Schwinger model at finite temperature and density with classical-quantum hybrid algorithm

Akio Tomiya, IPUT Osaka
akio_AT_yukawa.kyoto-u.ac.jp

自己紹介
素粒子物理、機械学習

なにをしてる人？

素粒子物理の理論的研究をしています。

機械学習を理論計算の効率化に使いたいです。

主な論文 https://scholar.google.co.jp/citations?user=LKVqy_wAAAAJ

Detection of phase transition via convolutional neural networks
A Tanaka, A Tomiya
Journal of the Physical Society of Japan 86 (6), 063001
ニューラルネットを使った相検出

Evidence of effective axial $U(1)$ symmetry restoration at high temperature QCD
A Tomiya, G Cossu, S Aoki, H Fukaya, S Hashimoto, T Kaneko, J Noaki, ...
Physical Review D 96 (3), 034509
格子QCDを用いたU(1)量子異常の消失の証拠

Digital quantum simulation of the schwinger model with topological term via adiabatic state preparation
B Chakraborty, M Honda, T Izubuchi, Y Kikuchi, A Tomiya
arXiv preprint arXiv:2001.00485
量子コンピュータ

略歴

2010 ：兵庫県立大学理学部物質科学科卒、超伝導

2015 ：大阪大学で博士号取得。素粒子論。

2015 - 2018 : 華中師範大学でポスドク (中国、武漢)

2018 - 2021 : 理研/BNLでポスドク (米国、NY)

2021 - ：大阪国際工科専門職大学、助教

Outline

1. Background motivation
   (Why quantum algorithms are needed?)

2. Statistical thermodynamics with density matrix

3. QFT with Hamiltonian & Schwinger model

4. VQE and beta VQE

5. Simulation results

6. Summary

Background motivation:
Why quantum algorithms are needed?

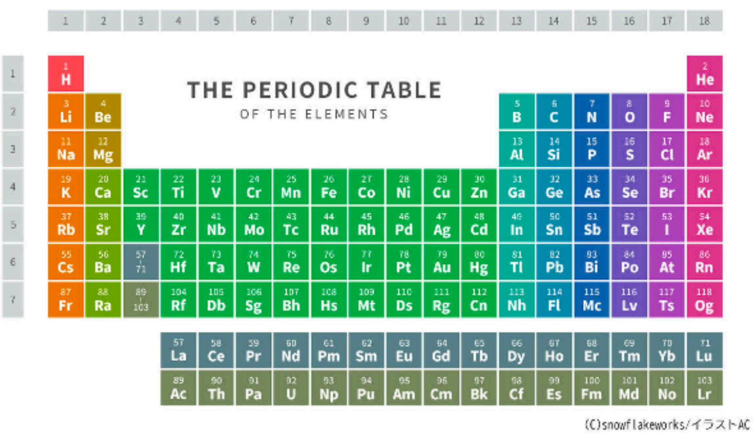
理論物理って何をするの？

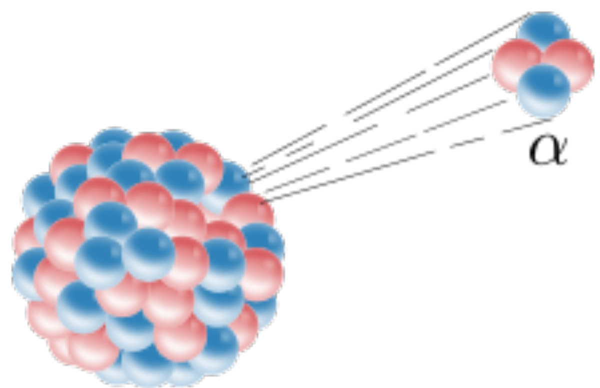
物理学の大きさによる分類

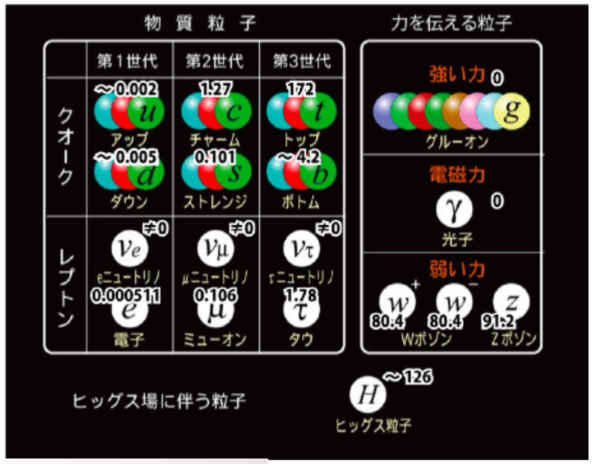
Akio Tomiya

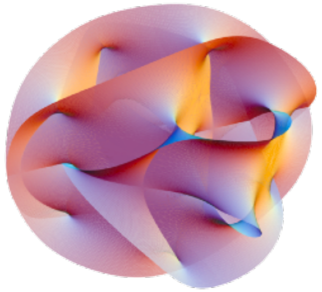
実験できる限界

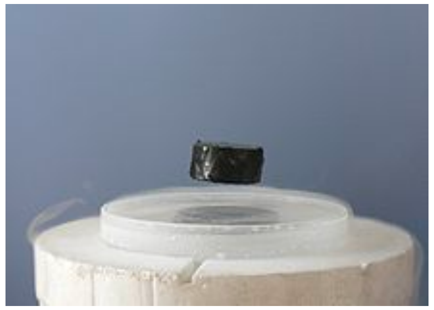
1eV	10^4 eV = 10keV	10^6 eV = 1MeV	10^9 eV = 1GeV	10^19 GeV
	10^[-8] cm	10^[-10]cm	10^[-13]cm	10^[-22]cm
	物性物理	原子核物理	素粒子物理	弦理論











電気・磁気的な性質？
磁石ってなんで磁石？

どの元素が安定？
原子核の融解温度

原子核作れる？
素粒子は何個ある？

素粒子は導ける？
時空誕生の謎

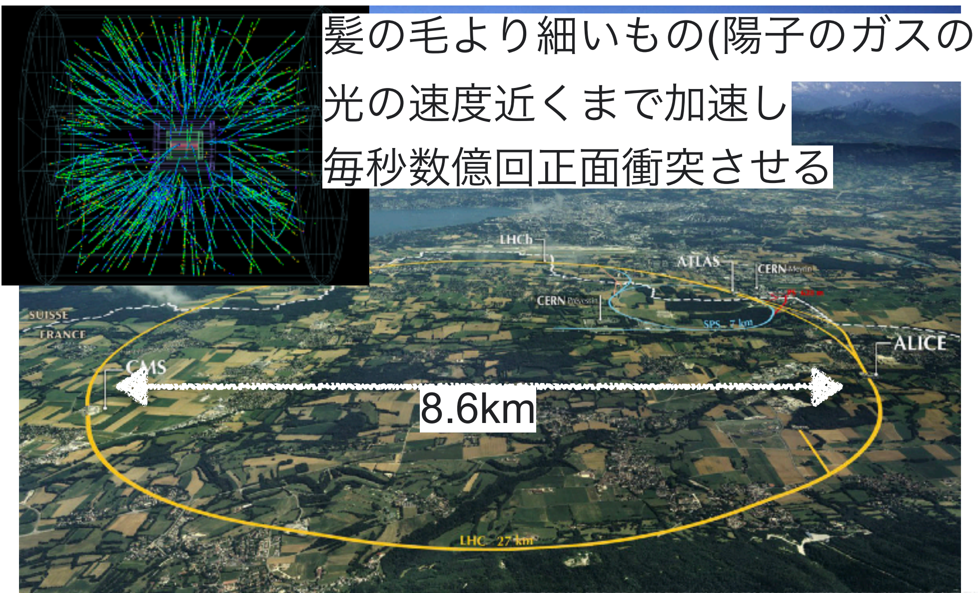
この辺りが私の専門

理論物理って何をするの？

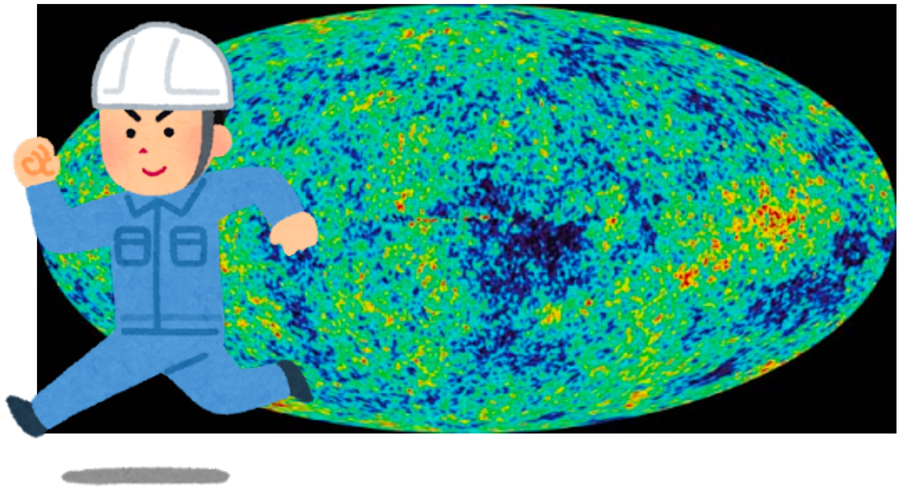
Akio Tomiya

数学や数値計算を使ってこの世の物質とその間のルールを理解する

実験物理や観測



髪の毛より細いもの(陽子のガスの塊)を
光の速度近くまで加速し
毎秒数億回正面衝突させる



質量
散乱
…
(大量の)
データ

予言

理論物理

データ間に関係を見つけ、
モデル(ハミルトニアンなどの
ユニバーサルなエネルギー関数)を作る
新たな現象を予言
予言は実験でチェック

↓辺りが私の専門

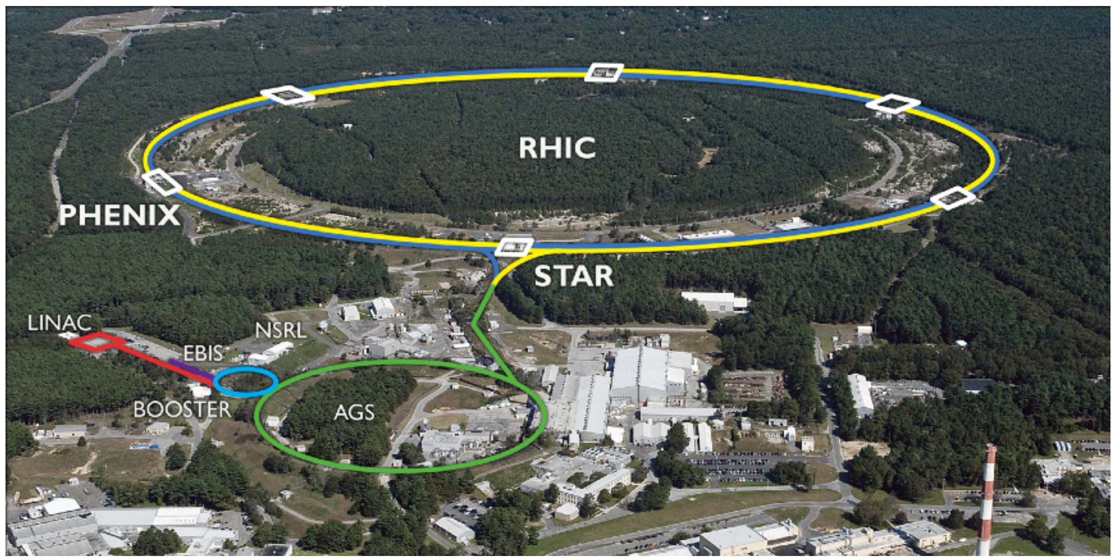
予言には計算が必要
手計算 or 数値計算(スパコンも使う)

仮想的な理論同士の関係なども調べる
(思わぬ所で役立ったりする)
計算手法の提案 etc

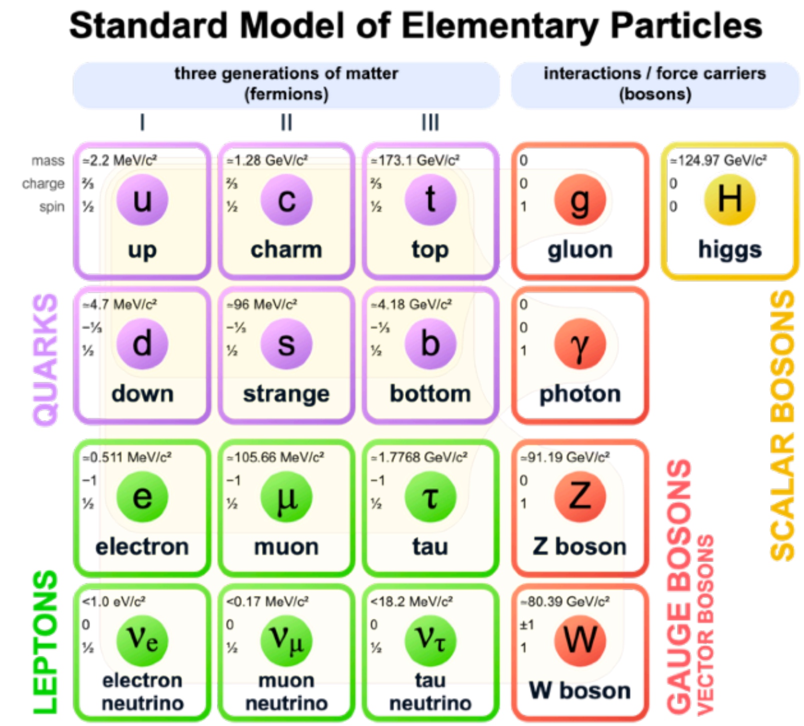
Akio Tomiya

Intro: QCD?

Fundamental theory inside of nucleus

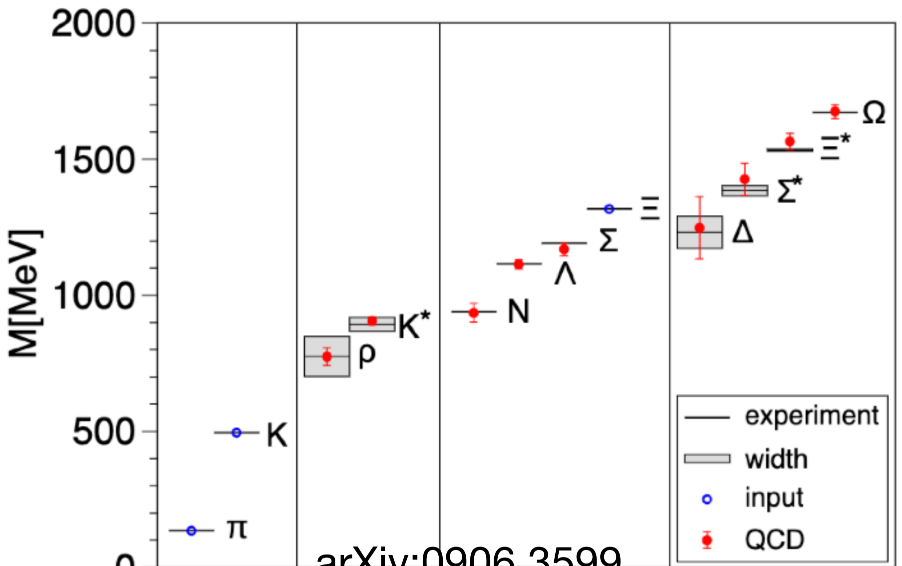


?



compare

Input



calculate

$$Z = \int \mathcal{D}A\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{iS}$$

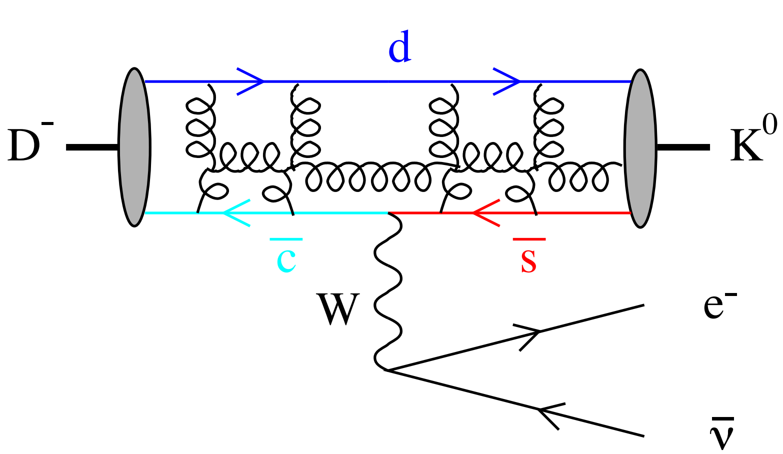
Motivation, Big goal

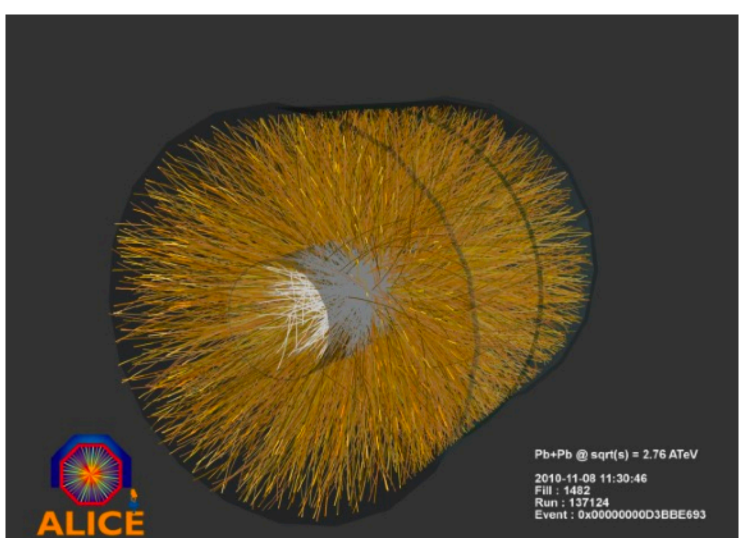
Non-perturbative calculation of QCD is important

QCD in 3 + 1 dimension

$$S = \int d^4x \left[-\frac{1}{4} \mathrm{tr}\, F_{\mu\nu} F^{\mu\nu} + \bar{\psi}\left(i\partial\!\!\!/ - gA\!\!\!/ - m \right)\psi \right]$$

$$Z = \int \mathscr{D}A \mathscr{D}\bar{\psi} \mathscr{D}\psi e^{iS} \qquad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - ig[A_\mu, A_\nu]$$





- This describes…
  - inside of hadrons (bound state of quarks), mass of them
  - scattering of gluons, quarks
  - Equation of state of neutron stars, Heavy ion collisions, etc
- **Non-perturbative effects are essential.** How can we deal with?
  - Confinement
  - Chiral symmetry breaking

Motivation, Big goal

LQCD = Non-perturbative calculation of QCD

QCD in 3 + 1 dimension

$$S = \int d^4x \left[-\frac{1}{4}\mathrm{tr}\, F_{\mu\nu}F^{\mu\nu} + \bar{\psi}\left(\mathrm{i}\not\partial - g\not A - m\right)\psi \right]$$

$$Z = \int \mathscr{D}A\mathscr{D}\bar{\psi}\mathscr{D}\psi e^{\mathrm{i}S} \qquad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - \mathrm{i}g[A_\mu, A_\nu]$$

QCD in Euclidean 4 dimension ($t \to -\mathrm{i}t$, <u>same hamiltonian</u>)

$$S = \int d^4x \left[+\frac{1}{4}\mathrm{tr}\, F_{\mu\nu}F^{\mu\nu} + \bar{\psi}\left(\not\partial - g\not A - m\right)\psi \right]$$

$$Z = \int \mathscr{D}A\mathscr{D}\bar{\psi}\mathscr{D}\psi e^{-S}$$

← This can be regarded as a statistical system

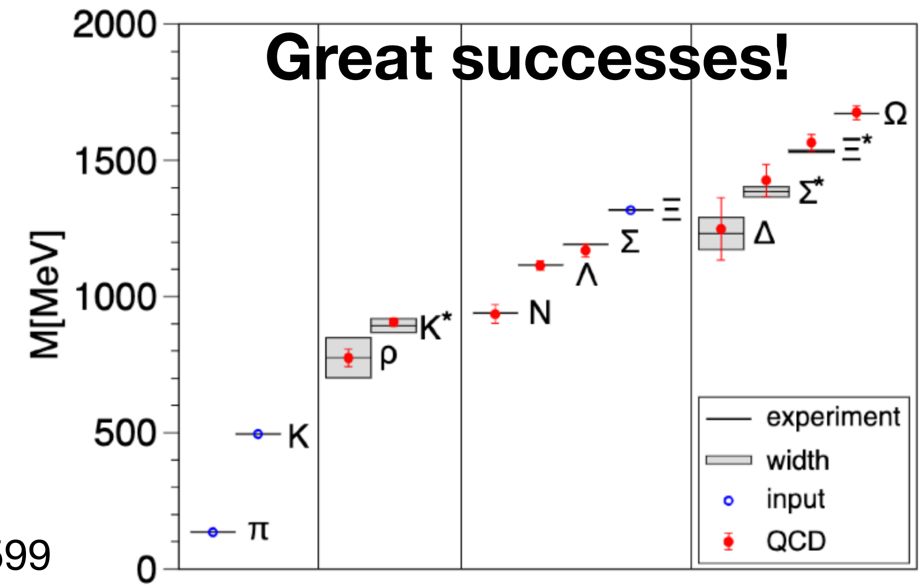
- Standard approach: Lattice QCD with Imaginary time and Monte-Carlo
  - LQCD = QCD + cutoff + irrelevant ops. = “Statistical mechanics”
  - Mathematically well-defined quantum field theory
  - **Quantitative** results are available = Systematic errors are controlled

Motivation, Big goal

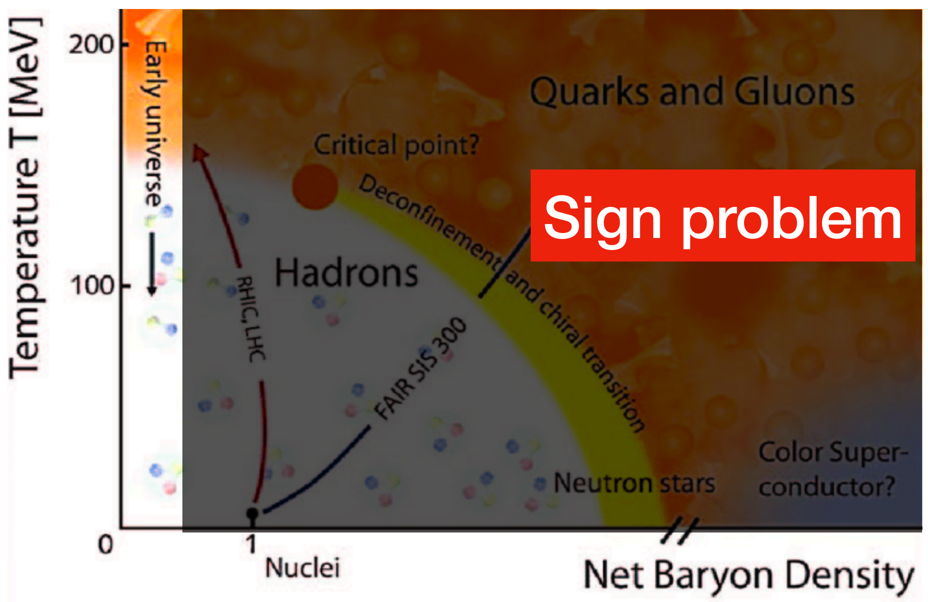
Sign problem prevents using Monte-Carlo

- Monte-Carlo is very powerful method to evaluate expectation values for "statistical system", like lattice QCD in imaginary time

$$\langle O[U]\rangle = \frac{1}{N_{\rm conf}}\sum_{c}^{N_{\rm conf}} O[U_c] + \mathcal{O}\left(\frac{1}{\sqrt{N_{\rm conf}}}\right) \qquad U_c \leftarrow P(U) = \frac{1}{Z}e^{-S[U]} \in \mathbb{R}_+$$



arXiv:0906.3599



- However, if we have, real time, finite theta, finite baryon density case, we cannot we use Monte-Carlo technique because $e^{-S[U]}$ becomes complex. This is no more probability.
- <u>Hamiltonian formalism does not have such problem! But it requires huge memory to store quantum states, which cannot realized even on supercomputer.</u>
- Quantum states should not be realized on classical computer but on quantum computer (Feynman 1982)

Previous works

Akio Tomiya

μ = 0 is good on Classical, T=0 is good for Quantum

lattice field theory calculations on Classical machines based on $U(\tau) = \mathrm{e}^{-\hat{H}\tau}$

$$P(U) = \frac{1}{Z} e^{-S[U]} \det(D[U] + m)^2$$

Since 1980 (M. Creutz)~

This P cannot be regarded as probability for μ ≠ 0

Quantum machines can realize (any) unitary evolutions (Solovay Kitaev theorem),

$$U(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t}$$

Phys.Rev.D 105 (2022) 9, 094503 etc

No problem for μ≠0 because we can only use unitary gates (operators)

Also “simple evolution” (short circuit) is preferred for near-term devices

We need a method to calculate T>0 and μ≠0 for QCD for near-term quantum devices

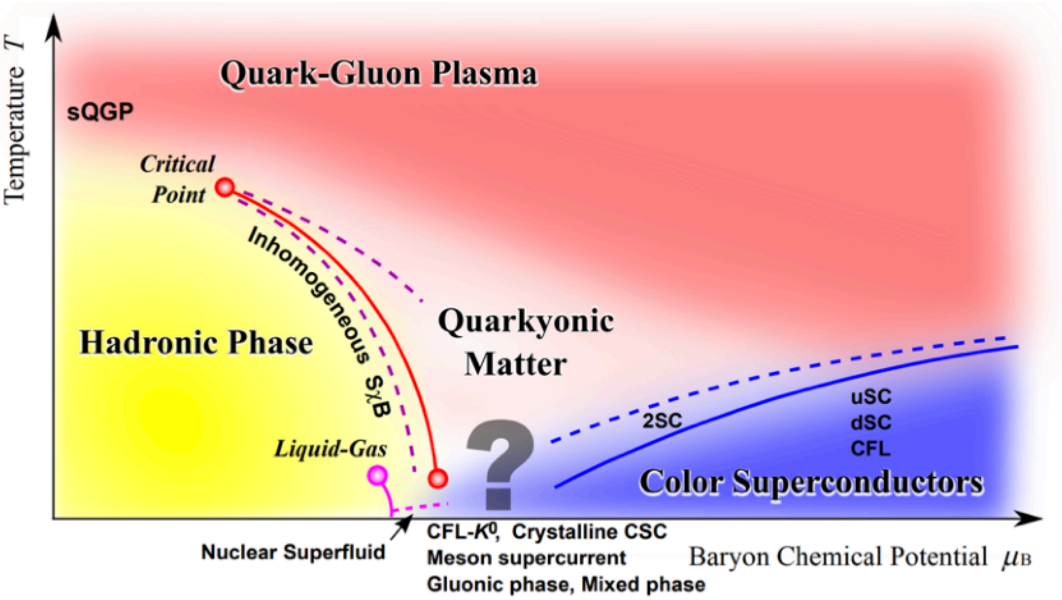
Akio Tomiya

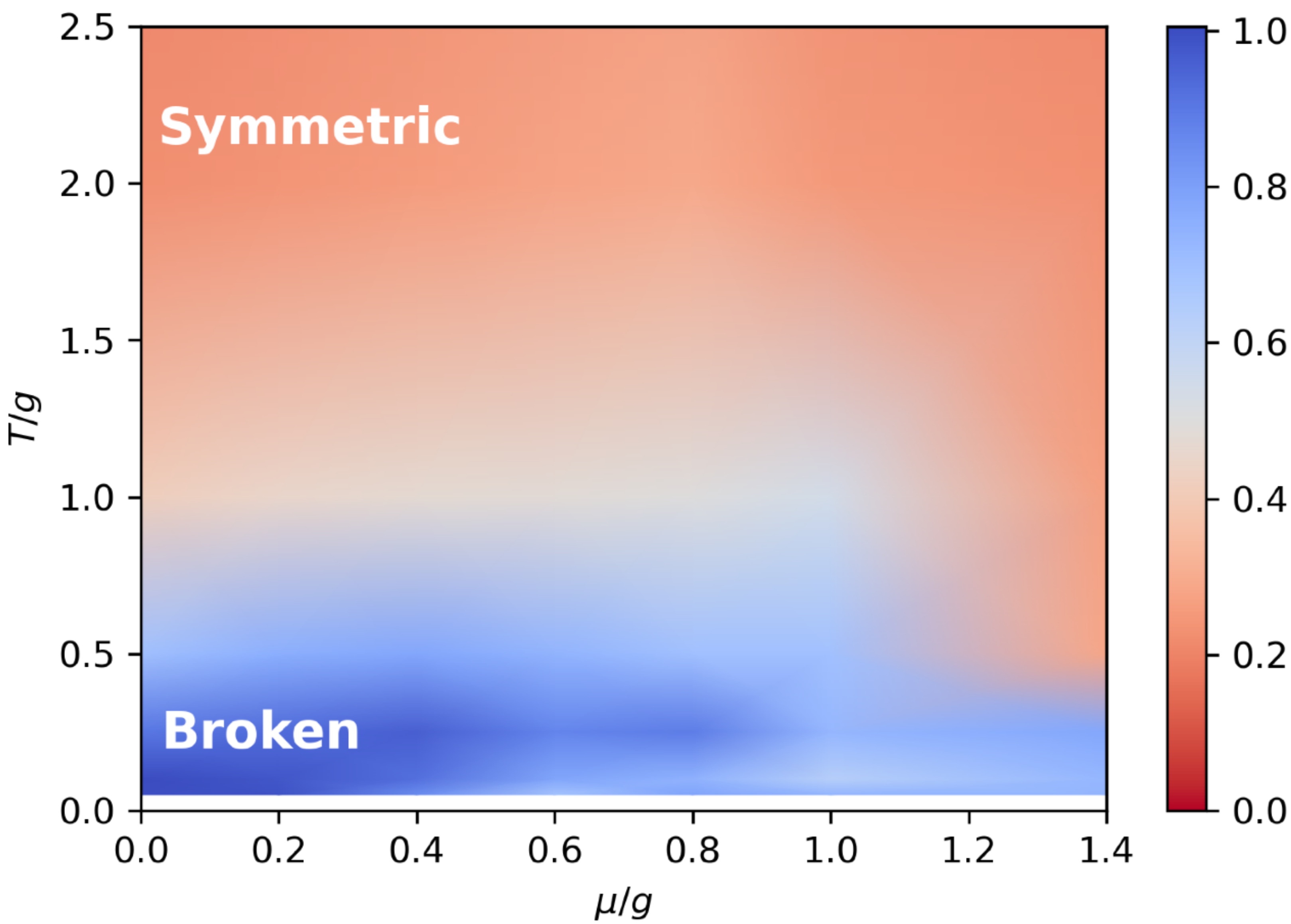
Summary of this talk

Chiral PT with quantum algorithm + machine learning

AT arXiv: 2205.08860

Fukushima , Hatsuda
Rept.Prog.Phys.74:014001,2011





I investigated T-mu phase diagram using quantum algorithm & neural network (β-VQE, No sign problem) for Schwinger model

Statistical mechanics with density matrix

Density matrix

Akio Tomiya

Feynman's introduction of statistical mechanics

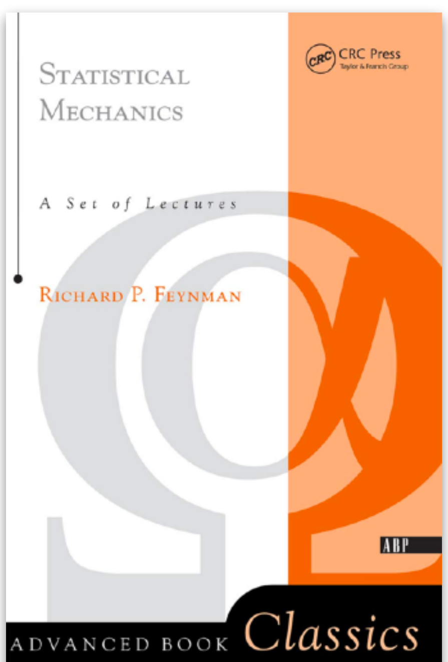
Pure states: $\rho_{\text{pure}} = |\Psi\rangle\langle\Psi|$ $\qquad \langle O \rangle = \mathrm{Tr}[O\rho_{\text{pure}}] = \langle\Psi|O|\Psi\rangle$

Mixed states:

$$\rho_{\text{mixed}} = \sum_i w_i |\psi_i\rangle\langle\psi_i| \qquad \langle O \rangle = \mathrm{Tr}[O\rho_{\text{mixed}}]$$

w_i represents probability to find a pure state $|\psi_i\rangle$

thermal states(grandcanonical): Mixed states with $w_i = Z^{-1}\mathrm{e}^{-\frac{1}{T}(E_i - \mu n_i)}$



or we choose,

$$\rho_{T,\mu} = \frac{1}{Z}\mathrm{e}^{-\frac{1}{T}(\hat{H} - \mu\hat{N})} \qquad \langle O \rangle_{T,\mu} = \mathrm{Tr}[O\rho_{T,\mu}]$$

What we need to evaluate

$$\langle O \rangle = \mathrm{Tr}[O\rho]$$

Density matrix

Akio Tomiya

Quantum version of probability distribution

Thermal-quantum average in general

$$\langle O \rangle = \mathrm{Tr}[O\rho]$$

General Properties of density matrix ρ

- Hermitian (namely diagonalizable), positive (semi) definite
- It unifies discretion of pure states and mixed states
- Normalized: $\mathrm{Tr}[\rho] = 1$
- We can regard ρ as quantum version of probability distribution p(x)
  - e.g.) $S = -\int dx\, p(x) \log p(x)$ (Shannon entropy)

    <—> $S = -\mathrm{Tr}[\rho \log \rho]$ (Von-Neumann entropy)
- Distance between two density matrices = quantum relative entropy (later)

QFT with Hamiltonian & Schwinger model
(Schwinger model as a spin model)

QFT with Hamiltonian

Akio Tomiya

1.Hは共通、t が違う 2.経路積分では有限温度境界条件

H : 場のハミルトニアン(第2量子化ハミルトニアン)

実時間発展を見たい

有限温度を考えたい

ミンコフスキー場の理論: M^{d+1}

ユークリッド場の理論: S^1 x M^d

正準量子化 $U(t) = \mathrm{e}^{-\mathrm{i}tH}$

ユークリッド化(t → τ)

$t = -\mathrm{i}\tau$

ミンコフスキー化(τ → t)

$U(\tau) = \mathrm{e}^{-\tau H}$ 正準量子化

摂動論

$$\langle OO(t) \rangle = \langle \Omega | \hat{\mathrm{T}} O(0) O(t) | \Omega \rangle$$

$$|\Omega\rangle \sim \lim U(t) |0\rangle$$

$$\langle OO(\tau) \rangle = \mathrm{Tr}[O(0)O(\tau)\rho]$$

今回の計算

$$\rho = U(\tau)/Z$$

経路積分

$$Z = \int \mathscr{D}\bar{\psi}\mathscr{D}\psi \mathrm{e}^{\mathrm{i}S^M}$$

経路積分

$$Z = \int \mathscr{D}\bar{\psi}\mathscr{D}\psi \mathrm{e}^{-S^E}$$

摂動論

$$S^M = \int_{-\infty}^{\infty} dt \int d^d x \, \mathscr{L}^M(x, t)$$

$$S^E = \int_0^{1/T} d\tau \int d^d x \, \mathscr{L}^E(x, \tau)$$

普段の格子QCD

フェルミオン有限温度境界条件: 経路積分の計算が、付加条件なしで演算子形式のフェルミオン的な場のTr とつながるための条件)

$$\psi(\tau + 1/T, \vec{x}) = -\psi(\tau, \vec{x})$$

導出1: 自由グリーン関数の周期性

導出2: コヒーレント状態を用いた経路積分から

Schwinger model

Akio Tomiya

＝2D QED: Solvable at m=0, similar to QCD in 4D.

Schwinger model = QED in 1+1 dimension

$$S = \int d^2x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} \left(\mathrm{i} \partial\!\!\!/ - g A\!\!\!/ - m \right) \psi + \frac{g\theta}{4\pi} \epsilon_{\mu\nu} F^{\mu\nu} \right]$$

<u>**Similarities to QCD in 3+1**</u>

- Confinement
- Chiral symmetry breaking (different mechanism), gapped even m=0

$$\langle \overline{\psi} \psi \rangle = -\frac{\mathrm{e}^{\gamma} g}{\pi^{3/2}} = -g 0.16 \cdots$$

- Topological term can be included as in QCD
- Vacuum decay by external electric field (Schwinger effect)

Hamiltonian of Schwinger model

＝2D QED: Solvable at m=0, similar to QCD in 4D.

Schwinger model = QED in 1+1 dimension

$$S = \int d^2x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} \left(i\partial\!\!\!/ - gA\!\!\!/ - m \right) \psi \right]$$

- Strategy

1. Derive Hamiltonian with gauge fixing
2. Rewrite gauge field to fermions using Gauss' law
3. Use Jordan-Wigner transformation → Spin system

Why? next page

Hamiltonian of Schwinger model

Akio Tomiya

Schwinger model in spin language

Schwinger model = QED in 1+1 dimension

$$S = \int d^2x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} \left(i\partial\!\!\!/ - gA\!\!\!/ - m \right) \psi \right]$$

- Strategy(1gauge fix, 2Gauss' law, 3Jordan-Wigner trf)

Schwinger model on the lattice (staggered fermion, OBC, Spin rep.)

$$H = \frac{1}{4a} \sum_n \left[X_n X_{n+1} + Y_n Y_{n+1} \right] + \frac{m}{2} \sum_n (-1)^n Z_n + \frac{g^2 a}{2} \sum_n \left[\sum_{j=1}^{n} \left(\frac{Z_j + (-1)^j}{2} \right) + \epsilon_0 \right]^2$$

- Spin representation is necessary to use quantum device (Analogous to floating point rep. in classical machine)

- (QCD + QC also requires this strategy)

Hamiltonian of Schwinger model

＝2D QED: Solvable at m=0, similar to QCD in 4D.

(detail)

Schwinger model = QED in 1+1 dimension

$$S = \int d^2x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} \left(i\partial\!\!\!/ - gA\!\!\!/ - m \right) \psi \right]$$

$$\Pi(x) = \frac{\partial \mathscr{L}}{\partial \dot{A}^1(x)} = \dot{A}(x) = E(x)$$

$A_0 = 0$

$$\begin{cases} H = \int dx \left[-i\bar{\psi}\gamma^1(\partial_1 + igA_1)\psi + m\bar{\psi}\psi + \frac{1}{2}\Pi^2 \right] \\ \partial_x E = g\bar{\psi}\gamma^0\psi \end{cases}$$

(Gauss' law constraint)

This constrains time evolution to be gauge invariant

Lattice Hamiltonian formalism

Hamiltonian on a discrete space

(detail)

Schwinger model in continuum

$$H = \int dx \left[-\mathrm{i}\bar{\psi}\gamma^1(\partial_1 + \mathrm{i}gA_1)\psi + m\bar{\psi}\psi + \frac{1}{2}\Pi^2 \right]$$

Gauss' law $\partial_x E = g\bar{\psi}\gamma^0\psi$

$$-\frac{1}{g}\Pi(x) \to L_n$$

$$-agA_1(x) \to \phi_n$$

upper componentof $\psi \to \chi_{\text{even-site}}$

lower componentof $\psi \to \chi_{\text{odd-site}}$

Schwinger model on the lattice (staggered fermion)

$$H = -\frac{\mathrm{i}}{2a}\sum_{n=1}^{N-1}\left[\chi_{n+1}^\dagger e^{-\mathrm{i}\phi_n}\chi_n - \chi_n^\dagger e^{\mathrm{i}\phi_n}\chi_{n+1}\right] + m\sum_{n=1}^{N}(-1)^n\chi_n^\dagger\chi_n + \frac{g^2a}{2}\sum_{n=1}^{N-1}L_n^2$$

Gauss' law $L_n - L_{n-1} = \chi^\dagger\chi_n - \frac{1}{2}\left(1-(-1)^n\right)$

Lattice Schwinger model = spin system

Akio Tomiya

Gauge trf, open bc, Gauss law -> pure fermionic system

(detail)

Schwinger model on the lattice (staggered fermion)

$$H = -\frac{\mathrm{i}}{2a}\sum_{n=1}^{N-1}\left[\chi_{n+1}^{\dagger}\mathrm{e}^{-\mathrm{i}\phi_n}\chi_n - \chi_n^{\dagger}\mathrm{e}^{\mathrm{i}\phi_n}\chi_{n+1}\right] + m\sum_{n=1}^{N}(-1)^n\chi_n^{\dagger}\chi_n + \frac{g^2 a}{2}\sum_{n=1}^{N-1}\boxed{L_n^2}$$

Gauss' law $\boxed{L_n - L_{n-1} = \chi^{\dagger}\chi_n - \frac{1}{2}\left(1-(-1)^n\right)}$

$L_0 = \epsilon_0 \in \mathbb{R}$ (**open B.C.**), **and insert "Gauss' law"**

$$\begin{cases} U_n = \prod_{j=1}^{n-1}\mathrm{e}^{-\mathrm{i}\phi_j} \\ \chi_n \to U_n\chi_n \\ \mathrm{e}^{-\mathrm{i}\phi_{n-1}} \to U_{n-1}\mathrm{e}^{-\mathrm{i}\phi_{n-1}}U_n^{\dagger} \end{cases}$$

remnant gauge transformation

Schwinger model on the lattice (staggered fermion, OBC)

$$H = -\frac{\mathrm{i}}{2a}\sum_{n}\left[\chi_{n+1}^{\dagger}\chi_n - \chi_n^{\dagger}\chi_{n+1}\right] + m\sum_{n}(-1)^n\chi_n^{\dagger}\chi_n + \frac{g^2 a}{2}\sum_{n}\left[\boxed{\sum_{j}^{n}\left(\chi_j^{\dagger}\chi_j - \frac{1-(-1)^j}{2}\right) + \epsilon_0}\right]^2$$

Lattice Schwinger model

Akio Tomiya

We requires anticommutations to fermions

(detail)

Schwinger model on the lattice (staggered fermion, OBC)

$$H = -\frac{\mathrm{i}}{2a}\sum_{n}\left[\chi_{n+1}^{\dagger}\chi_{n} - \chi_{n}^{\dagger}\chi_{n+1}\right] + m\sum_{n}(-1)^{n}\chi_{n}^{\dagger}\chi_{n} + \frac{g^{2}a}{2}\sum_{n}\left[\sum_{j}^{n}\left(\chi_{j}^{\dagger}\chi_{j} - \frac{1-(-1)^{j}}{2}\right) + \epsilon_{0}\right]^{2}$$

System is quantized by assuming the canonical anti-commutation relation

$$\{\chi_j^{\dagger}, \chi_k\} = \mathrm{i}\delta_{jk} \qquad j, k = \text{site index}$$

On the other hand, Pauli matrices satisfy anti-commutation as well

$$\{\sigma^{\mu}, \sigma^{\nu}\} = 2\delta_{\mu\nu}\mathbf{1} \qquad \mu, \nu = 1,2,3$$

Quantum spin-chain case, each site has Pauli matrix, but they are “commute”.

We can absorb difference of statistical property using Jordan Wigner transformation

Jordan-Wigner transformation:

$$\chi_n = \frac{X_n - \mathrm{i}Y_n}{2}\prod_{j<n}(\mathrm{i}Z_j)$$

X_j: Pauli matrix of x on site j

Y_j: Pauli matrix of y on site j

Z_j: Pauli matrix of z on site j

This guarantees the statistical property

This (re)produces correct Fock space.

We can rewrite the Hamiltonian in terms of spin-chain

Lattice Schwinger model = spin system

Akio Tomiya

Jordan-Wigner transformation: Fermions ~ Spins

(detail)

Schwinger model on the lattice (staggered fermion, OBC)

$$H=-\frac{\mathrm{i}}{2a}\sum_n\left[\chi_{n+1}^\dagger\chi_n-\chi_n^\dagger\chi_{n+1}\right]+m\sum_n(-1)^n\chi_n^\dagger\chi_n+\frac{g^2a}{2}\sum_n\left[\sum_j^n\left(\chi_j^\dagger\chi_j-\frac{1-(-1)^j}{2}\right)+\epsilon_0\right]^2$$

$$\begin{cases}\chi_n=\dfrac{X_n-\mathrm{i}Y_n}{2}\displaystyle\prod_{j<n}(\mathrm{i}Z_j)\\ \chi_n^\dagger=\dfrac{X_n+\mathrm{i}Y_n}{2}\displaystyle\prod_{j<n}(-\mathrm{i}Z_j)\end{cases}$$

Jordan-Wigner transformation

X_j: Pauli matrix of x on site j

Y_j: Pauli matrix of y on site j

Z_j: Pauli matrix of z on site j

Schwinger model on the lattice (staggered fermion, OBC, Spin rep.)

$$H=\frac{1}{4a}\sum_n\left[X_nX_{n+1}+Y_nY_{n+1}\right]+\frac{m}{2}\sum_n(-1)^nZ_n+\frac{g^2a}{2}\sum_n\left[\sum_{j=1}^n\left(\frac{Z_j+(-1)^j}{2}\right)+\epsilon_0\right]^2$$

[Y. Hosotani 9707129]

State preparation, VQE and Beta-VQE

State preparation, VQE and Beta-VQE

State preparation is hard

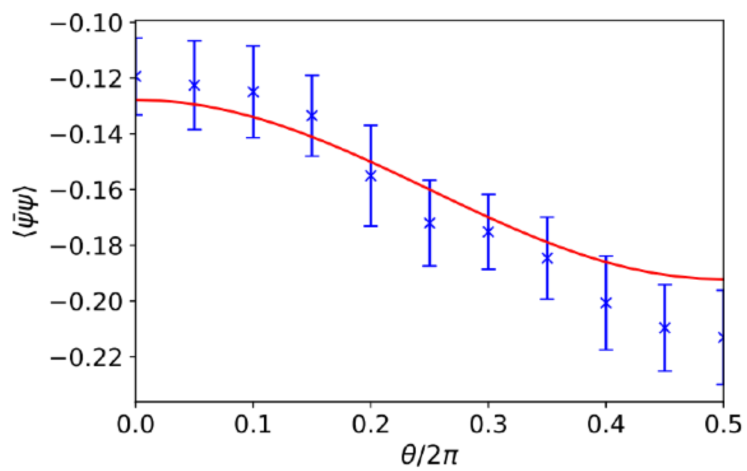
We are interested in expectation value with true ground state for Hamiltonian

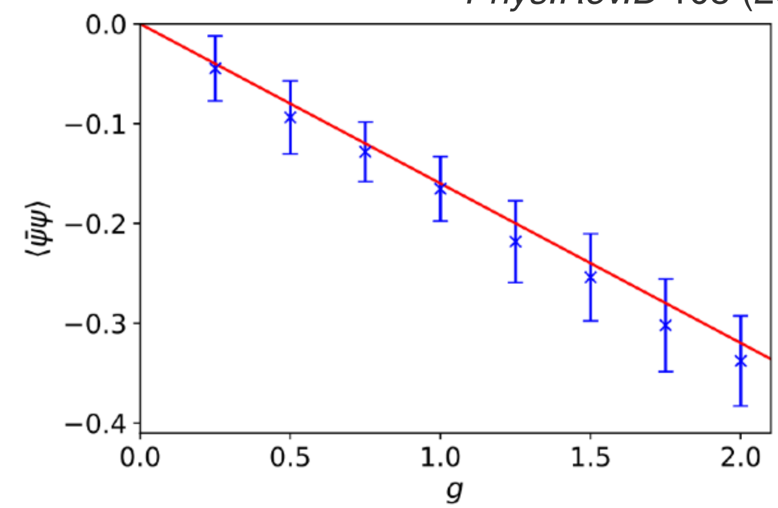
$$\langle O \rangle = \langle \Omega | O | \Omega \rangle$$

For the actual ground state $H|\Omega\rangle = E_0|\Omega\rangle$

On the quantum algorithm, the ground state can be prepared using adiabatic state preparation = long unitary evolution

B Chakraborty, M Honda, T Izubuchi, Y Kikuchi, AT
Phys.Rev.D 105 (2022) 9, 094503





BUT, Near term quantum devices are only capable to deal with simple (short) circuit since technology has been developing

Variational approaches help to evaluate the ground state to evaluate the expectation value = Variational Quantum Eigen-solver (VQE)

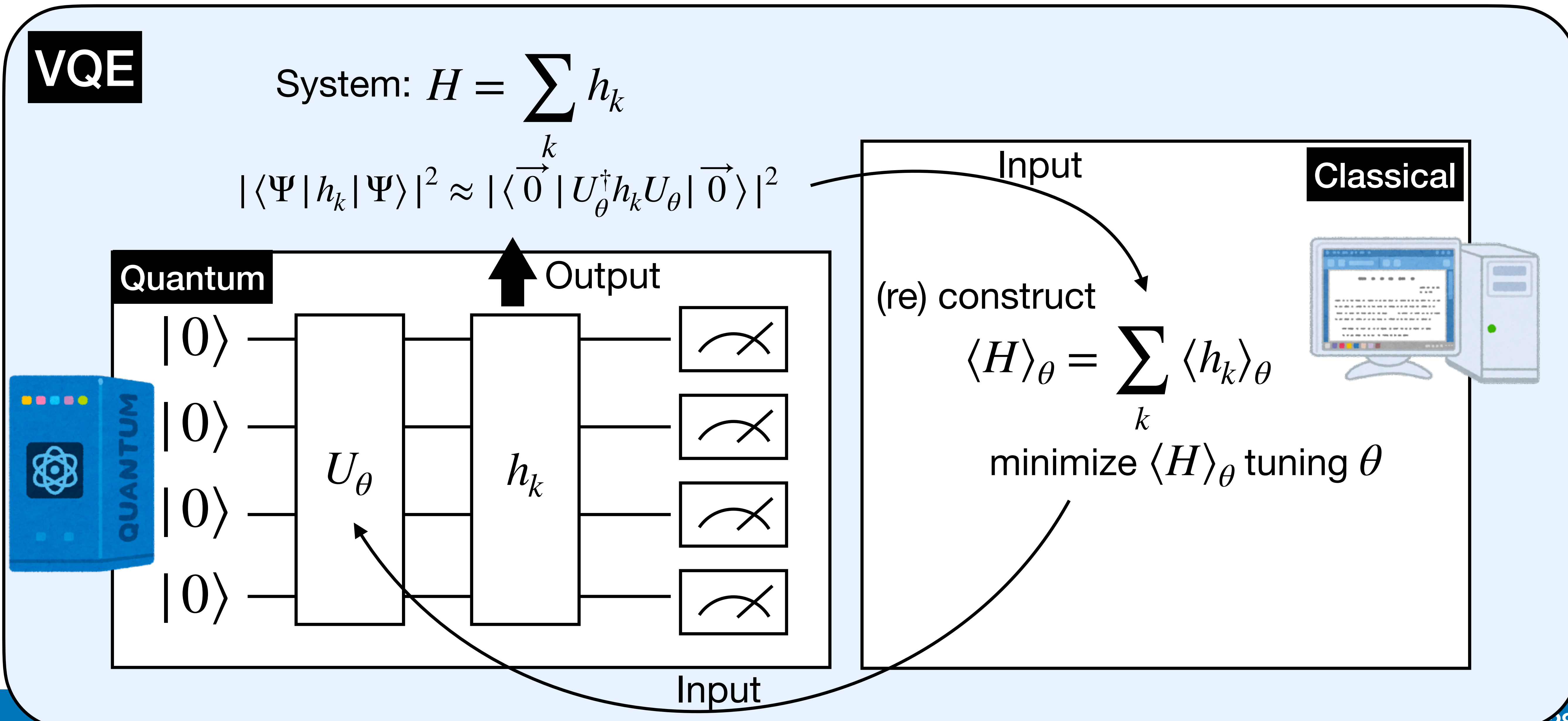
VQE (Variational quantum eigen-solver) 1/2

Akio Tomiya

Variational approach to prepare a pure state

1304.3061

- (Iterative) Variational method with quantum and classical machines to prepare a pure state
- We use a product state, $|\vec{0}\rangle = |0\rangle \otimes |0\rangle \otimes |0\rangle \otimes |0\rangle \otimes \cdots = \bigotimes |0\rangle$, which is easy to prepare
- Try to mimic $|\Psi\rangle \approx U_\theta|\vec{0}\rangle$ by tuning θ for the ground state $|\Psi\rangle$. Used to calculate $|\langle\Psi|O|\Psi\rangle|^2$
- U_θ : unitary circuit acting on more than 2 qubits. θ: Parameters. Like combinations of $U^{\mathrm{CNOT}}_{1\to 2}\mathrm{e}^{-i\theta_1 Y_1/2}$



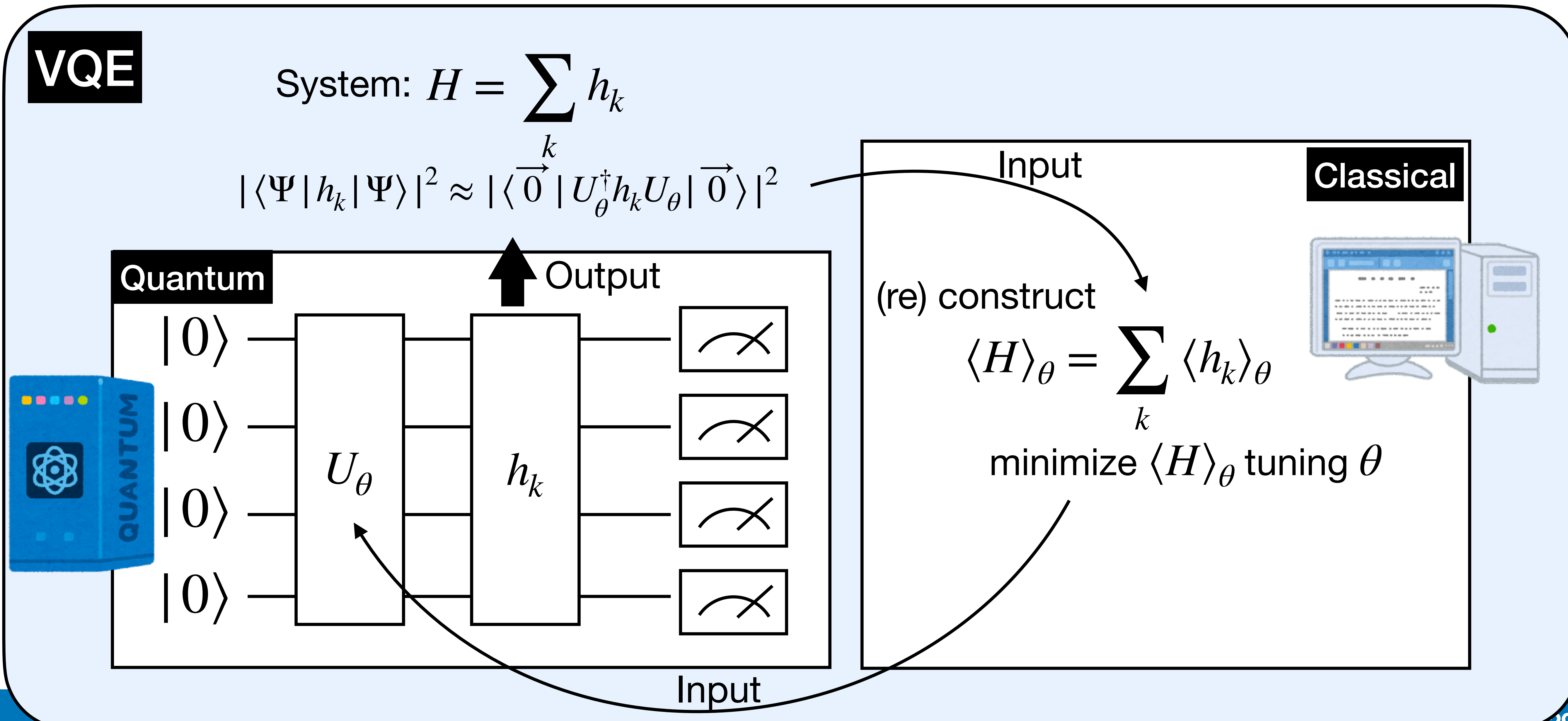
VQE (Variational quantum eigen-solver) 2/2

Akio Tomiya

Variational approach in density matrix

1304.3061

- Target density matrix: $\rho = |\Psi\rangle\langle\Psi|$, $\mathrm{tr}\,\rho = 1$ (e.g. Ground-state of H)
- We mimic $|\Psi\rangle \approx U_\theta|\vec{0}\rangle$ by tuning θ
  - Equivalently, $\rho_\theta = U_\theta|\vec{0}\rangle\langle\vec{0}|U_\theta$, $\mathrm{tr}\,\rho_\theta = 1$, $\langle\Psi|O|\Psi\rangle \approx \mathrm{Tr}[\rho_\theta O]$



Beta VQE 1/4

Extended VQE for mixed states

Jin-Guo Liu+ 1902.02663

- $\rho_\Theta = \sum_{\{\vec{x}\}} p_\phi[\vec{x}]\ U_\theta | \vec{x} \rangle \langle \vec{x} | U_\theta$ as an ansatz (mixed state)
    - $\vec{x} = (x_1, x_2, x_3, \cdots, x_k, \cdots)^\top$, and $x_k \in \{0,1\}$
    - $p_\phi[\vec{x}]$: Parametrized joint distribution for a configuration of $\vec{x}$, normalized. ϕ is a set of parameters.
    - $\Theta = \theta \cup \phi$ (quantum and classical parameters)
    - $| \vec{x} \rangle = | x_1 \rangle \otimes | x_2 \rangle \otimes | x_3 \rangle \otimes \cdots \otimes | x_k \rangle \otimes \cdots$, a product state
- This ansatz is correctly normalized: $\mathrm{Tr}[\rho_\Theta] = \sum_{\{\vec{x}\}} p_\phi[\vec{x}]\ \mathrm{Tr}[U_\theta | \vec{x} \rangle \langle \vec{x} | U_\theta] = \sum_{\{\vec{x}\}} p_\phi[\vec{x}]\ = 1$
- $\langle O \rangle_{T,\mu} \approx \mathrm{Tr}[\rho_\Theta O]$, if $\rho_\Theta \approx \rho$ for $\rho = \dfrac{1}{Z} \mathrm{e}^{-\frac{1}{T}(\hat{H} - \mu \hat{N})}$

Beta VQE 2/4

Extended VQE for mixed states

Jin-Guo Liu+ 1902.02663

- How can we realize $\rho_\Theta \approx \rho$ for $\rho = \frac{1}{Z} e^{-\frac{1}{T}(\hat{H} - \mu \hat{N})}$
- Minimize Kullback–Leibler–*Umegaki* divergence (pseudo-distance)
  - $D(\rho_\Theta | \rho) = \mathrm{Tr}[\rho_\Theta \ln \frac{\rho_\Theta}{\rho}] = \mathrm{Tr}[\rho_\Theta \ln \rho_\Theta] - \mathrm{Tr}[\rho_\Theta \ln \rho]$
  - Relative entropy for density matrices (Classical ver. is called KL div.)
  - This is bounded $D(\rho_\Theta | \rho) \geq 0$ and saturated iff $\rho_\Theta = \rho$
  - In practice, we minimize shifted one,

$$\mathscr{L}(\Theta) = D(\rho_\Theta | \rho) - \underbrace{\ln Z}_{\mathrm{const}} = \mathrm{Tr}[\rho_\Theta \ln \rho_\Theta] + \frac{1}{T}\mathrm{Tr}[\rho_\Theta(\hat{H} - \mu \hat{N})]$$

Note (skip)

Akio Tomiya

We can define, a loss function, $\tilde{\mathscr{L}}(\Theta) = D(\rho_\Theta||\rho)$

$$\rho_{T,\mu} = \frac{1}{Z_{T,\mu}} \mathrm{e}^{-\frac{1}{T}(\hat{H}-\mu\hat{N})}$$

$$D(\rho_\Theta||\underset{T,\mu}{\rho}) = \mathrm{Tr}\,[\rho_\Theta \log \frac{\rho_\Theta}{\rho_{T,\mu}}], \tag{24}$$

$$= \mathrm{Tr}\,[\rho_\Theta \log \rho_\Theta] - \mathrm{Tr}\,[\rho_\Theta \log \rho_{T,\mu}], \tag{25}$$

$$= \mathrm{Tr}\,[\rho_\Theta \log \rho_\Theta] - \mathrm{Tr}\,[\rho_\Theta \log \frac{1}{Z_{T,\mu}} \mathrm{e}^{-\frac{1}{T}(\hat{H}-\mu\hat{N})}], \tag{26}$$

$$= \mathrm{Tr}\,[\rho_\Theta \log \rho_\Theta] + \mathrm{Tr}\,[\rho_\Theta \log Z_{T,\mu}] + \frac{1}{T}\mathrm{Tr}\,[\rho_\Theta(\hat{H} - \mu\hat{N})], \tag{27}$$

$$= \mathrm{Tr}\,[\rho_\Theta \log \rho_\Theta] + \mathrm{Tr}\,[\rho_\Theta] \log Z_{T,\mu} + \frac{1}{T}\mathrm{Tr}\,[\rho_\Theta(\hat{H} - \mu\hat{N})], \tag{28}$$

$$= \mathrm{Tr}\,[\rho_\Theta \log \rho_\Theta] + \underset{\text{(const in }\Theta)}{\log Z_{T,\mu}} + \frac{1}{T}\mathrm{Tr}\,[\rho_\Theta(\hat{H} - \mu\hat{N})]. \tag{29}$$

The last line follows because ρ_Θ is normalized.

In practice, we use,

$$\mathscr{L}(\Theta) = \tilde{\mathscr{L}}(\Theta) - \log Z_{T,\mu} = \mathrm{Tr}\,[\rho_\Theta \log \rho_\Theta] + \frac{1}{T}\mathrm{Tr}\,[\rho_\Theta(\hat{H} - \mu\hat{N})]. \tag{30}$$

Namely,

$$\mathscr{L}(\Theta) = \mathrm{Tr}\,[\rho_\Theta \log \rho_\Theta] + \frac{1}{T}\mathrm{Tr}\,[\rho_\Theta \mathscr{H}], \tag{31}$$

Beta VQE 3/4

Extended VQE for mixed states

Jin-Guo Liu+ 1902.02663

- $\mathscr{L}(\Theta) = \mathrm{Tr}[\rho_\Theta \ln \rho_\Theta] + \frac{1}{T}\mathrm{Tr}[\rho_\Theta(\hat{H} - \mu\hat{N})]$
  - $\mathrm{Tr}[\rho_\Theta \log \rho_\Theta] = \sum_{\{\vec{x}\}} p_\phi(\vec{x}) \log p_\phi(\vec{x})$
- We need two derivatives
  - $\frac{\partial}{\partial\phi}\mathscr{L}(\Theta) = \frac{\partial}{\partial\phi}\sum_{\{\vec{x}\}} p_\phi(\vec{x})[\log p_\phi(\vec{x})]$: Classical
  - $\frac{\partial}{\partial\theta}\mathscr{L}(\Theta) = \frac{1}{T}\frac{\partial}{\partial\theta}\langle\vec{x}\,|\,U_\theta^\dagger \mathscr{H} U_\theta\,|\,\vec{x}\rangle]$: Quantum

p: a neural network
-> gradient descent

REINFORCE algorithm

Beta VQE 4/4

Extended VQE for mixed states

Jin-Guo Liu+ 1902.02663

- We minimize the loss function $\mathscr{L}(\Theta) = \mathrm{Tr}[\rho_\Theta \ln \rho_\Theta] + \frac{1}{T}\mathrm{Tr}[\rho_\Theta(\hat{H} - \mu\hat{N})]$
  - Variational bound: $\mathscr{L}(\Theta) - \log Z_{T,\mu} \geq 0$
  - We use SU(4) ansatz for each 2 qubits for U_θ (let me skip)
- *Advantage* of beta VQE
  - No sign problem, even with the chemical potential
  - Bounded variational approximation
- *Disadvantage*
  - Systematic error
  - Need numerical resource if we use a classical machine

MADE: Masked Auto-encoder for Distribution Estimation

1502.03509

I (mostly) skip this section in the seminar

1502.03509

Summary of MADE

(simple) Neural network for probability estimation

- MADE = Masked Auto-encoder for Distribution Estimation
- Auto-encoder is a neural network
- It can mimic a joint distribution of binary variables
  - (x_1, x_2, x_3, x_4) is distributed as $p(x_1, x_2, x_3, x_4) \equiv p[\overrightarrow{x}]$
- It is categorized as a generative model (as normalizing flow)
- It is correctly, normalized

Simulation results

Simulation results

Simulation setup

AT arXiv: 2205.08860

- g = 1, Nx = (4, 6), 8, 10, 1/T = [0.5-20.0], mu= [0-1.4], 4 lattice spacings 1/2a = [0.5-0.35]
- We do not take large volume limit but take continuum limit
    - (Practically, Nx>10 cannot be calculated on our numerical resources)
    - (My previous work shows data from Nx>12 are essential to take stable large volume limit though)
- Beta VQE:
    - Unitary = SU(4) ansatz
    - Classical weight = MADE
- Training epoch is 500, sampling = 5000
- Observables
    - Variational free energy (exact and variational one)
    - (Translationally invariant) Chiral condensate

Simulation results

Akio Tomiya

Variational free energy is O(1), Nx=10

AT arXiv: 2205.08860

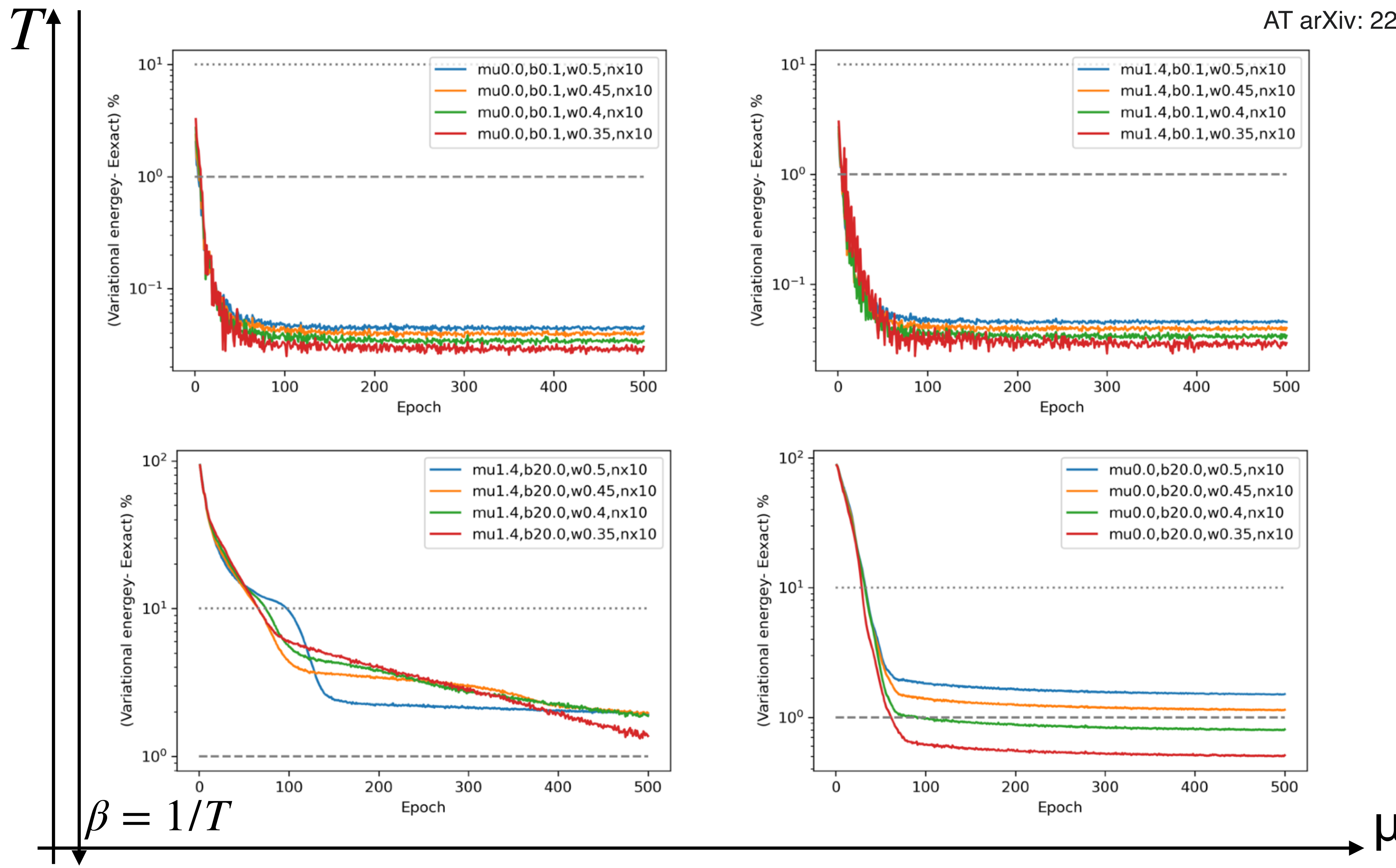
μ/g	g/T	N_x	w/g	$\mathcal{L} - \ln Z$	$-\ln Z$	Diff (%)
0.0	0.1	4	0.5	-27.779	-27.781	0.00804
0.0	0.1	4	0.35	-27.807	-27.808	0.005
0.0	0.1	10	0.5	-70.686	-70.718	0.0459
0.0	0.1	10	0.35	-71.744	-71.765	0.0302
0.0	0.5	4	0.5	-5.792	-5.802	0.185
0.0	0.5	4	0.35	-5.885	-5.891	0.105
0.0	0.5	10	0.5	-17.133	-17.25	0.68
0.0	0.5	10	0.35	-18.849	-18.934	0.448
0.0	10.0	4	0.5	-1.748	-1.75	0.161
0.0	10.0	4	0.35	-1.829	-1.829	0.0184
0.0	10.0	10	0.5	-8.218	-8.341	1.48
0.0	10.0	10	0.35	-9.98	-10.03	0.496
0.0	20.0	4	0.5	-1.492	-1.739	14.2
0.0	20.0	4	0.35	-1.653	-1.806	8.46
0.0	20.0	10	0.5	-8.202	-8.328	1.51
0.0	20.0	10	0.35	-9.955	-10.006	0.509
1.4	0.1	4	0.5	-28.021	-28.023	0.00697
1.4	0.1	4	0.35	-27.989	-27.991	0.00755
1.4	0.1	10	0.5	-70.842	-70.874	0.0453
1.4	0.1	10	0.35	-71.742	-71.763	0.0291
1.4	0.5	4	0.5	-6.784	-6.789	0.0609
1.4	0.5	4	0.35	-6.644	-6.647	0.0327
1.4	0.5	10	0.5	-17.989	-18.104	0.636
1.4	0.5	10	0.35	-19.445	-19.534	0.456
1.4	10.0	4	0.5	-3.708	-3.71	0.0728
1.4	10.0	4	0.35	-3.63	-3.669	1.07
1.4	10.0	10	0.5	-10.067	-10.243	1.71
1.4	10.0	10	0.35	-11.763	-11.862	0.837
1.4	20.0	4	0.5	-3.673	-3.681	0.218
1.4	20.0	4	0.35	-3.621	-3.669	1.31
1.4	20.0	10	0.5	-10.028	-10.224	1.92
1.4	20.0	10	0.35	-11.699	-11.862	1.37

Simulation results

Akio Tomiya

Variational free energy is O(1), Nx=10

AT arXiv: 2205.08860



1. Mild dependence on μ
2. Hard for T -> 0 (large deviation) as expected

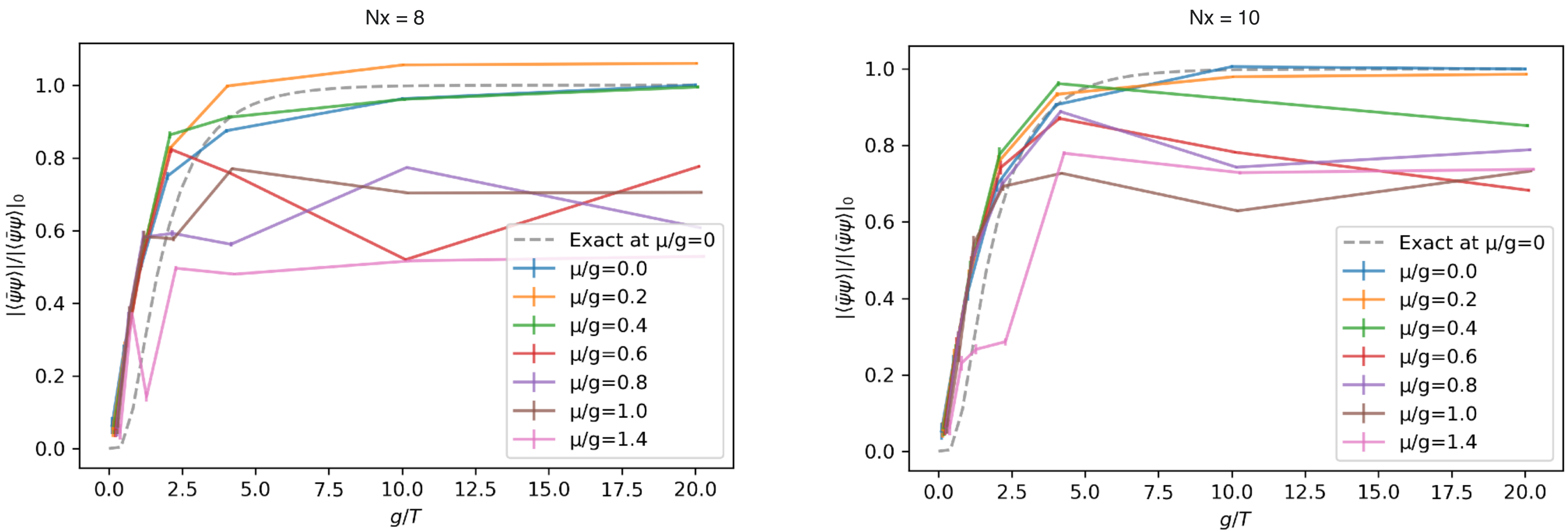
Simulation results

Continuum extrapolation for Nx = 8, 10

Akio Tomiya

AT arXiv: 2205.08860

So far it looks good



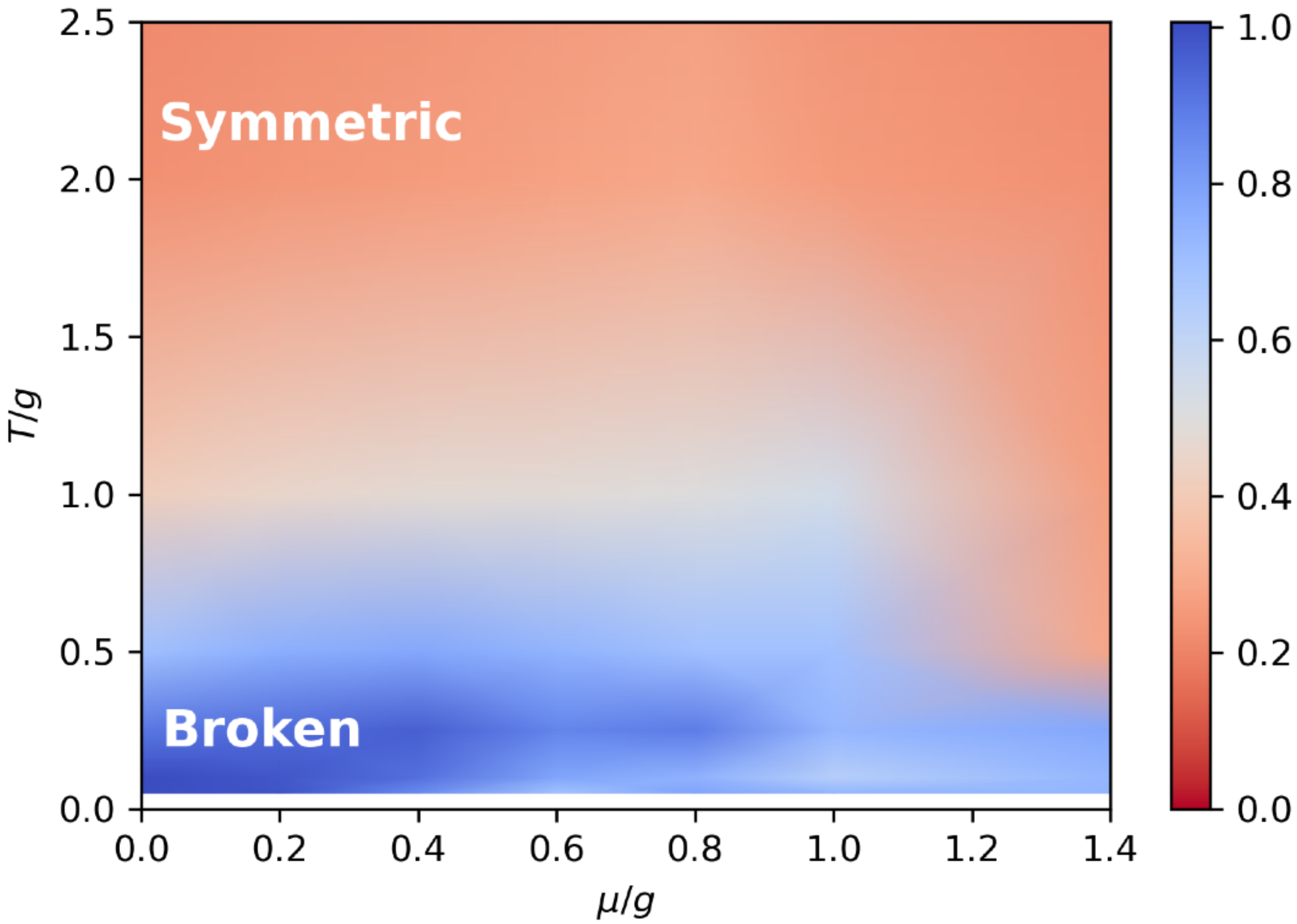
We use Nx = 10 results for the phase diagram

Simulation results

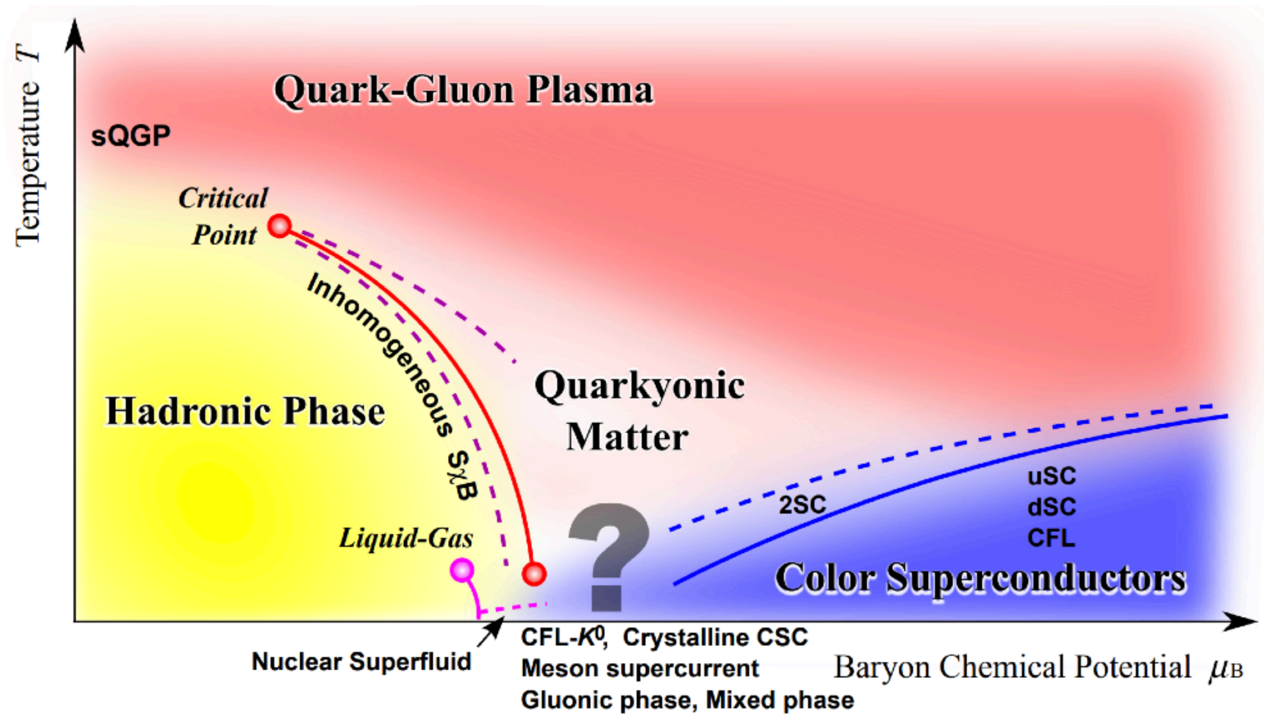
Continuum extrapolation for Nx = 10

AT arXiv: 2205.08860

$$\frac{\langle \overline{\psi}\psi \rangle_{T,\mu}}{\langle \overline{\psi}\psi \rangle_{0.05,0}}$$

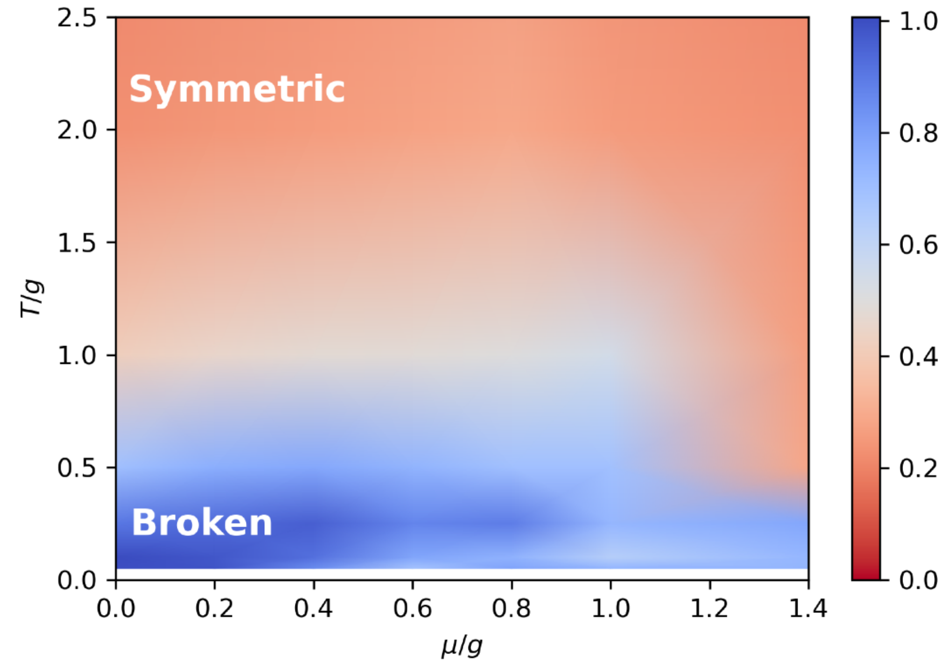


Fukushima , Hatsuda
Rept.Prog.Phys.74:014001,2011



Summary

AT arXiv: 2205.08860



- We investigate T-μ phase diagram for Schwinger model
- Continuum extrapolation has been evaluated
- Variational approach do not show difficulty for our parameter regime
- Towards to go large volume, optimization of code, GPU version, tensor network (real device?)
- Towards to investigate QCD. We need theoretical development to represent SU(3) variables with qubits (several candidates are avalable)