Quantum Simulation of Finite Temperature Schwinger Model via Quantum Imaginary Time Evolution

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based on the ongoing work with

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Finite-T QFT on quantum computers (QC)

Motivation

Quantum Simulation of finite-temperature and -density QCD

...Sign problem

$\Rightarrow$Lattice Monte Carlo method fails

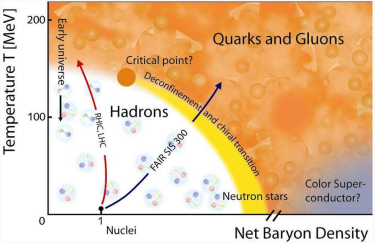
How to simulate finite-T QFTs on QC?

Mixed nature of thermal states

Finite T $\sim$ Imaginary time evolution

(non-unitary operation) $\Rightarrow$ Difficult on QC

[Aarts 2015]



Our work:

Simulate finite-T Schwinger model based on a quantum-classical hybrid algorithm

Introduction

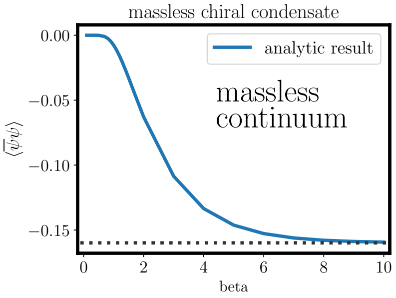
Schwinger model

- Schwinger model = 1+1 dim U(1) gauge theory

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

- Similarity to QCD
  - Chiral symmetry breaking ($\sim$chiral condensate $\langle\bar{\psi}\psi\rangle$)
  - Topological θ term $\Rightarrow$sign problem
  - Confinement/Screening
- Properties
  - Analytically solvable in the massless case
  - At finite-T...
    $\langle\bar{\psi}\psi\rangle \approx 0$ at low β ($\beta = 1/T$)
    $\langle\bar{\psi}\psi\rangle \neq 0$ at high β

[Sachs,Wipf 2010]



Qubit description of Schwinger model

- Spin Hamiltonian of Schwinger model

$$H = \frac{1}{4a}\sum_{n=1}^{N-1}\left[X_nX_{n+1} + Y_nY_{n+1}\right] + \frac{m}{2}\sum_{n=1}^{N}(-1)^n Z_n + \frac{ag^2}{2}\sum_{n=1}^{N-1}\left[\sum_{i=1}^{n-1}\frac{Z_i + (-1)^i}{2} + \frac{\theta}{2\pi}\right]^2$$

  a: lattice spacing, N: system size, g: coupling constant, m: fermion mass

  Here we have...

  - Discretized using Kogut-Susskind formalism
  - Solved the Gauss's law constraint and imposed the open b.c.
    $\Rightarrow$Remove U(1) gauge field
  - Used Jordan-Wigner transformation
    $\Rightarrow$Map fermions to spin degrees of freedom
- Nonlocal terms appear due to solving Gauss's law
- Chiral condensate $\langle\bar{\psi}\psi\rangle = \frac{1}{N}\sum_{i=1}^{N}(-1)^i\frac{1+\langle Z_i\rangle}{2a}$.

Finite-T QFT on QC

- Thermal states are mixed states:
  (e.g.) Gibbs state

$$\rho_\beta = Z^{-1} e^{-\beta \hat{H}}, \quad \langle \mathcal{O} \rangle_\beta^{\text{ens}} = Z^{-1}\,\mathrm{Tr}(\mathcal{O}\rho_\beta), \quad (Z = \mathrm{Tr}\,\rho_\beta)$$

  $\Rightarrow$ Mixed state: Difficult to prepare on QC
- Attempts of thermal state preparation on QC so far
  - Quantum thermal reservoir (e.g.) [Terhal+ 2000]
  - Quantum Metropolis sampling (e.g.) [Temme+ 2011]
  - ...

  $\Rightarrow$Requires numbers of samples or ancilla qubits that scale with system size

Thermal Pure Quantum (TPQ) state [Sugiura,Shimizu 2011] [Sugiura,Shimizu 2013]

- Typical pure state in thermal system
- Able to calculate local thermodynamic quantities
- Definition:
  For any mechanical variable ($\sim$ local observable) A,

$$\mathrm{P}\left(\left|\langle\psi|\hat{A}|\psi\rangle_{TPQ} - \langle\hat{A}\rangle^{\mathrm{eq}}_{E,N}\right| \geq \epsilon\right) \leq \eta_\epsilon(N)$$

$\langle\cdot\rangle^{\mathrm{eq}}_{E,N}$: thermal average

$\eta_\epsilon(N)$: function s.t. vanishes as $N \to \infty$

Thermal Pure Quantum (TPQ) state [Sugiura,Shimizu 2011] [Sugiura,Shimizu 2013]

- We use canonical TPQ:

$$|\beta, N\rangle \equiv e^{-\frac{\beta}{2}\hat{H}} |\psi_R\rangle \qquad (|\psi_R\rangle \text{ : random state })$$

- Average of initial random state

$$\overline{\left(\langle\hat{A}\rangle^{\mathrm{TPQ}}_{\beta,N} - \langle\hat{A}\rangle^{\mathrm{ens}}_{\beta,N}\right)^2} \to 0 \quad \text{w/ Thermodynamic limit} \quad N \to \infty$$

- (cf.) Grand Canonical TPQ state [Sugiura 2014]:
  We can easily introduce density

$$|\beta, \mu, N\rangle \equiv e^{-\frac{\beta}{2}(\hat{H}-\mu\hat{N})} |\psi_R\rangle \qquad \left(\hat{N} \text{ : number operator}\right)$$

Preparing TPQ state on QC

Preparation of canonical TPQ state $|\beta, N\rangle \equiv \exp\left(-\frac{\beta}{2}\hat{H}\right)|\psi_R\rangle$ on QC

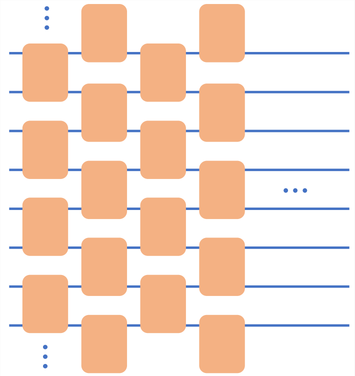
$\Rightarrow$ **Two tasks**

1. Preparation of random state $|\psi_R\rangle$
   ...Random state (unitary t-design) based on random circuits [Hunter-Jones 2019]
2. Implementation of non-unitary operation $\exp\left(-\frac{\beta}{2}\hat{H}\right)$
   - Variational method [McArdle+ 2018]
   - Probabilistic method [Liu+ 2020]
   - <u>Quantum Imaginary Time Evolution (QITE)</u> [Motta+ 2020]

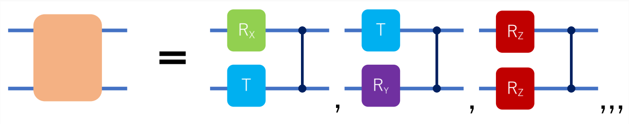
Algorithm

Random state preparation

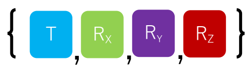
Random state (unitary t-design) based on random circuits[Hunter-Jones 2019]
...built from staggered layers of 2-site unitaries



- Each gate consists of single qubit gates randomly chosen from a universal gate set, and control-Z gate:

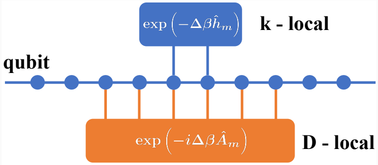


- Universal gate set (e.g.) :



- Achieve k-design with $O(Nk)$ depth

QITE algorithm: Calculation step



1. Trotterization $e^{-\frac{\beta}{2}\hat{H}} \simeq (e^{-\Delta\beta\hat{h}_1} e^{-\Delta\beta\hat{h}_2} \dots)^{n_{step}}$
2. Substitute local non-unitary operation with larger unitary operation

$$Ce^{-\Delta\beta\hat{h}_1}|\psi\rangle \simeq e^{-i\Delta\beta\hat{A}}|\psi\rangle$$

3. Expand $\hat{A}$ with Pauli strings and parameter $\mathbf{a}$

$$\hat{A}(\mathbf{a}) = \sum_{i_1\dots i_k} a_{i_1\dots i_k} \underbrace{\hat{\tau}_{i_1}\dots\hat{\tau}_{i_k}}_{\text{Pauli matrices}} \equiv \sum a_I\hat{\sigma}_I \qquad (\hat{\sigma}_I \in \{I, X, Y, Z\}^{\otimes D})$$

4. Determine the optimal parameter $\mathbf{a} = \{a_I\}$
   Then perform real time evolution $(I = 1 \sim 4^D)$

$$e^{-\frac{\beta}{2}\hat{H}}|\psi_R\rangle \simeq \left(\prod_m e^{-\Delta\beta\hat{h}_m}\right)^{n_{step}}|\psi_R\rangle \simeq \left(\prod_l \prod_I e^{-i\Delta\beta a_I\hat{\sigma}_I}\right)^{n_{step}}|\psi_R\rangle$$

Bottleneck of QITE algorithm

- For each term $e^{-\Delta\beta\hat{h}_m}$, we approximate $|\Phi\rangle_T$ with $|\Phi\rangle_A$:

$$\begin{aligned}\text{target state} \quad |\Phi\rangle_T &= Ce^{-\Delta\beta\hat{h}_m}|\psi\rangle \qquad \left(C = \langle\psi|e^{-2\Delta\beta\hat{h}_m}|\psi\rangle^{-1/2}\right)\\ \text{approximate state} \quad |\Phi\rangle_A &= e^{-i\Delta\beta\hat{A}(\mathbf{a})}|\psi\rangle\end{aligned}$$

$$\hat{A}(\mathbf{a}) = \sum a_I\hat{\sigma}_I \quad \left(\hat{\sigma}_I \in \{I, X, Y, Z\}^{\otimes D}\right)$$

- Find the optimal parameter $\mathbf{a}$ to minimize $\|\ |\Phi\rangle_T - |\Phi\rangle_A\ \|$

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

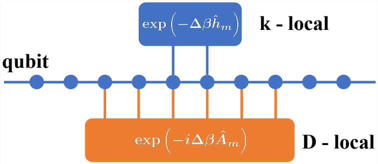
$$\text{w/} \quad S_{IJ} = \langle\psi\,|\hat{\sigma}_I\hat{\sigma}_J|\,\psi\rangle\,, \quad b_I = -2c^{-1/2}\,\mathrm{Im}\langle\psi|\hat{\sigma}_I\hat{h}_m|\psi\rangle$$

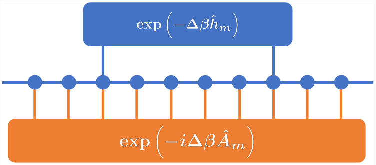
- Measure $\langle\psi\,|**|\,\psi\rangle$ on QC
  Solve the optimization problem by CG algorithm on CC
- Need to calculate $4^D \times 4^D$ matrix

QITE algorithm: Nonlocality

- It works well with local Hamiltonians
  (e.g.) Heisenberg model [Motta+ 2020],
  NJL model [Czajka+ 2022],
  (Z_2 gauge theory (TPQ) [Davoudi+ 2022])
- We can increase system size with fixed D

$\Rightarrow$ **How about Schwinger model, which includes non-local terms?**



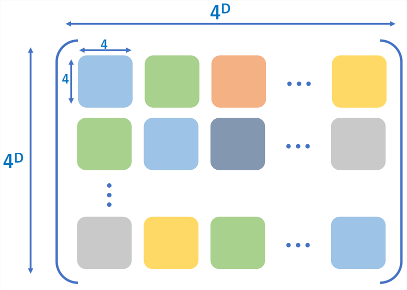


Practical improvements of QITE (Our idea)

To reduce cost and memory, we focus on the structure of $\mathbf{S}$

1. Decompose $\mathbf{S}$ into 4×4 matrix
2. Independent elements = only first row (up to phase)

$\mathbf{S} =$



$\Rightarrow$ Result: cost and memory $O(16^D) \rightarrow O(4^D)$

Calculation setup

- Schwinger model Hamiltonian
  (Staggered fermion, Jordan-Wigner transformation, Gauss's law, open b.c.)

$$H = \frac{1}{4a}\sum_{n=1}^{N-1}\left[X_n X_{n+1} + Y_n Y_{n+1}\right] + \frac{m}{2}\sum_{n=1}^{N}(-1)^n Z_n + \frac{ag^2}{2}\sum_{n=1}^{N-1}\left[\sum_{i=1}^{n-1}\frac{Z_i + (-1)^i}{2} + \frac{\theta}{2\pi}\right]^2$$

- Parameters

  $N = 4 - 12, \;\; a = 0.8, \;\; g = 1.0,$

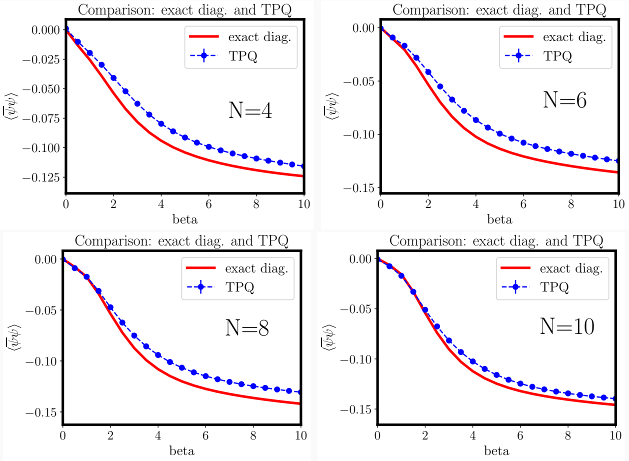
  $m = 0.00$: Exact solvable $\rightarrow$ feasibility test

  $m = 0.15$ with θ : prediction

  averaged over 100 initial random states
- Methods:
  1. Exact diagonalization (exact at finite N)
  2. TPQ (classical algorithm)
  3. QITE (quantum algorithm, statevector simulation)

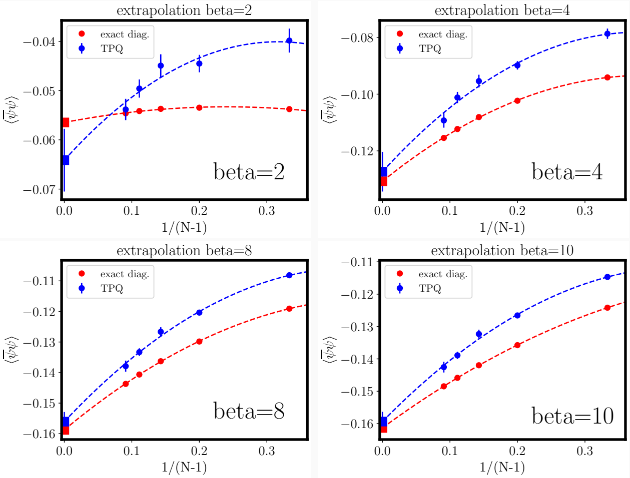
Results

Comparison: TPQ vs Exact diagonalization (massless case)



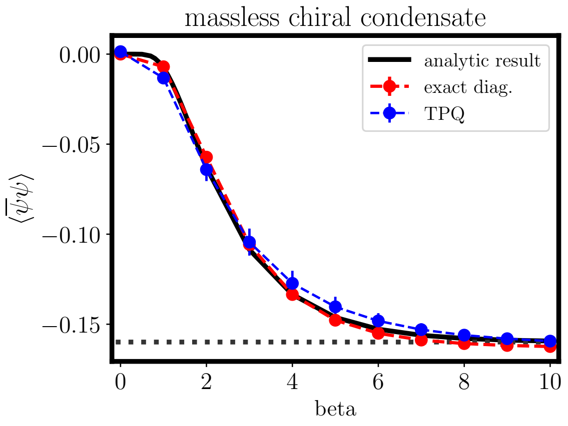
- At finite N, TPQ $\neq$ exact diag.
- At $\beta \simeq 0$ or ∞, TPQ $=$ exact diag.

Extrapolation toward thermodynamic limit (massless case)



- $1/(N-1)$ Extrapolation by quadratic function
- Extrapolated results of TPQ are consistent with one of exact diag. at $N \to \infty$ (within the statistical errors)

Thermodynamic limit of chiral condensate (massless case)



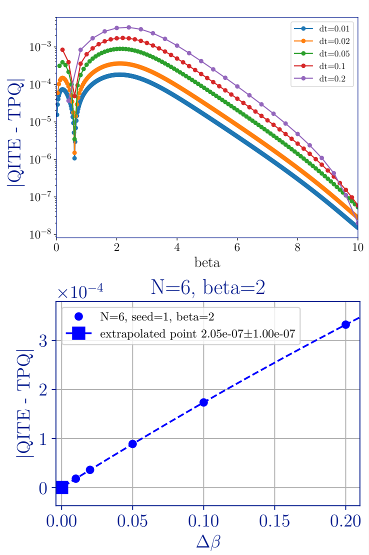
- Analytic result of massless chiral condensate at continuum: [Sachs,Wipf 2010]

$$\langle\overline{\psi}\psi\rangle = -\frac{m_\gamma}{2\pi} e^\gamma e^{2I(\beta m_\gamma)}$$

$$I(x) = \int_0^\infty \frac{1}{1-e^{x\cosh(t)}} dt$$

- At zero-T [Gross+ 1996], $\langle\overline{\psi}\psi\rangle = -e\frac{\exp(\gamma)}{2\pi^{3/2}} \simeq -0.1599$

Comparison: QITE vs TPQ (massless case)



- Perform QITE algorithm with $N = 6, \Delta\beta = 0.01 - 0.2$
- We found the difference between TPQ and QITE scales $O(\Delta\beta)$
- Systematic error from $\Delta\beta$ is under control

Summary of feasibility test (massless case)

TPQ $\Leftrightarrow$ Exact diagonalization

- At small system size, TPQ$\neq$ exact diag.
- TPQ $=$ exact diag. with larger N
- **Thermodynamic limit of TPQ results reproduces the analytic result**

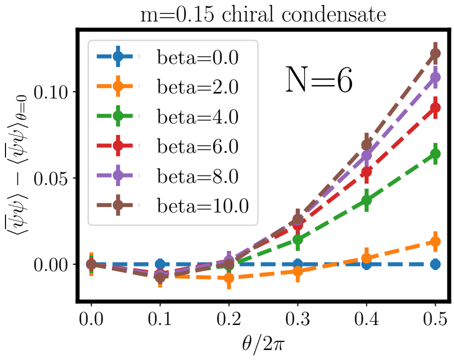
QITE $\Leftrightarrow$ TPQ

- QITE has a digitization error
- It scales properly and is controllable

TPQ + QITE works well!

We need to take (1) $\Delta\beta \to 0$, and (2) $N \to \infty$ extrapolation for accurate estimation

θ dependence of chiral condensate (massive case)

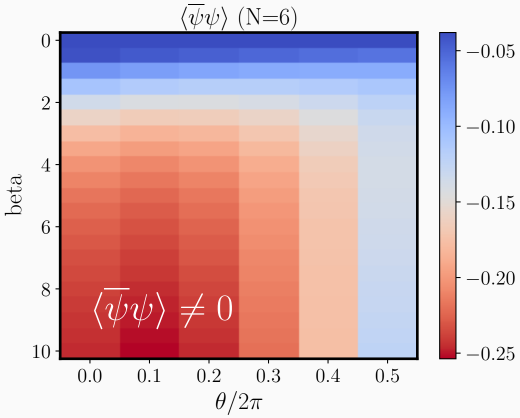


- QITE result
- Vertical axis denotes

$$\langle\overline{\psi}\psi\rangle_{\beta,\theta} - \langle\overline{\psi}\psi\rangle_{\beta,\theta=0}$$

- Low/High beta
  ...small/large θ-dependence

θ dependence of chiral condensate (massive case)



- $\langle\bar{\psi}\psi\rangle \neq 0$ at high β and small θ
- In large θ, chiral symmetry seems to be restored
- Taking thermodynamic limit: ongoing work

$\Rightarrow$ **TPQ+QITE works at massive and nonzero θ region !**

Summary and Discussion

Summary

- We investigated the Schwinger model at finite T with TPQ and QITE
- Non-locality oh the Hamiltonian requires large D, but we improved the QITE method and successfully handled large enough number of site
- TPQ result is consistent with T-dependence of chiral condensate at thermodynamic limit (massless case)
- Our method can be extend to massive and nonzero θ region
- Our calculations have been done classically, but **completely implementable on quantum circuits**

Discussion

- Application to other systems (higher dim., non-Abelian, **finite dinsity**,...)
- Implementation on real devices (VITE? connectivity?)
- Non-locality: Further improvements?
- Imaginary time evolution with local hamiltonian and **Gauss' law projection** [Davoudi+ 2022]

Thank you!

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TPQ (Thermal pure quantum) state

TPQ state … Pure state that approximates the thermal state

- Definition:

$$\mathrm{P}\left(\left|\langle\psi|\hat{A}|\psi\rangle_{TPQ} - \langle\hat{A}\rangle^{\mathrm{eq}}_{E,N}\right| \geq \epsilon\right) \leq \eta_\epsilon(N)$$

$\langle\cdot\rangle^{\mathrm{eq}}_{E,N}$: ensemble average

$\eta_\epsilon(N)$: function s.t. vanishes as $N \to \infty$

- Canonical TPQ state[Sugiura,Shimizu 2013]:

$$|\beta, N\rangle \equiv e^{-\frac{\beta}{2}\hat{H}}\,|\psi_R\rangle \qquad (\ |\psi_R\rangle\ :\ \text{random state}\ )$$

- Grand Canonical TPQ state[Sugiura 2014]:

$$|\beta, \mu, N\rangle \equiv e^{-\frac{\beta}{2}(\hat{H}-\mu\hat{N})}\,|\psi_R\rangle \qquad \left(\hat{N}\ :\ \text{number operator}\right)$$

QITE - practical improvements

- Utilizing the efficient Pauli measurement
  "Pauli word" W: $W = W_1 W_2 \dots W_N \in \{X, Y, Z\}^N$
  (e.g.) 10-sites

$$
\begin{aligned}
W &= XYZXYZXYZX \\
&= XYZ\ XYZ\ XYZ\ X \to \langle X_1 Y_2 Z_3 \rangle\ ,\ \langle X_4 Y_5 Z_6 \rangle\ ,\ \langle X_7 Y_8 Z_9 \rangle
\end{aligned}
$$

Improvement

Memory: $O(16^D) \to O(4^D)$

Calculation cost: $O(16^D) \to O(4^D)$ ($\to O(3^D)$)