021)

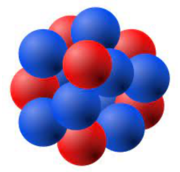
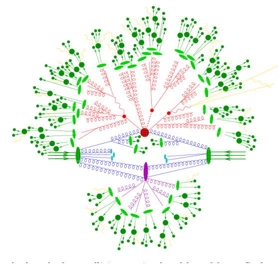
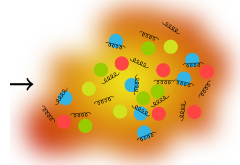


$P_0(t)$ **fraction of pairs that remains in "bound state"**



Summary

Quantum computing offers potential opportunities to vastly expand our understanding of QCD

- Many-body nuclear structure 
- Real-time dynamics of scattering and hadronization 
- High-temperature/density QCD 
- …

Short-term: Current quantum hardware is too small and noisy to achieve quantum advantage, but it is an important time to explore potential applications

Long-term: Determining whether QCD can be simulated efficiently by quantum computers will give us profound insights about nature