Quantum computing for nuclear matter at finite temperature

Dan-Bo Zhang

South China Normal University

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Collaborator: Tianyin Li, Xudan Xie, Xingyu Guo, Wai Kin Lai, Xiaohui Liu, Enke Wang, Hongxi Xing, Dan-Bo Zhang, Shi-Liang Zhu

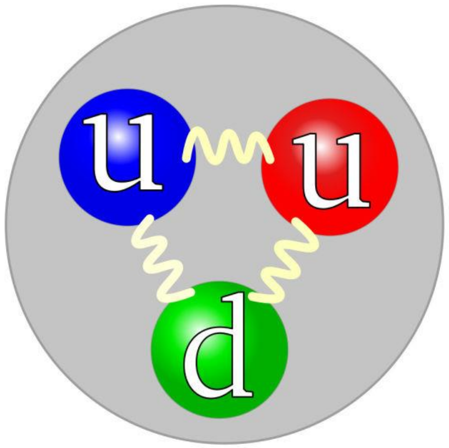
量子计算与高能核物理交叉前沿讲习班

Outlines

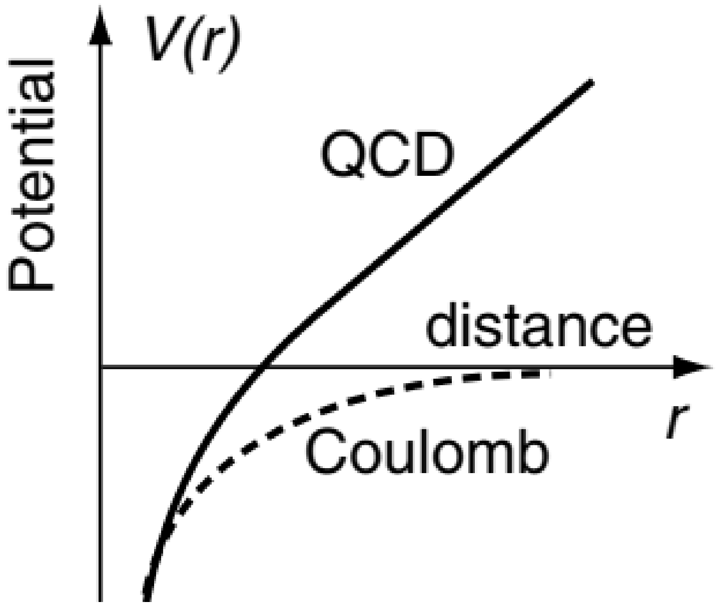
- nuclear matter as quantum many-body system
- quantum algorithm for finite-temperature systems
- demo: 1+1D Schwinger model
- discussion: phase diagram, non-abelian…

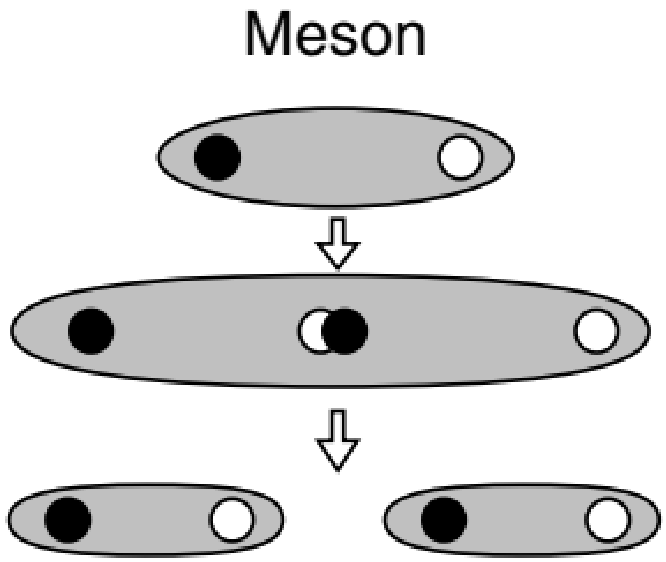
Confinement and QCD

proton



Strong interaction:
No single quark observed in nature

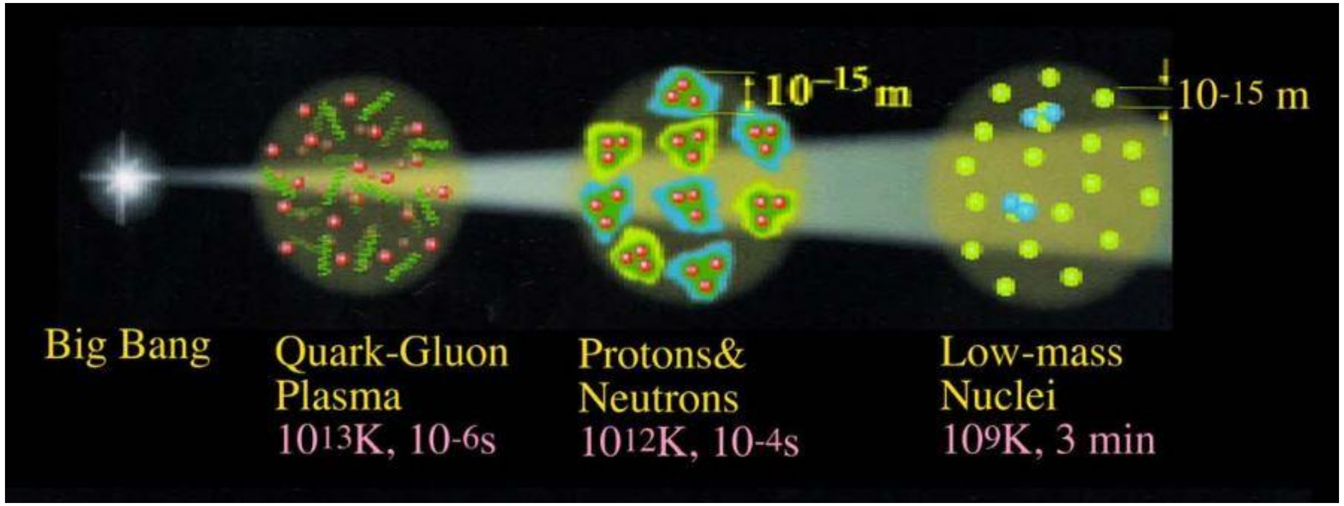




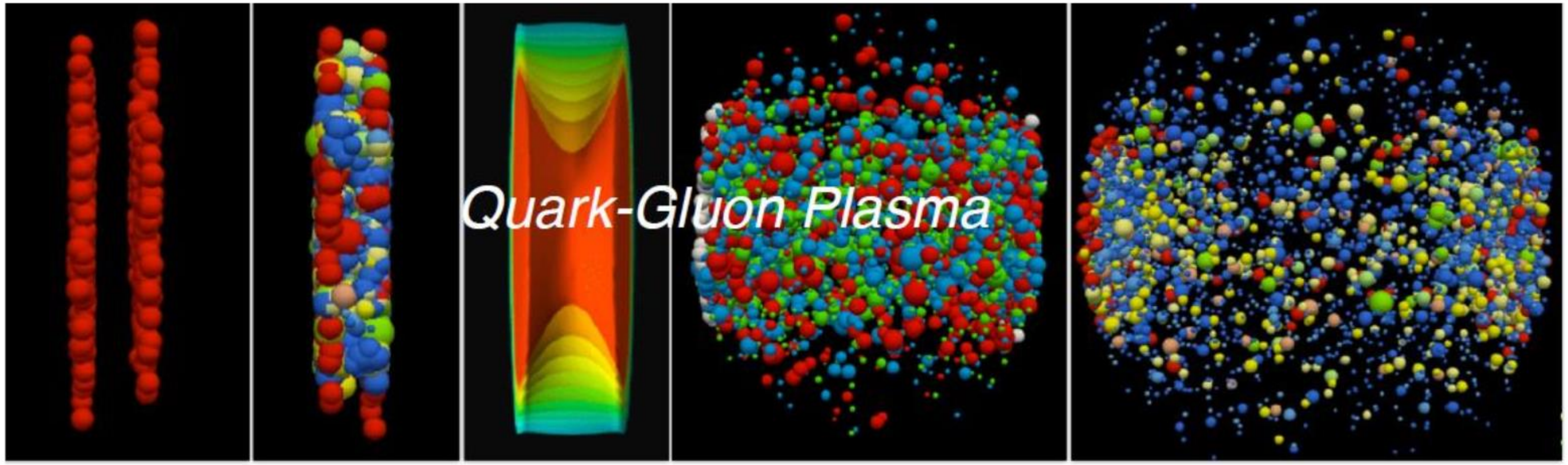
Deconfinement

- Early stage of universe

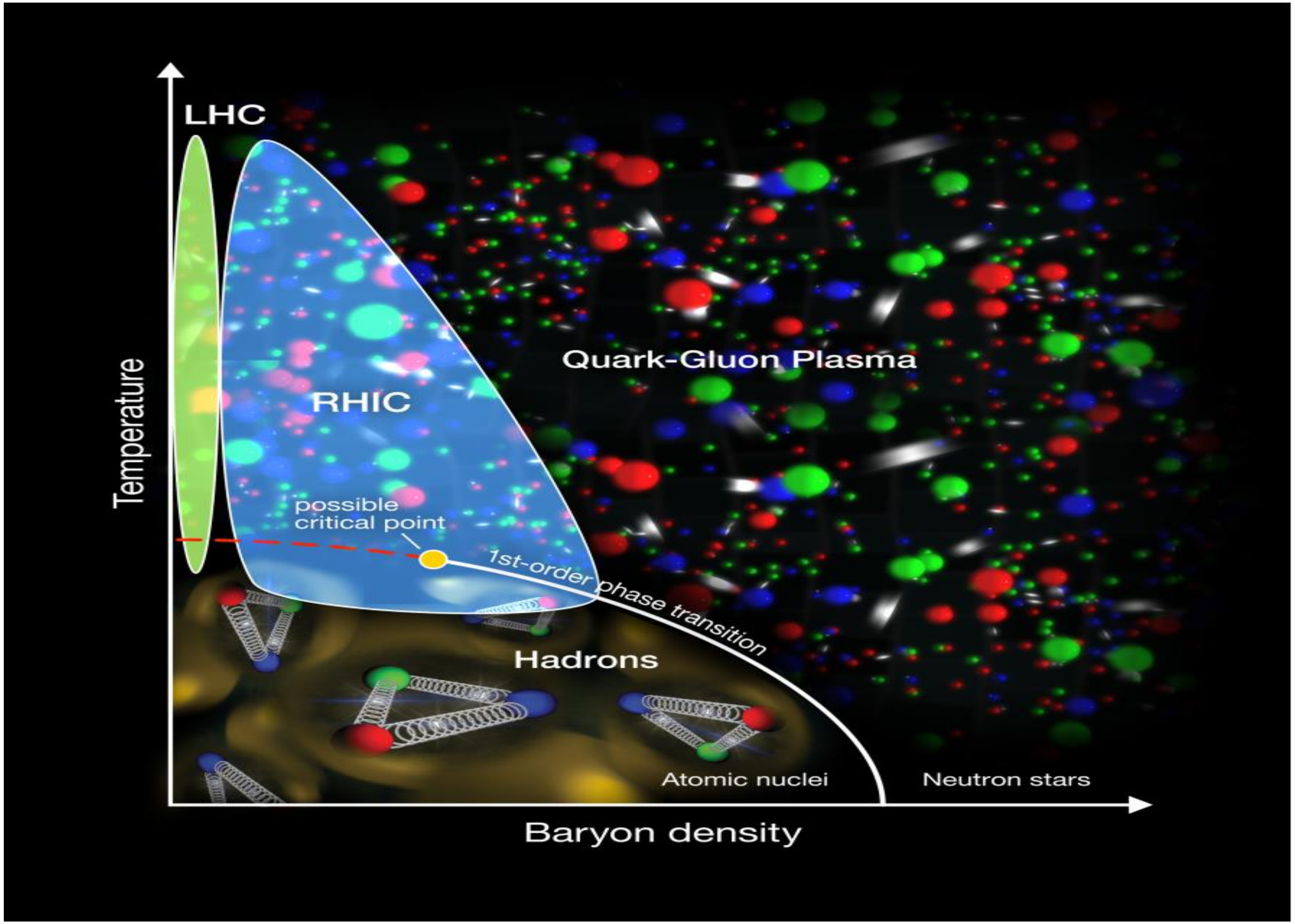
  (can quantum computer simulate the evolution of universe?)



- Nuclear collisions



QCD phase diagram



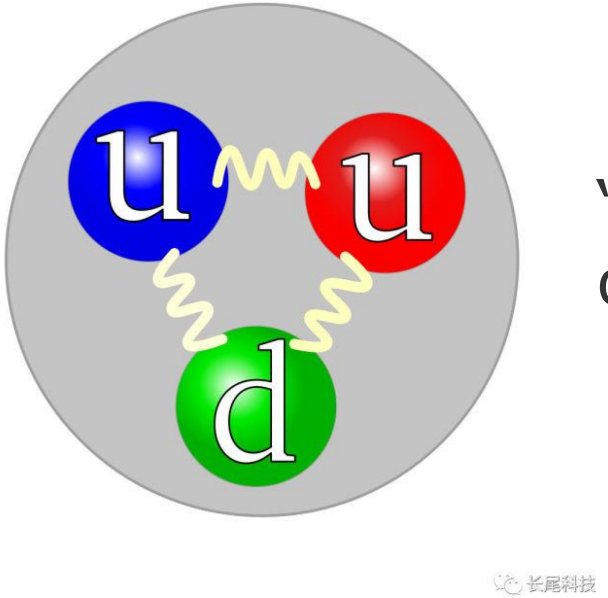
Quantum many-body System of quarks and gluons.

Sign problem at finite-temperature & finite-density

See 丁亨通

Parton picture for a hadron

Quark model,
By Gell-Mann
1964



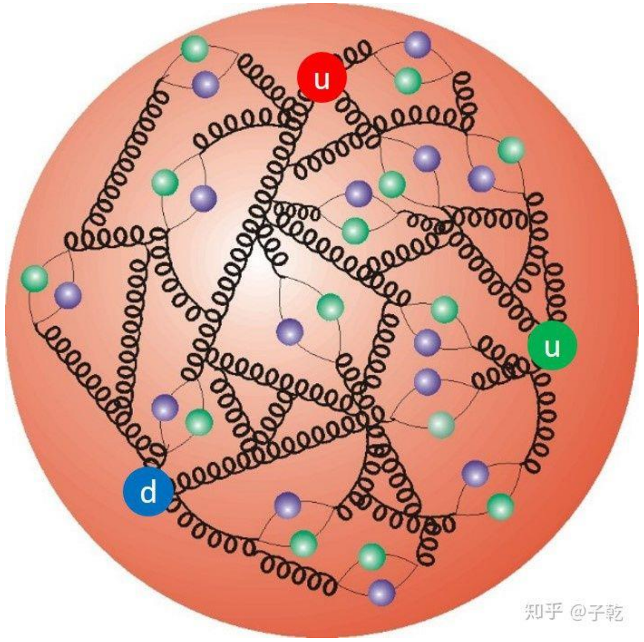
See 杨一玻

$$v \to c$$

Close to light speed

“Very High-Energy Collisions of Hadrons”

Parton model,
By Feynman,
1969

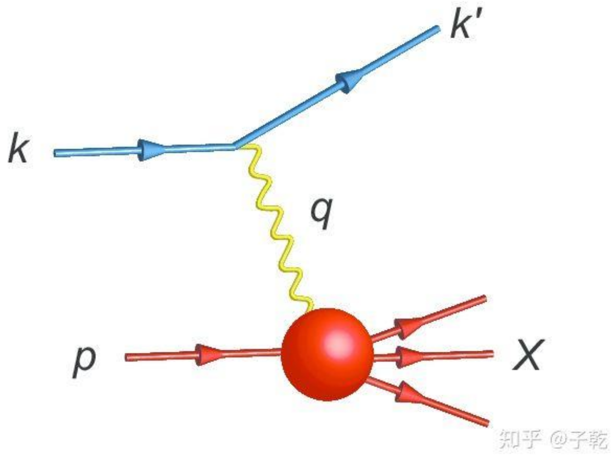


Quantum many-body system

See 周剑

How to “see” parton

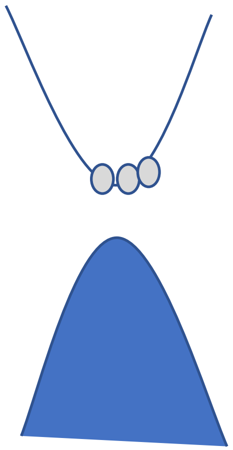
- Experiment: Deep inelastic scattering



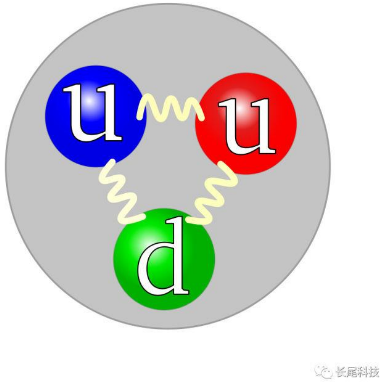
- Dynamical correlator (light-cone):

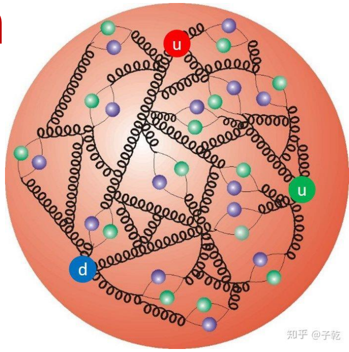
$$f_{q/h}(x) = \int \frac{dz}{4\pi} e^{-ixM_h z}$$
$$\times \langle h| \underline{e^{iHt}\bar{\psi}(0,-z)e^{-iHt}}\gamma^+\psi(0,0)\,|h\rangle$$

$\cancel{t = z}$



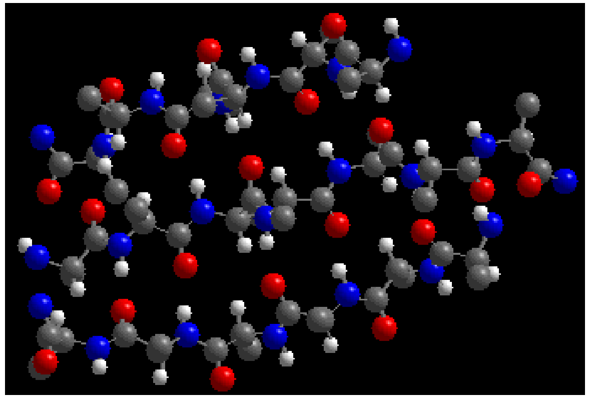
Real-time evoluiton

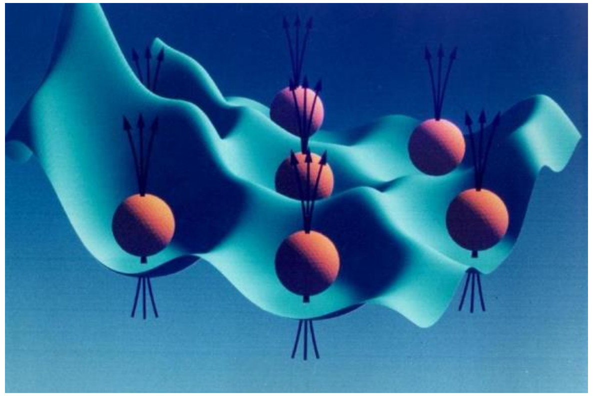




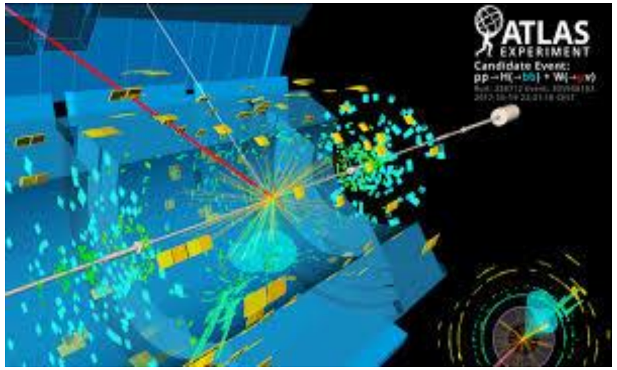
Many-body state of a proton is complicated!

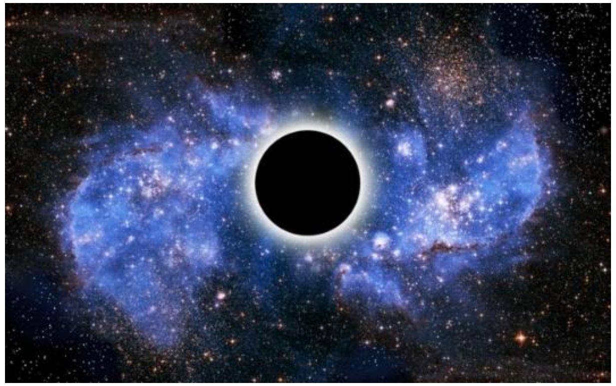
Feynman: a controllable quantum system can simulate other quantum systems





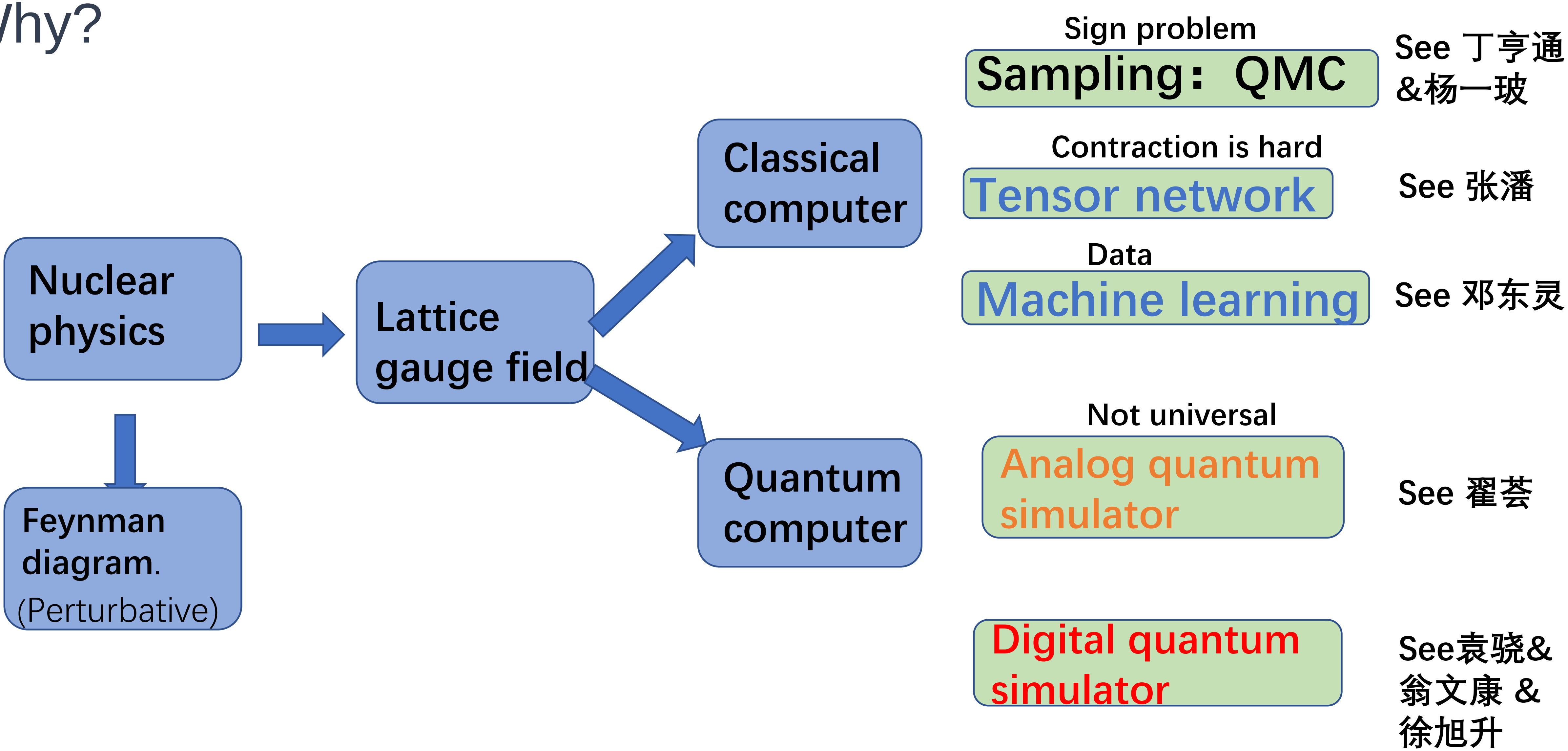
Quantum computer





Nuclear physics on a quantum computer

Why?



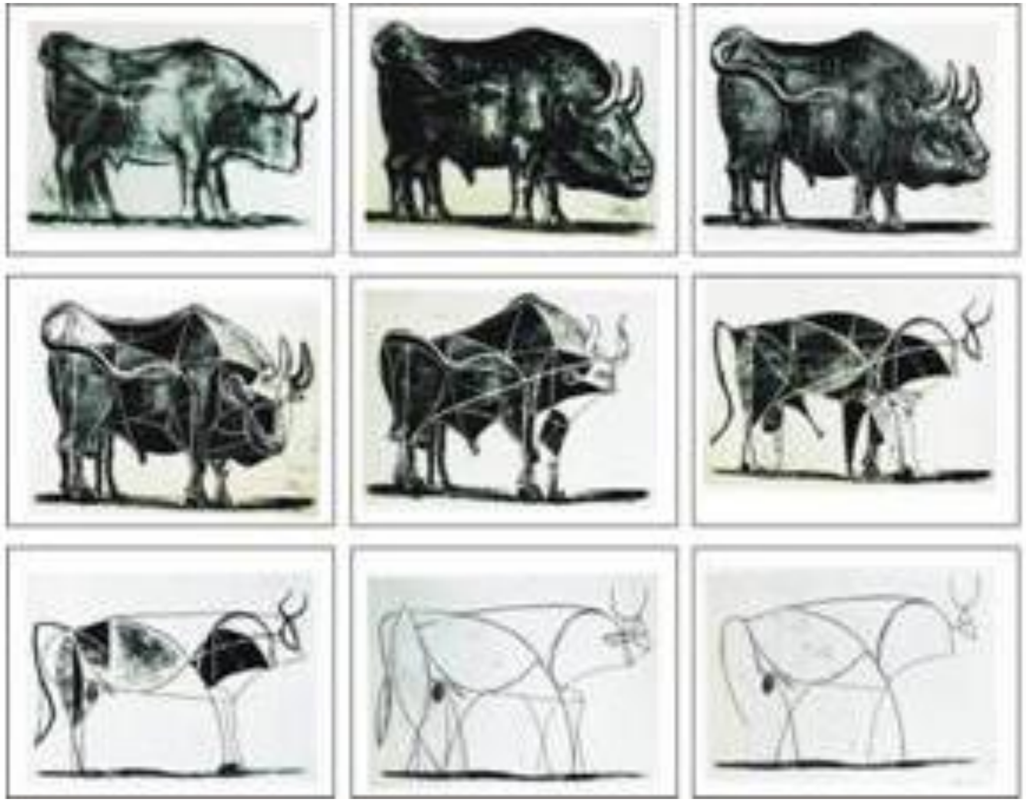
What make QCD special on a quantum computer?

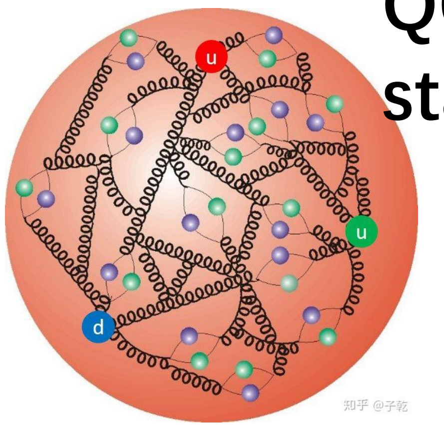
QCD	mapping	Quantum computer
• fermion with flavor, spin, color	$\xrightarrow{\text{JW transf}}$	• qubit
• gluon (continuous-variable)	$\xrightarrow{\text{Digitalization}}$	• qubit
• local gauge-invariance	$\xrightarrow[\text{(Gauss law)}]{\text{Local constraint}}$	• physical Hilbert space
• continue limit		• renormalizaiton?

seems too hard on near-term quantum computers

Nuclear matter in the eye of an artist

毕加索眼里的牛





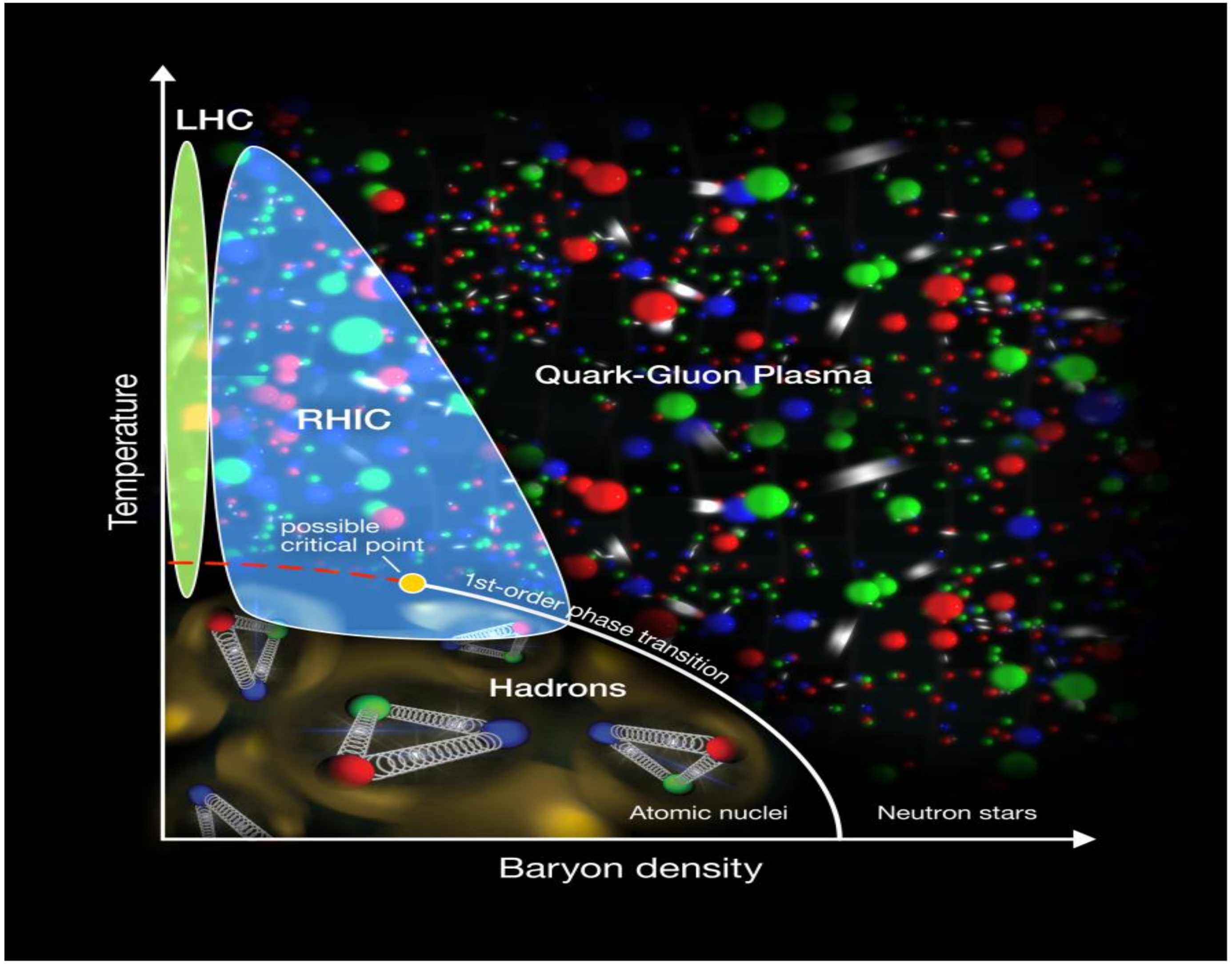
QCD at current stage is too hard

losing details but not the key features

?

Starting with some “toy models”, play with quantum computers

QuNu Collaboration @ SCNU



1. Hadron structure, simulated with 1+1D NJL model (no gauge field, only contact interaction)

- **Parton distribution function**

TYL, XYG, WKL, XHL, EKW, HX, **DBZ**, SLZ
PhysRevD.105.L111502(2022)

- **Light-Cone Distribution Amplitudes**

TYL, XYG, WKL, XHL, EKW, HX, **DBZ**, SLZ
arXiv:2207.13258 (2022)

2. Deconfinement at high temperature, simulated with 1+1D Schwinger model

XDX, XYG, HX,ZYX, **DBZ**, SLZ
PhysRevD.106.054509(2022)

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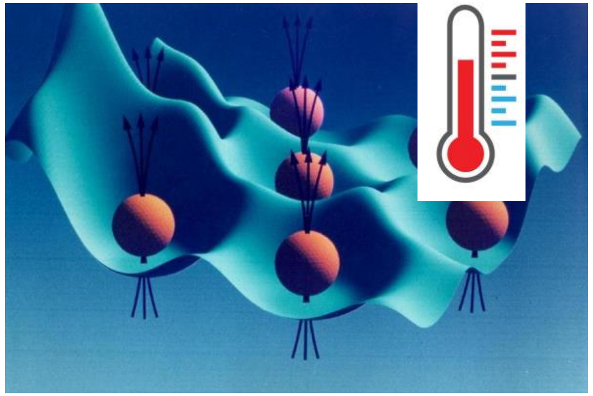
Simulation of finite-temperature quantum systems



- Important as the nature lives at finite-T

$$\rho(\beta) = e^{-\beta H}/Z(\beta)$$

$$Z(\beta) = \mathrm{Tr} e^{-\beta H} \quad T = 1/\beta$$

Mixed state: classical distribution of eigenstates of H

Nielson & chuang's textbook (2002)

should be weak. Obtaining ρ_{therm} for arbitrary H and T is generally an exponentially difficult problem for a classical computer. Might a quantum computer be able to solve this efficiently? We do not yet know.

- Quantum simulation / algorithm
  - imaginary time evolution
  - variational method by minimizing free energy

Poulin & Wocjan, PRL, 2009
Mario Motta, etc., Nat. Phys. 2019
Dan-Bo Zhang, etc., PRL, 2021

J. Wu & T. H. Hsieh, PRL, 2019
Liu, Mao, Zhang & Wang, 2021

Mixed state on a quantum computer?

- U|0>: quantum computer naturally for pure states!
  - mixed states in real quantum computers due to noises? Not controllable

- Mixed state from a trace of pure state

$$\rho = \mathrm{Tr}_B |\psi\rangle \langle\psi|$$

Schmidt decomposition $|\psi\rangle = \sum_i \sqrt{\lambda_i}\, |\psi_i^A\rangle \otimes |\psi_i^B\rangle$ $\quad \rho = \sum_i \lambda_i |\psi_i^A\rangle \langle\psi_i^A|$

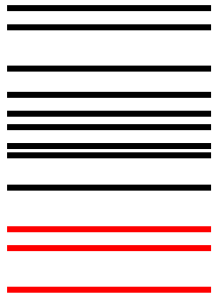
- Mixed state as a classical distribution of pure state

$$\rho = \sum_i \lambda_i |\psi_i^A\rangle \langle\psi_i^A|$$

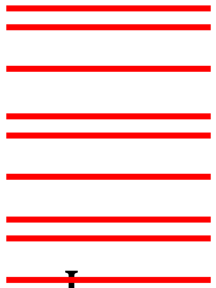
With a prob λ_i , generate a state $|\psi_i^A\rangle$

Complexity of Gibbs state

- low-temperature limit: large weighting on low-lying eigenstates



- high-temperature limit: almost equal-weighting
- infinite temperature: completely mixed state: the easiest one!

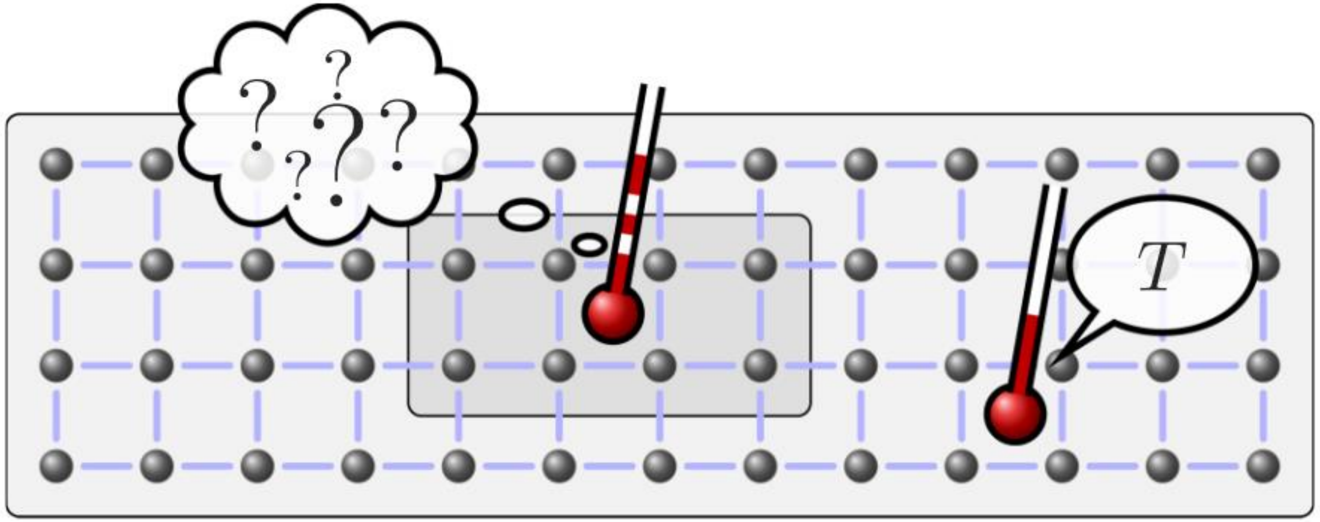


$$\mathrm{I}_{2^n}/2^n = 1/2^n \sum_i |\varphi_i><\varphi_i| = \frac{\mathrm{I}_2}{2} \otimes \frac{\mathrm{I}_2}{2} \otimes \ldots \frac{\mathrm{I}_2}{2}$$

Just product of one-qubit completely mixed state

- Locality of temperature

Phys. Rev. X **4**, 031019(2014)
Phys. Rev. X **11** 011047 (2021)



define temperature at length scale

$\mathcal{O}(\beta^{2/3})$

- **Infinite-T, totally local**
- **High-T, easy problem. Many methods work**

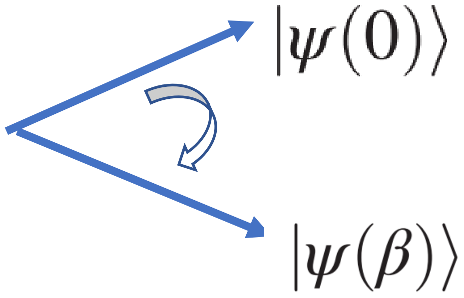
Gibbs states: imaginary time evolution

- Thermofield double (TFD) state (purification of Gibbs state)

$$|\psi(\beta)\rangle = \sum_n \frac{e^{-\beta E_n/2}}{\sqrt{\mathcal{Z}(\beta)}} |u_n^*\rangle_A \otimes |u_n\rangle_B \qquad \rho(\beta) = \mathrm{Tr}_A |\psi(\beta)\rangle\langle\psi(\beta)|$$

$$|\psi(\beta)\rangle = \sqrt{C} I \otimes e^{-\beta H/2} |\psi(0)\rangle \qquad |\psi(0)\rangle = (1/\sqrt{D}) \sum_n |n\rangle_A \otimes |n\rangle_B$$

- Implement imaginary time evolution (non-unitary operator) on quantum computer
  - find an (approximately) equal unitary operator
  - unitary evolution + projection

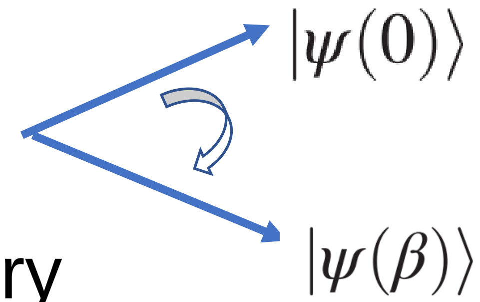


Quantum imaginary time evolution

Mario Motta, etc., Nat. Phys. 2019

- Trotter decomposition $\hat{H} = \sum_m \hat{h}[m]$

$$\mathrm{e}^{-\beta \hat{H}} = (\mathrm{e}^{-\Delta\tau\, \hat{h}[1]}\mathrm{e}^{-\Delta\tau\, \hat{h}[2]} \dots)^n + \mathcal{O}(\Delta\tau);\ n = \frac{\beta}{\Delta\tau}$$



- For each small imaginary-time evolution, find an unitary operation

$$|\bar{\Psi}'\rangle \equiv c^{-1/2}\, e^{-\Delta\tau \hat{h}[l]}|\Psi\rangle = e^{-i\Delta\tau \hat{A}[l]}|\Psi\rangle \qquad \hat{A}[l] = \sum_I a[l]_I \hat{\sigma}_I$$

Solve linear problem on classical Computer

$$\left(\mathbf{S} + \mathbf{S}^T\right)\mathbf{a}[l] = -\mathbf{b}$$

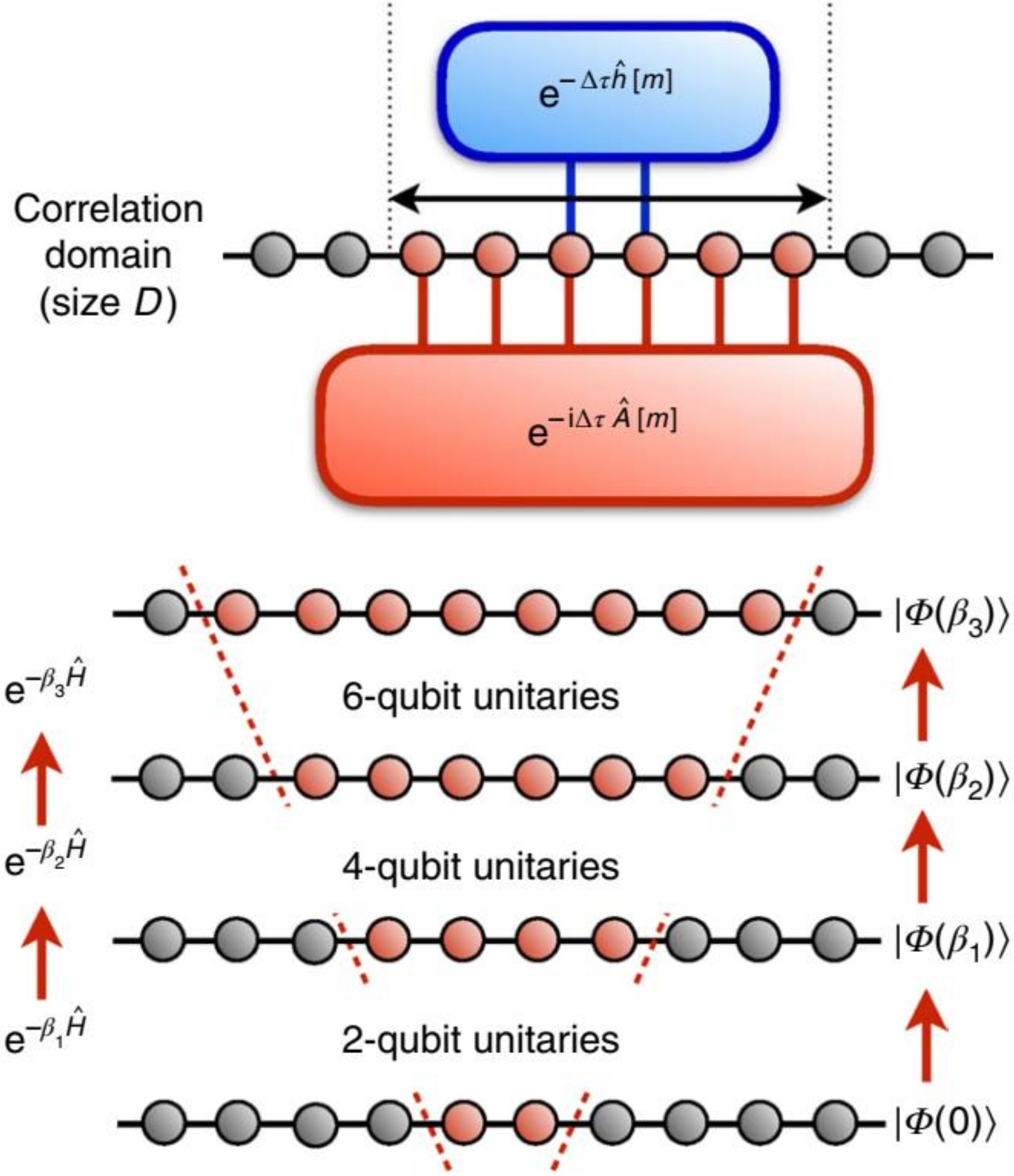
Measure on quantum computer

$$S_{IJ} = \langle\Psi|\hat{\sigma}_I^\dagger \hat{\sigma}_J|\Psi\rangle \quad ,$$

$$b_I = i\,\langle\Psi|\hat{\sigma}_I^\dagger|\Delta_0\rangle - i\,\langle\Delta_0|\hat{\sigma}_I|\Psi\rangle$$

Also see 袁骁： variational imaginary time evolution

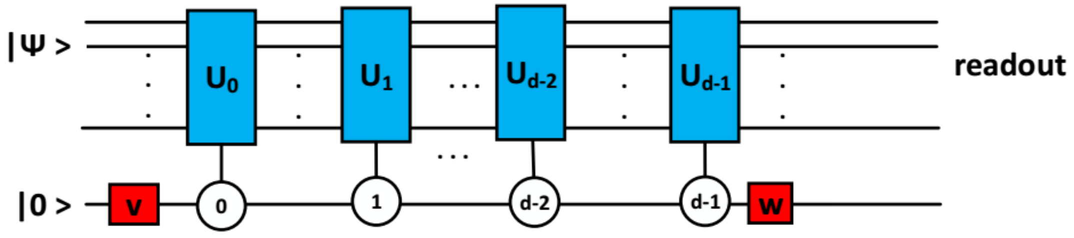
Few-qubit imaginary time evolution may corresponds to multi-qubit real-time evolution



Linear-combination-of-unitaries(LCU)

- An nonunitary operator can be expressed as a linear combination of unitaries, with $\log_2 d$ auxiliary qubits

$$L_r = \sum_{i=0}^{d-1} r_i U_i$$



Gui-Lu Long, 2002

A. M. Childs etc., , Siam. J. Comput. 46, 1920 (2017)

- Imaginary time evolution, by Fourier transformation

$$e^{-\beta h/2} = \int_{-\infty}^{\infty} dp R(\beta, p) e^{-ihp}, \qquad R(\beta, p) = \frac{2}{\pi} \frac{\beta}{\beta^2 + 4p^2}$$

Also see 袁骁：
universal cooling
（hybrid quantum-classical）

- Discretization of integral?
- Integral of unitaries with an auxillary continuous-variable(qumode)!

Qubits and Qumodes

- Qubit (discrete variable) : superposition of |0> and |1>

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

- Qumode (continuous variable) : “position” $|p\rangle$, “momentum” $|q\rangle$

$$[\hat{q},\hat{p}] = i\hbar$$

$$|p\rangle = \int dq e^{ipq}|q\rangle \qquad |\psi\rangle = \int dq\psi(q)\,|q\rangle = \int dp\psi(p)\,|p\rangle$$

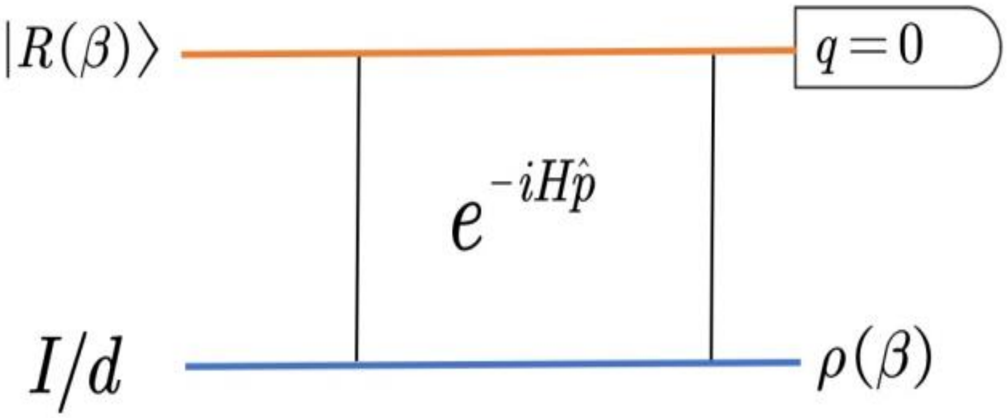
Undergrad math for a simple quantum algorithm

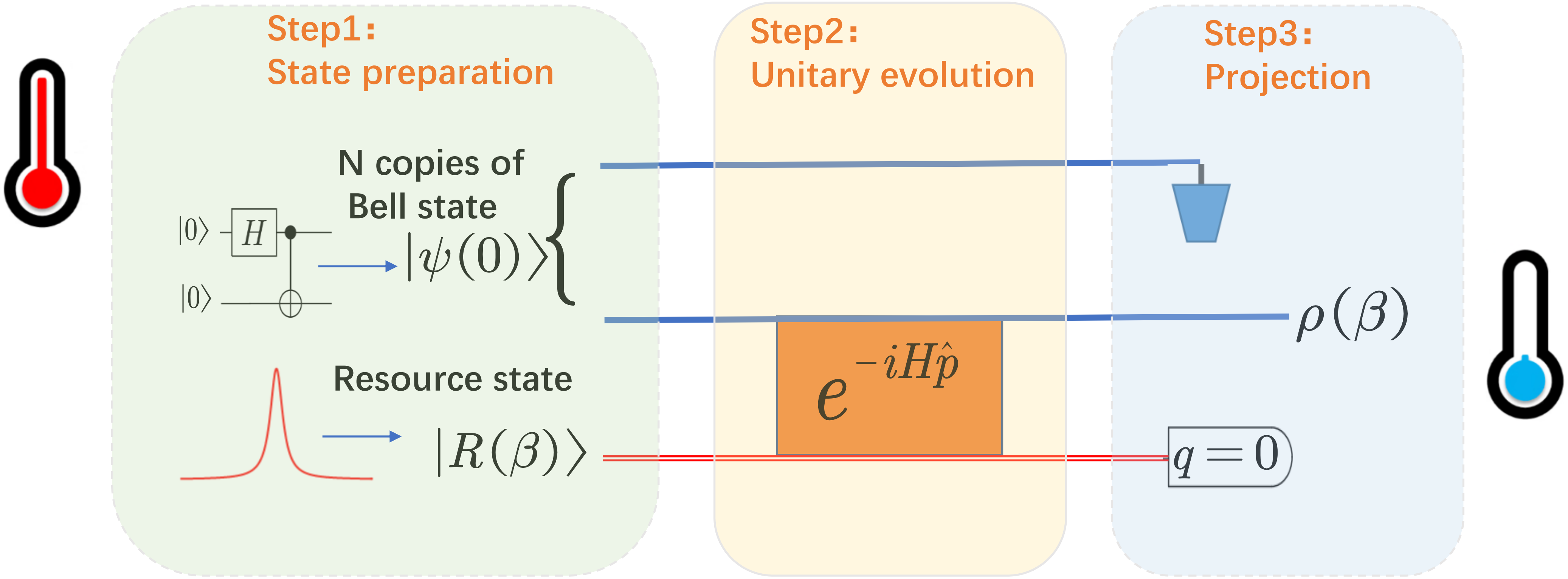
- Continuous-Variable Assisted Thermal Quantum Simulation

Dan-Bo Zhang, etc., PRL,127, 020502 (2021)

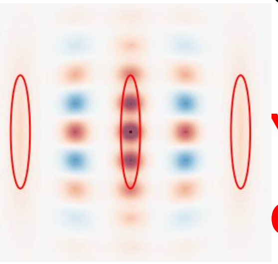
$$e^{-\beta h/2} = \int_{-\infty}^{\infty} dp R(\beta, p) e^{-ihp}, \qquad R(\beta, p) = \frac{2}{\pi} \frac{\beta}{\beta^2 + 4p^2}$$

$$e^{-\beta H/2} = \int_{-\infty}^{\infty} dp R(\beta, p) e^{-iHp} \propto \langle 0_q | e^{-iH\hat{p}} | R(\beta) \rangle \qquad |R(\beta)\rangle = \sqrt{\beta\pi} \int_{-\infty}^{\infty} dp R(\beta, p) |p\rangle_p$$





Can resource state R efficiently prepared?

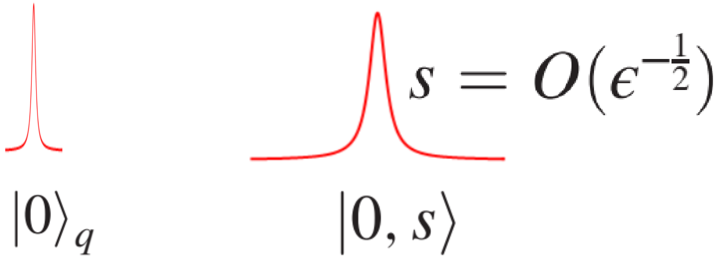


Yes, rapid progress on bosonic code

How to implement the evolution?

Yes. Efficient with Trotterizaton

The projection can be made only with finite squeezing!



Test: simulate quantum critical regime

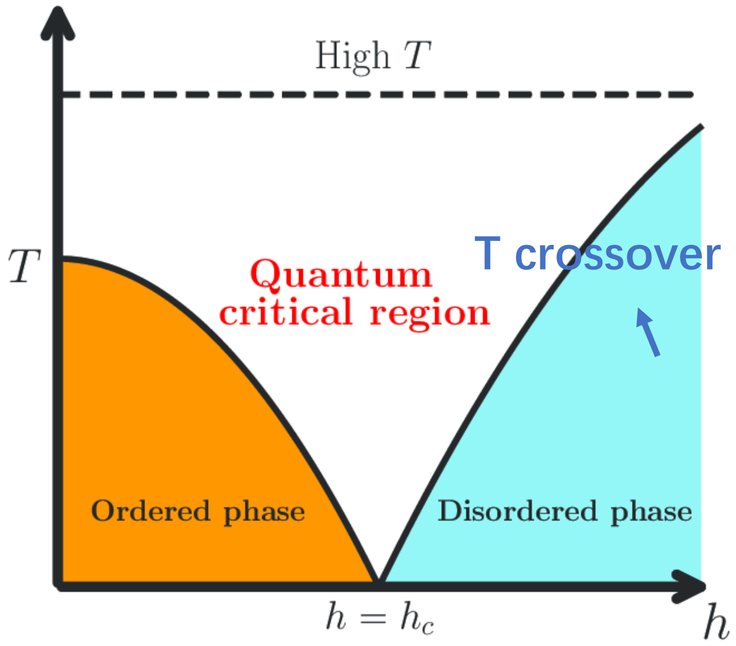
- quantum phase transition occurs at T=0,

but the quantum critical point affects physics at finite T, e.g., high-Tc superconductor

- quantum critical region: interplay

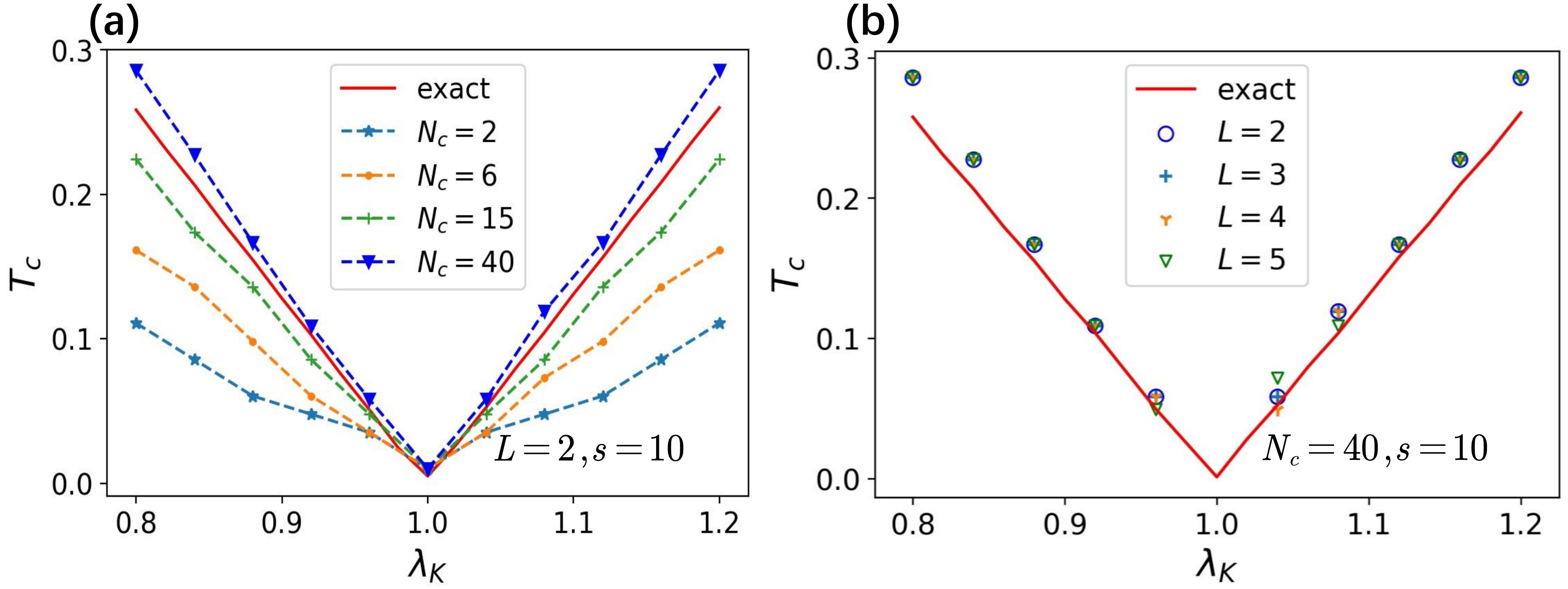
between quantum and thermal fluctuations

- a testbed for quantum simulation



Analog of QCD phase diagram?

- p-wave superconductor on a ring $H_K = -J\sum_{i=1}^{L}(c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger + \mathrm{H.c.}) - \mu\sum_{i=1}^{L} c_i^\dagger c_i$



Gibbs states: variational principle

- Zero temperature: ground state by minimizing the energy

$$\min_{\vec{\theta}} E\left(\vec{\theta}\right) \geqslant E_{gs}$$

- Finite temperature: minimizing free energy

$$Min_{\theta}\ F(\theta) := E(\theta) - TS(\theta) \geqslant\ F_0$$

Role of entropy: distribution!

Q: how to evaluate S? $S = -\mathrm{Tr}\,\rho\log\rho$

Not like a Hermitian operator

Measurement of entropy

- Measurement of observables $\mathbf{M} = \sum_i C_i \mathbf{P}_i \qquad \langle \mathbf{M} \rangle = \sum_i C_i \langle \mathbf{P}_i \rangle$

- Entropy is a function of state itself: statistics of the spectrum of density matrix
- Von-Neumann entropy $S = -\mathrm{Tr}\,\rho \log \rho = -\sum_i \lambda_i \log \lambda_i$

- Rényi entropy

$$S_n = \frac{1}{1-n} \log \mathrm{Tr}\,\rho^n$$

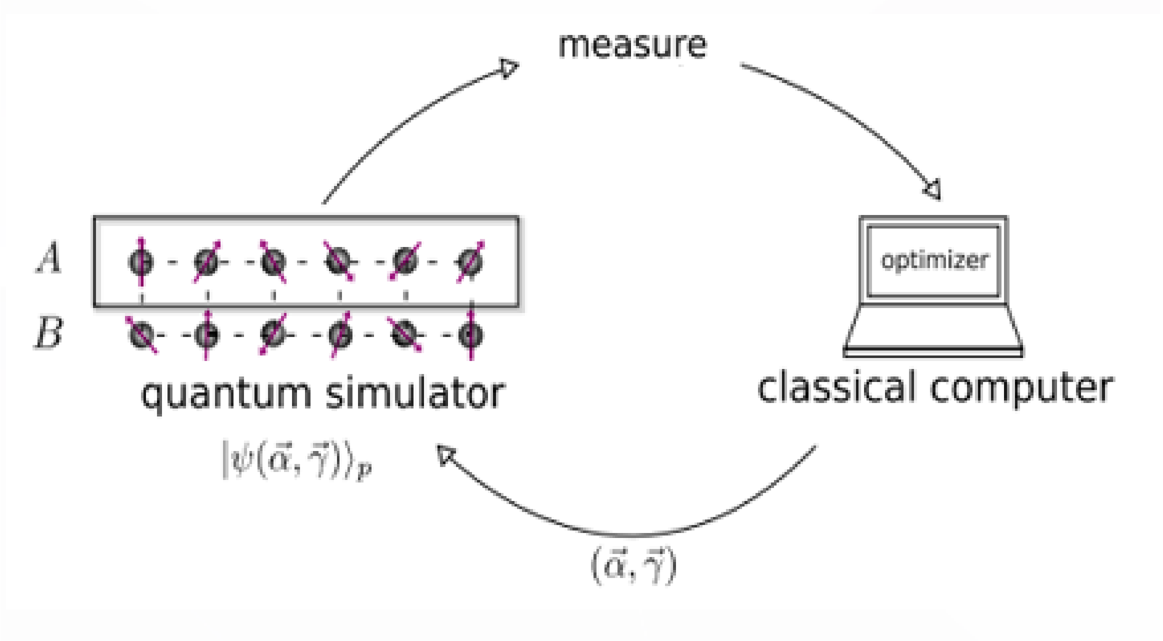
n=2, purity!

- **General Swap test with n copies**
- **Random measurements with t-design (t=n)**

Von-Neumann entropy is still hard to measure

Variational preparing TFD state

Jingxiang Wu and Timothy H. Hsieh, PRL 123, 220502 (2019)



$$|\boldsymbol{\varphi}(\boldsymbol{\alpha},\boldsymbol{\gamma})\rangle_{\boldsymbol{p}} = \prod_{i}^{p} e^{i\alpha_i H_{AB}} e^{i\gamma_i (H_A+H_B)/2} |\boldsymbol{TFD}(\mathbf{0})\rangle$$

Minimizing the infidelity:
(how to do the overlap? Moreover, global type cost, see 邓东灵)

$$F_p(\vec{\alpha},\vec{\gamma}) = 1 - |\langle \mathrm{TFD}(\beta)|\psi(\vec{\alpha},\vec{\gamma})\rangle_p|^2$$

Minimizing the free energy
(how to measure entropy?):

$$F_A = E_A - TS_A$$

Gibbs state as classical distribution of eigenstates

Jin-Guo Liu & Lei Wang, arXiv:1912.11381

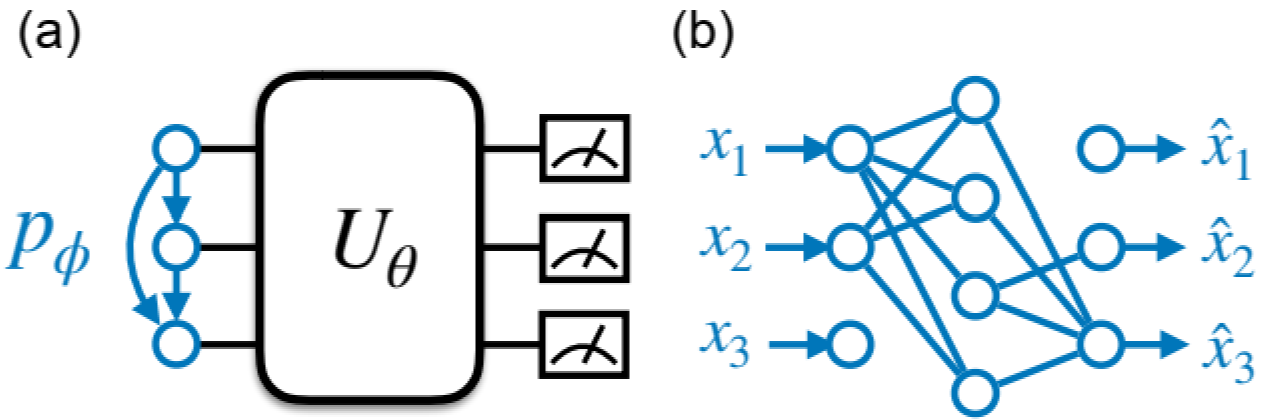
$$\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

Cooperation between classical neural network and variational quantum circuit!

$$\rho = \sum_x p_\phi(x) U_\theta |x\rangle\langle x| U_\theta^\dagger$$

Classical prob

$$S = -\sum_i p_i \log\, p_i$$



Minimizing the free energy

$$F_A = E_A - TS_A$$

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Model: 1+1D Schwinger model

- 1+1D quantum electrodynamics (U(1) gauge field)

$$\mathcal{L} = \bar{\psi}\left(\gamma^{\mu}(i\partial_{\mu} + gA_{\mu}) - m\right)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$

Electric flux

- 麻雀虽小， 五脏俱全。 Confinement, dynamical generated mass(gapped at m=0), chiral symmetry breaking…

- familiar to quantum computing community as easy to simulate. (Also see 翟荟, which is a Z_2 Schwinger Model)

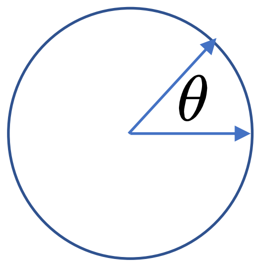
- Deconfinement at infinite temperature
  PRD 19.1188(1979)

Lattice Hamiltonian + Gauss law

U(1) gauge theory

- lattice Hamiltonian

$$H = \frac{1}{2a}\sum_{j=1}^{N-1}[\hat{\Phi}_j^{\dagger}\hat{U}_{j,j+1}\hat{\Phi}_{j+1} + h.c.] + m\sum_{j=1}^{N}(-1)^j\hat{\Phi}_j^{\dagger}\hat{\Phi}_j + \frac{g^2 a}{2}\sum_{j=1}^{N-1}\hat{L}^2_{j,j+1}$$



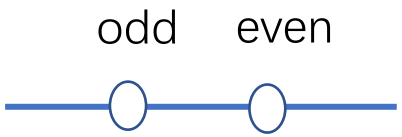
$$\hat{U}_{j,j+1} = e^{i\theta_{j,j+1}}$$

$$[\theta_{j,j+1}, L_{j',j'+1}] = -i\delta_{j,j}$$

$$\hat{U}|l\rangle = |l+1\rangle$$

- Gauss law: physical Hilbert space with local constraints

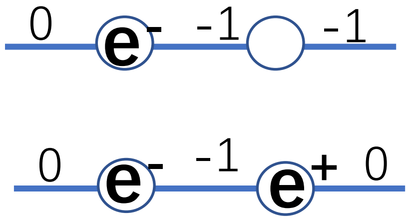
Stagger fermion



$$\hat{L}_{j,j+1} - \hat{L}_{j-1,j} = \hat{\Phi}_j^{\dagger}\hat{\Phi} - \frac{1-(-1)^j}{2}$$

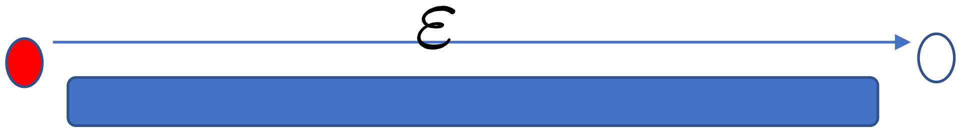
Odd: 0 (e^-), 1 (empty)

even: 1 (e^+), 0 (empty)



- Open boundary

Background field with a pair of charges



$$\hat{L}_{j,j+1} = \varepsilon + \sum_{l=1}^{j} [\hat{\Phi}_j^{\dagger}\hat{\Phi}_j - \frac{1-(-1)^l}{2}]$$

- and with $\hat{\Phi}_j \rightarrow \prod_{l=1}^{j-1} \hat{U}_{j,j+1}\hat{\Phi}_j$
- Hamiltonian with only fermions

$$H = \varpi \sum_{j=1}^{N-1} (\hat{\Phi}_j^{\dagger}\hat{\Phi}_{j+1} + h.c.) + m \sum_{j=1}^{N} (-1)^j \hat{\Phi}_j^{\dagger}\hat{\Phi}_j$$

$$+ \frac{g^2 a}{2} \sum_{j=1}^{N-1} \left\{ \varepsilon + \sum_{l=1}^{j} [\hat{\Phi}_j^{\dagger}\hat{\Phi}_j - \frac{1-(-1)^l}{2}] \right\}^2$$

- Jordan-Wigner transformation $\hat{\Phi}_j = \prod_{l=1}^{j-1}(i\sigma_l^z)\sigma_j^-$

$$H_\varepsilon = \varpi \sum_{j=1}^{N-1} [\hat{\sigma}_j^+ \hat{\sigma}_{j+1}^- + h.c.] + \frac{m}{2} \sum_{j=1}^{N} (-1)^j \hat{\sigma}_j^z$$

$$+ \underbrace{\frac{g^2 a}{2} \sum_{j=1}^{N-1} \left\{ \varepsilon + \sum_{l=1}^{j} \left[\hat{\sigma}_l^z + (-1)^l \right] \right\}^2}_{\text{Long range interaction}},$$

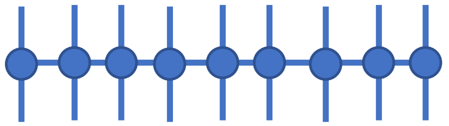
Long range interaction

Tensor network approach

Hamiltonian simulation of the Schwinger model at finite temperature

Boye Buyens, Frank Verstraete, and Karel Van Acoleyen
Phys. Rev. D **94**, 085018 – Published 21 October 2016

- **Matrix Product Operators to represent Gibbs states**



- **Works for infinite long chain with iTEBD. Free of sign problem.**

- **Gauge invariant enforced by projector P (Gauss law)**

$$\langle Q\rangle_\beta = \frac{\mathrm{tr}(PQPe^{-\beta H})}{Z(\beta)} \text{ with } Z(\beta) = \mathrm{tr}\left(Pe^{-\beta H}\right)$$

String tension: indicator of confinement/deconfinement

- String tension as the difference of free energies with/without a pair of charges at boundaries

$$\sigma_\varepsilon(\beta) = \frac{1}{Nga}\left(F_\varepsilon(\beta) - F_0(\beta) - f_\varepsilon\right)$$

H_0

H_ε

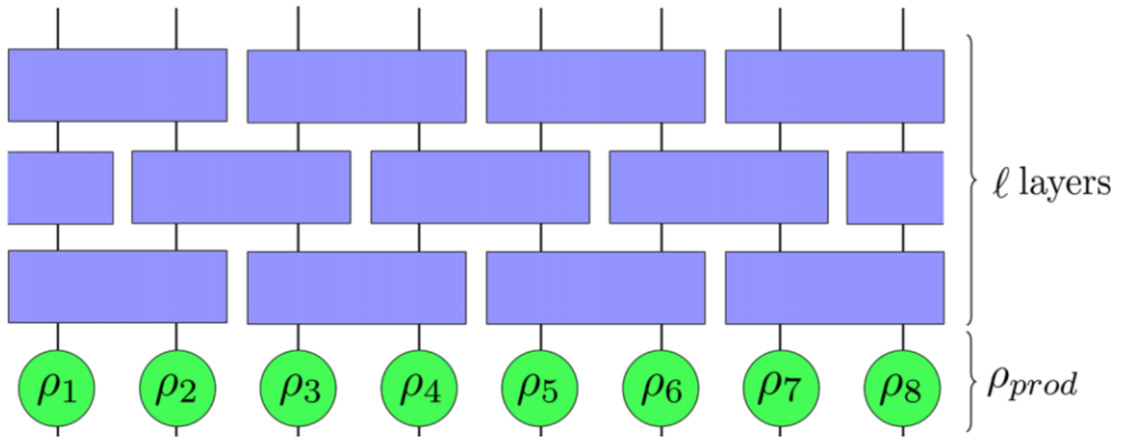
- **Zero T. A linear potential between two charges(qqbar)**

- **Increasing T: the string is weaken by thermal fluctuations of qqbar.**

First try with quantum algorithm

- Get free energy is necessary

- Method: variational quantum algorithm for evaluating the free energy



Product spectrum ansatz

$$\rho(\boldsymbol{\omega}) = U(\phi)\rho_0(\theta)U^\dagger(\phi)$$

Entropy not change with U

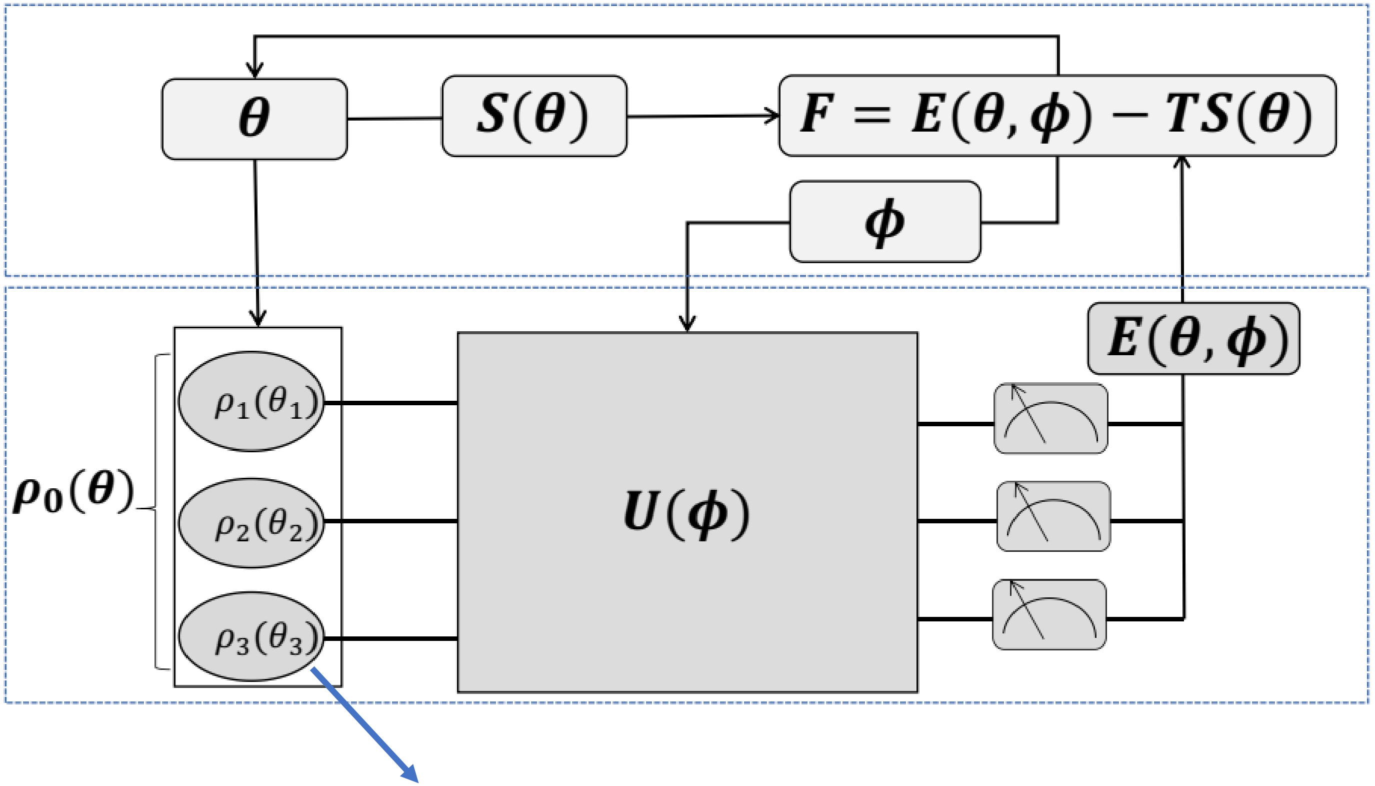
- **Minimize free energy:** $F(\beta) = E(\beta) - TS(\beta)$

Classical computer ($S(\beta)$)

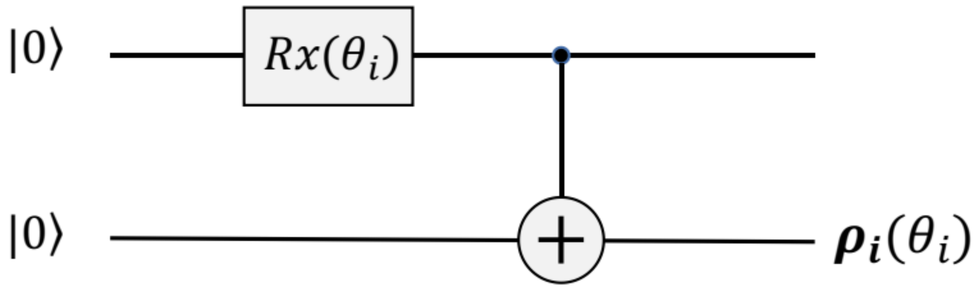
Quantum computer ($E(\beta)$)

Illustration of the algorithm

Hybrid quantum-classical optimization



One-qubit mixed state
from a two-qubit entangled state



How about finite-density?

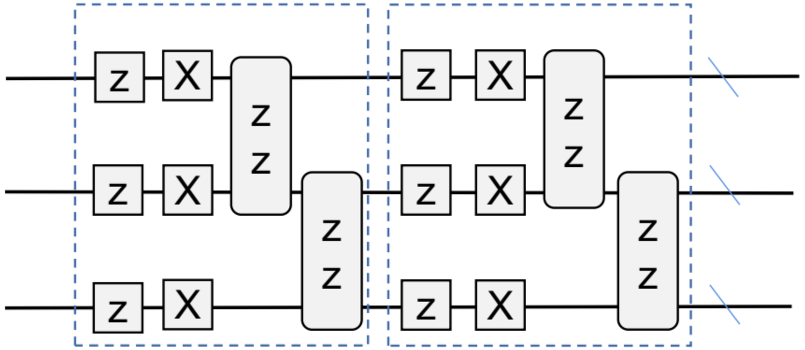
- For Monte Carlo, finite-density leads to sign problem

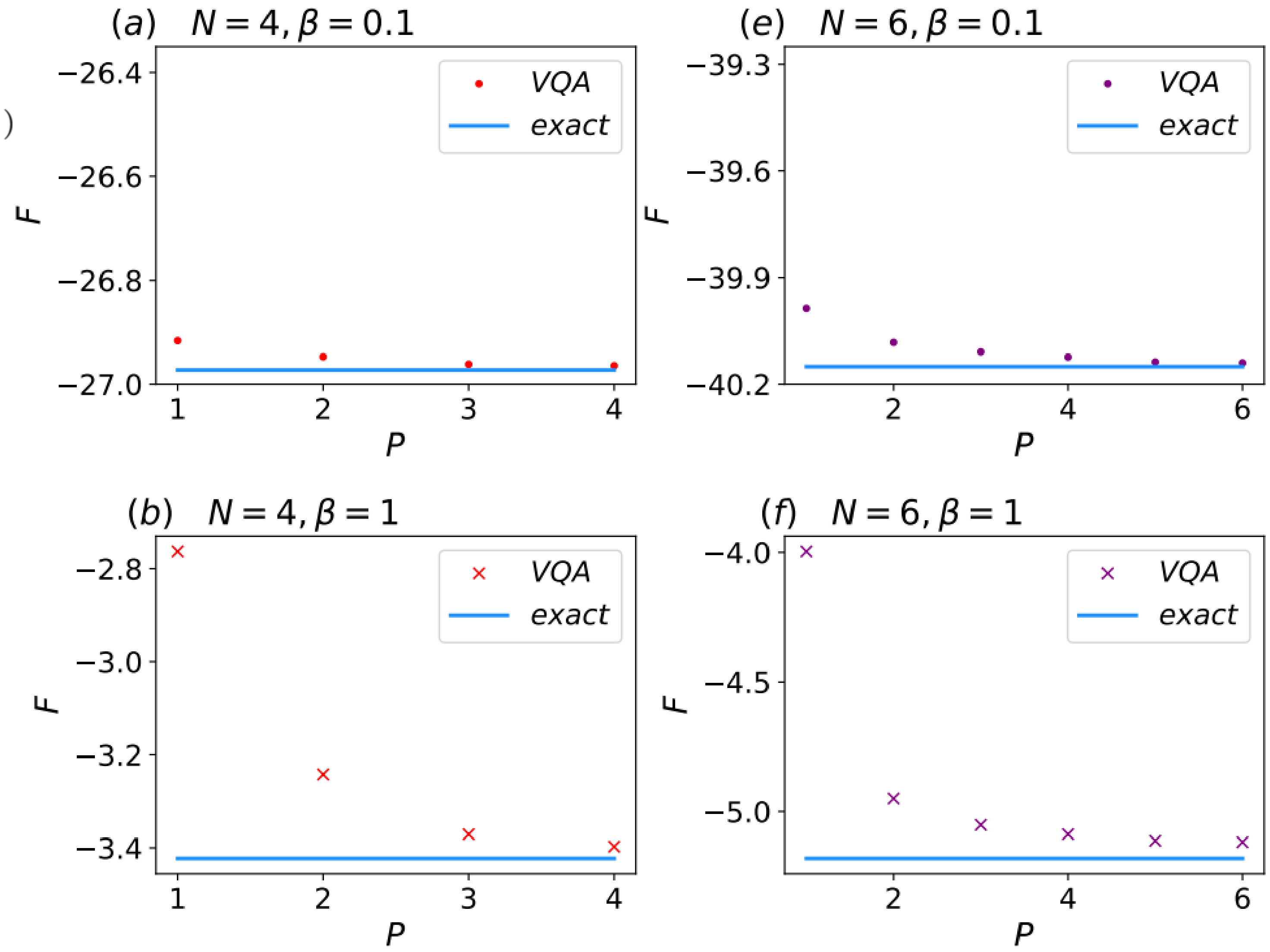
- Quantum computing puts finite-density and zero-density on the same footing by involving chemical potential

$$H_\varepsilon \Rightarrow G_\varepsilon(\mu) = H_\varepsilon - \frac{\mu}{2}\sum_{j=1}^{N} \hat{\sigma}_j^z$$

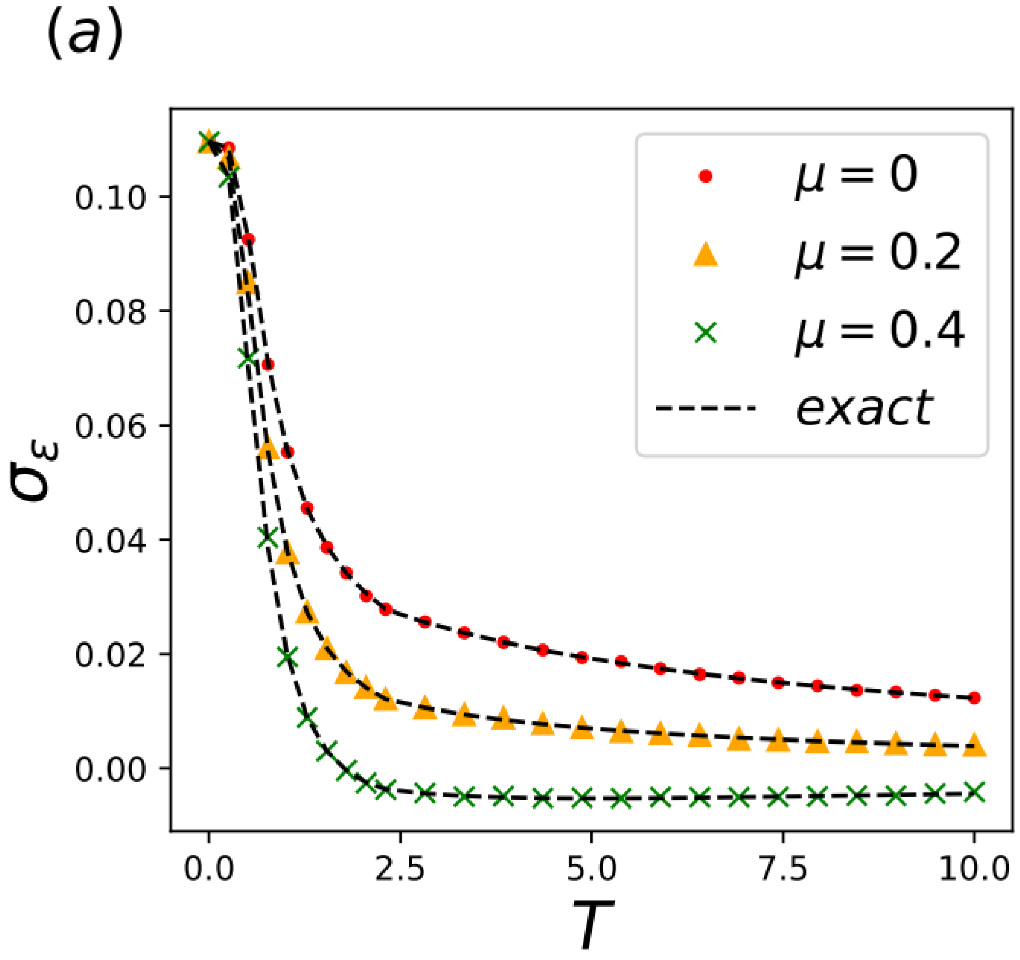
Results: accuracy vs circuit depth

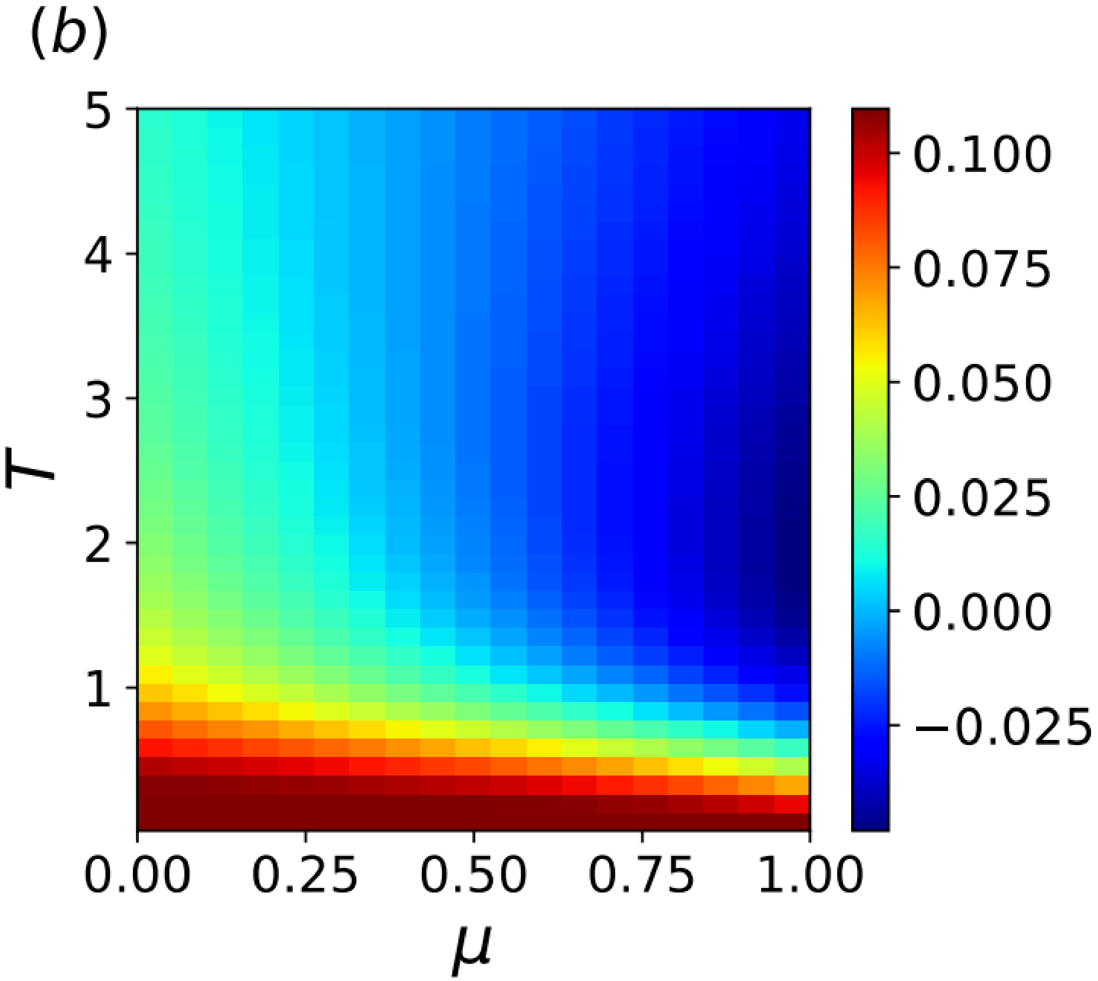
$$U(\phi) = \prod_{l=1}^{p} e^{-iH_{zz}(\alpha_l)} e^{-iH_x(\lambda_l)} e^{-iH_z(\zeta_l)}$$





String tension at finite-T finite-density

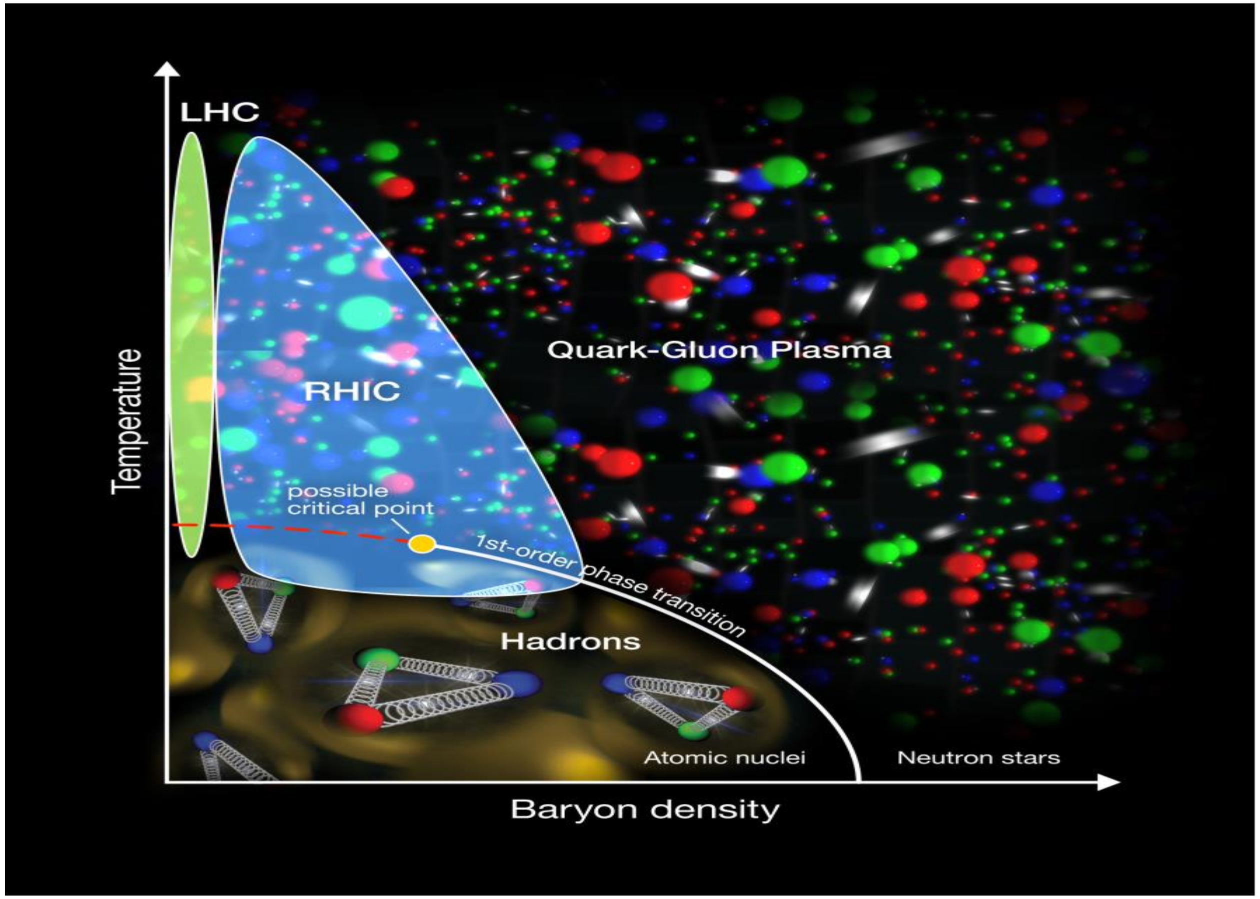




Outlines

- nuclear matter as quantum many-body system
- quantum algorithm for finite-temperature systems
- demo: 1+1D Schwinger model
- discussion: phase diagram, non-abelian…

Phase diagram of QCD



Textbook of statistical physics: if we can calculate free energy, then we can get everything

- Equation of state
- Critical point
- …

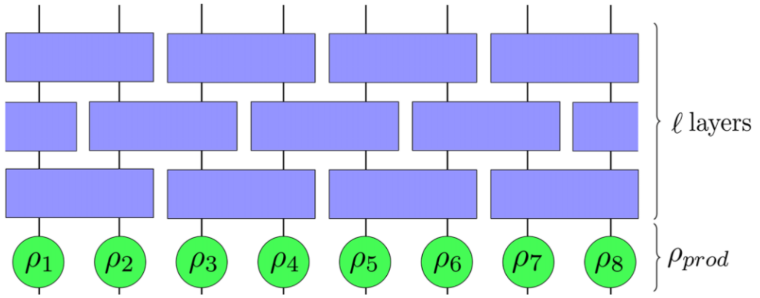
Q1: Can we efficiently and accurately calculate free energy on a quantum computer?

Q2: Can we really simulate QCD on a quantum computer?

Q1: quantum simulation of finite-T system

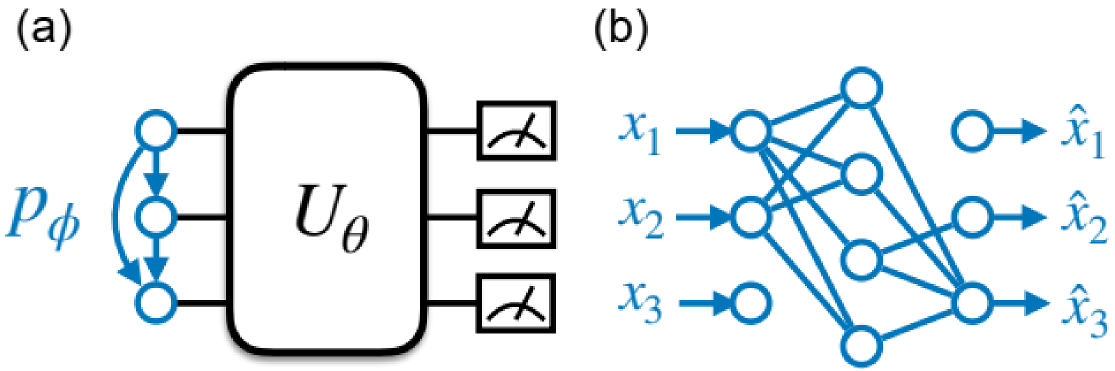
- **efficiently and accurately calculate free energy?**

$$\rho = \sum_x \underline{p_\phi(x)} U_\theta |x\rangle\langle x| U_\theta^\dagger$$



n may be not sufficient

How many parameters to determine the classical distribution?

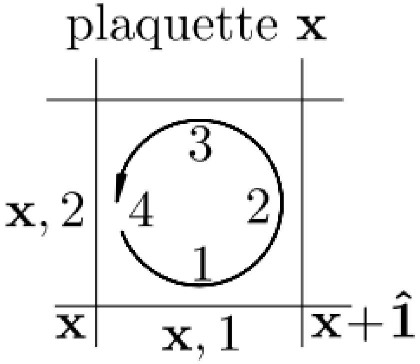


- **hard to optimize (Lei Wang)**
- **analog quantum simulator? but how to control temperature?**

Q2: simulate QCD

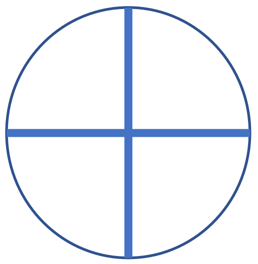
- 1+1D, no problem for even SU(2), SU(3), as gauge field can be eliminated by Gauss law.

- d+1D, even U(1) demands lots of quantum resource.



- digitalization of gauge field (see NuQS Collaboration)

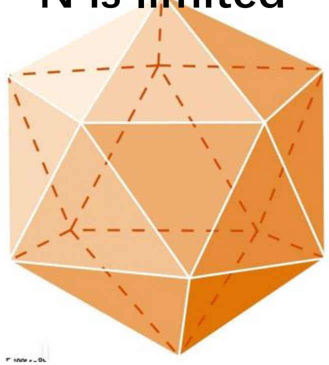
U(1) → Z_N, subgroup, approach U(1)



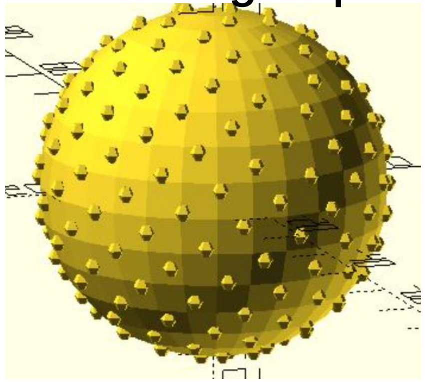
$\log_2 N$ **qubits**

SO(3) → Uniform covering?

N is limited



Not a group



Conclusion

- Simulate finite-temperature and finite-density systems with quantum computer. In principle, no problem.

- Simulate QCD phase diagram? Great challenge at mapping the lattice model on a quantum computer.