Quantum simulation of thermal field theories

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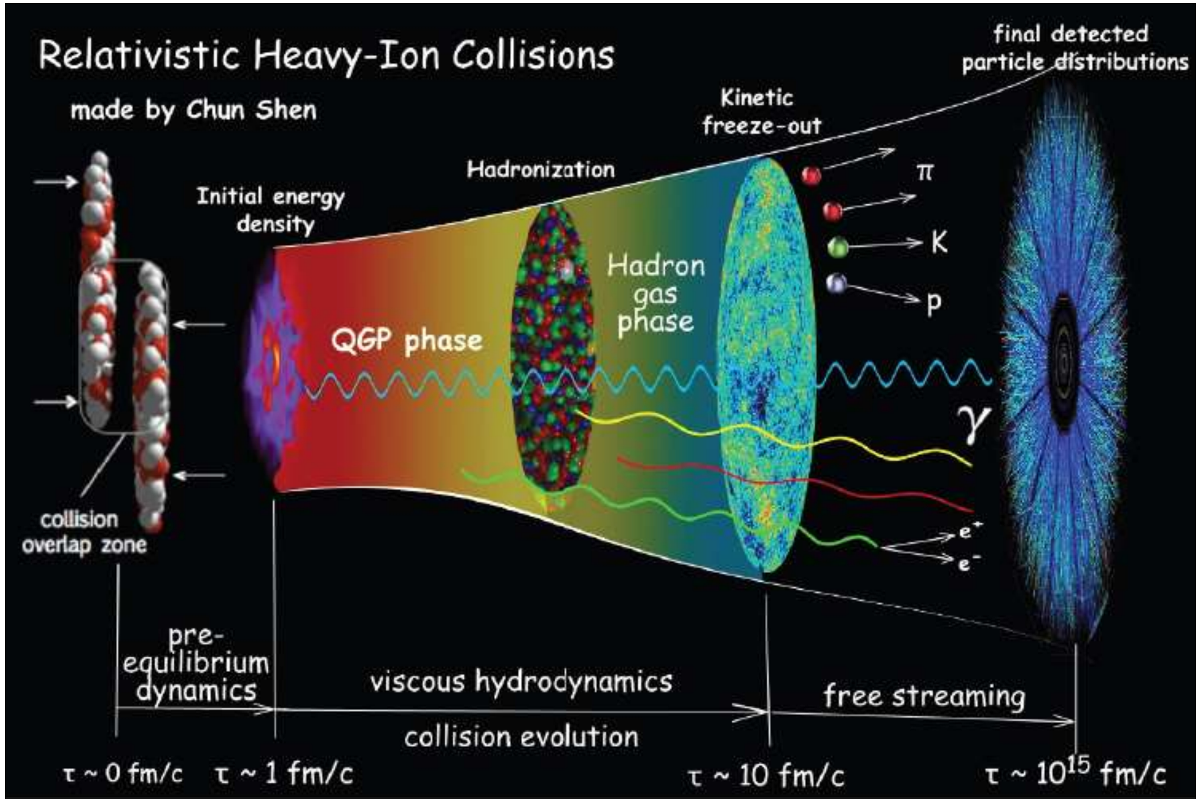
1.1 Introduction



- QGP constitutes one of the main research areas in QCD physics.
- Time evolution of QCD matter before thermalization has been studied using classical approaches such as classical field simulations or kinetic theory
- It has not yet been resolved from fundamental principles of QCD
- Lattice QCD is only applicable at low baryon densities where the numerical sign problem does not interfere with calculations

- Quantum computing is a potential tool for solving real-time dynamics from QCD first principles

1.2 State of the art in quantum computer technology

- Quantum computing (QC) is a rapidly-emerging technology that harnesses the laws of quantum mechanics to solve problems too complex for classical computers.
- Currently, we are in the Noisy Intermediate-Scale quantum (NISQ) era:
  - Quantum processors containing up to ~ 1000 qubits
  - Sensitive to their environment
  - Prone to quantum decoherence
- Quantum information science has proved useful in a broad range of physics applications
- Quantum simulation is potentially more advantageous in reducing the problem complexity from exponential to polynomial

IBM Condor employs over 1000 qubits ⇨

1.3 Quantum computing in quantum field theory

- ϕ^4 theory

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m_0^2\phi^2 - \frac{1}{4!}\lambda_0\phi^4$$

Jordan, Lee & Preskill, 2011 [arXiv:1112.4833]

Klco & Savage, 2018 [arXiv:1808.10378]

- Fermion fields

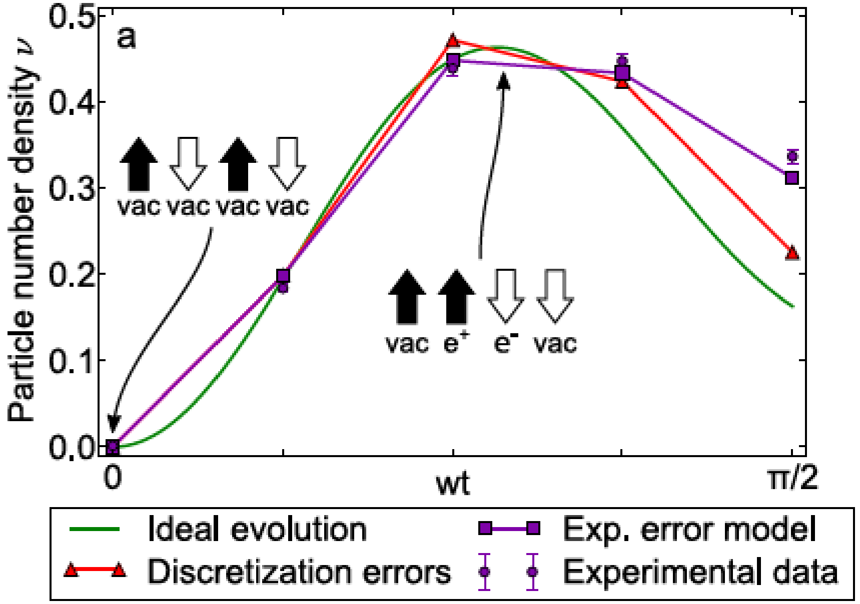
$$\mathcal{L} = \sum_{j=1}^{N}\bar{\psi}_j(i\gamma^\mu\partial_\mu - m)\psi_j + \frac{g^2}{2}\left(\sum_{j=1}^{N}\bar{\psi}_j\psi_j\right)^2$$

Jordan, Lee & Preskill, 2014 [arXiv:1404.7115]

- Schwinger model

$$\mathcal{L} = \bar{\psi}(i\not{D} - m)\psi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}$$

de Jong et al., 2022 [arXiv:2106.08394]



Martínez et al., 2016 [arXiv:1605.04570v1]

We study QFT in thermal equilibrium preparing for a broader study of real-time dynamics

1.4 Thermal field theory

- Thermal states are typically difficult to prepare on a circuit and involve non-unitary operations.
- Quantum imaginary time evolution **(QITE)** requires exponentially less space and time per iteration compared with their classical counterparts

Motta, 2019 [arXiv:1901.07653]

Expectation value $\langle \hat{O} \rangle_\beta \equiv Z_\beta^{-1} \mathrm{Tr}[e^{-\beta \hat{H}} \hat{O}]$ Partition function $Z_\beta \equiv \mathrm{Tr}[e^{-\beta \hat{H}}]$.

The trace can be calculated by summing the expectation values over the complete set of states

We focus on phase space distribution: $f_p^i = \left\langle \hat{a}_p^{i\,\dagger} \hat{a}_p^i \right\rangle_\beta$

2.1 Fermion fields in 1+1 dimensions

Lagrangian density $\mathcal{L} = \frac{1}{2}\bar{\psi}(i\partial - m)\psi - \mathcal{H}_I(\psi)$

Majorana fermions $\begin{cases} \psi^\dagger = \psi^T \\ \{\psi^\alpha(t,x), \psi^\beta(t,y)\} = \delta(x-y)\delta^{\alpha\beta} \end{cases}$

- Step 1: put the theory on a spatial lattice: $x \in \Omega_x \equiv \{0, a, \cdots, (N-1)a\}$ $\quad L \equiv aN$

$$\hat{H} = \frac{1}{2}\sum_n \bar{\psi}_n\left[-\frac{i}{2a}\gamma^1(\psi_{n+1} - \psi_{n-1}) + m\psi_n\right] - \frac{r}{4a}\sum_n \bar{\psi}_n(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + \hat{H}_I$$

with $\psi_n(t) \equiv \sqrt{a}\psi(t, na)$

Qian & Wu, 2024 [arXiv:2404.07912]

- Step 2: Map it onto qubits: N qubits needed to represent N Majorana fermions

One can use both coordinate and momentum space to represents on qubits

2.2 Representation in coordinate space

- Step 1: In terms of the creation/annihilation operators, the Hamiltonian may be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_I \qquad \hat{H}_0 = \sum_n \left[-i\frac{a_n a_{n+1} + a_n^\dagger a_{n+1}^\dagger}{2a} + m\left(a_n^\dagger a_n - \frac{1}{2}\right)\right]$$

$$\psi_n = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} a_n \\ a_n^\dagger \end{pmatrix} \qquad -\frac{r}{2a}\sum_n [a_n^\dagger(a_{n+1} - 2a_n + a_{n-1}) + 1]. \qquad \{a_n, a_{n'}^\dagger\} = \delta_{nn'}$$

- Step 2: Map it onto qubits using eigenstates of $a_n^\dagger a_n$ as the computation basis

$$|n_0 n_1 \cdots n_{N-1}\rangle_x = \prod_{i=0}^{N-1} (a_i^\dagger)^{n_i} |0\rangle_x \equiv (a_0^\dagger)^{n_0} (a_1^\dagger)^{n_1} \cdots (a_{N-1}^\dagger)^{n_{N-1}} |0\rangle_x,$$

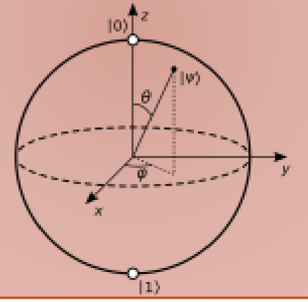
$$_x\langle n_0 n_1 \cdots n_{N-1}| = {}_x\langle 0| \prod_{i=N-1}^{0} (a_i)^{n_i} \equiv {}_x\langle 0|(a_{N-1})^{n_{N-1}}(a_{N-2})^{n_{N-2}} \cdots (a_0)^{n_0}$$

The fermions can be map to qubits using the Jordan-Wigner transformation

$$a_n^\dagger = \frac{\sigma_n^X - i\sigma_n^Y}{2}\prod_{i=0}^{n-1}\sigma_i^Z \qquad a_n = \frac{\sigma_n^X + i\sigma_n^Y}{2}\prod_{i=0}^{n-1}\sigma_i^Z$$

bit $\rightarrow \{0,1\}$

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



2.3 Representation in momentum space

➢ Step 1: Hamiltonian in terms of creation and annihilation operators in momentum space

1 $\tilde{a}_p^\dagger \equiv \frac{1}{\sqrt{N}} \sum_n e^{ipan} a_n^\dagger, \qquad \tilde{a}_p \equiv \frac{1}{\sqrt{N}} \sum_n e^{-ipan} a_n.$

$\Delta p \equiv 2\pi/L$

2 $\begin{pmatrix} \hat{a}_p^\dagger \\ \hat{a}_{-p} \end{pmatrix} = \frac{1}{2\sqrt{E_p}} \begin{pmatrix} \sqrt{p^+} + \sqrt{p^-} & \sqrt{p^+} - \sqrt{p^-} \\ \sqrt{p^-} - \sqrt{p^+} & \sqrt{p^+} + \sqrt{p^-} \end{pmatrix} \begin{pmatrix} \tilde{a}_p^\dagger \\ \tilde{a}_{-p} \end{pmatrix}$

3 $\hat{H}_0 \equiv \sum_p E_p (\hat{a}_p^\dagger \hat{a}_p - 1/2)$

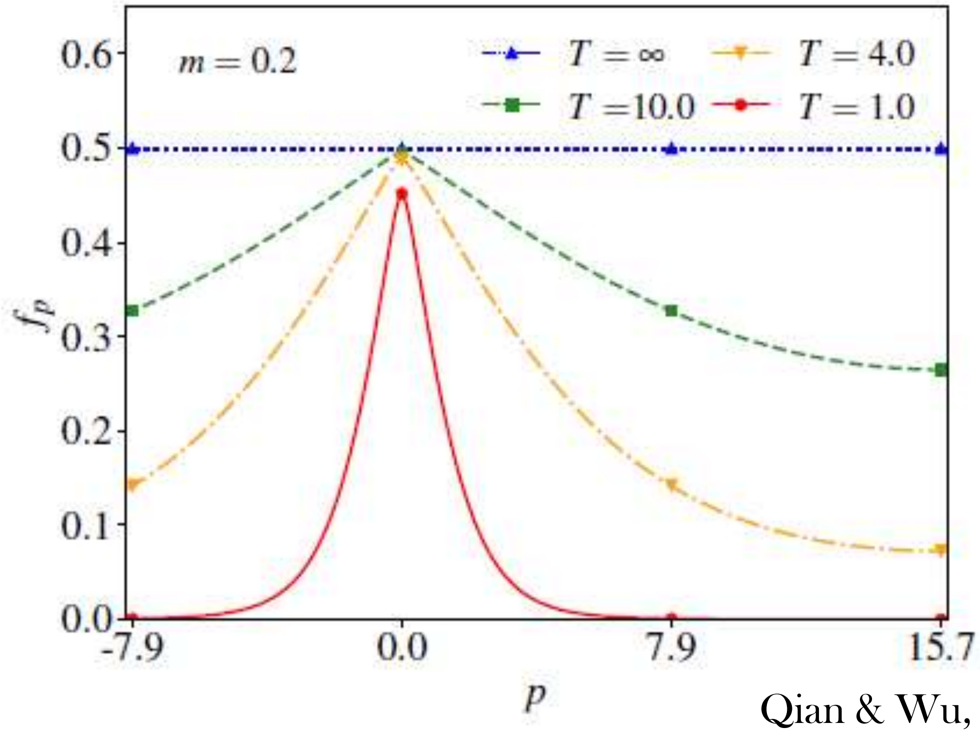
$E_p = \sqrt{\left(m + \frac{2r}{a} \sin^2 \frac{ap}{2}\right)^2 + p_a^2}$

➢ Step 2: Map it onto qubits using eigenstates of $a_p^\dagger a_p$ as the computation basis

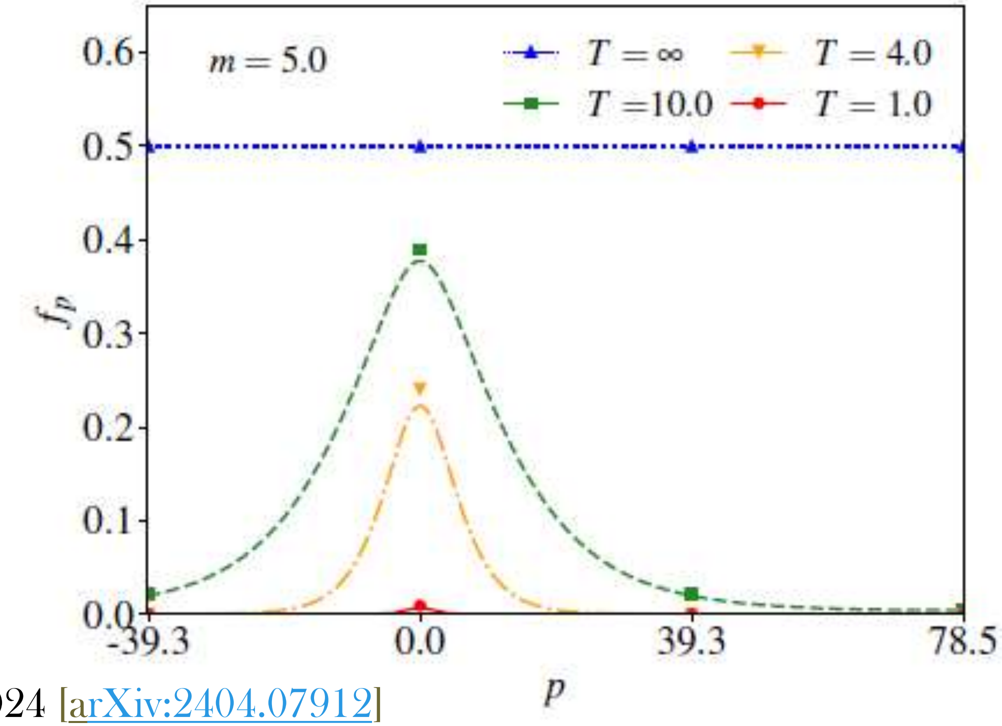
We use coordinate space (field operator space) for simulations and momentum space for analytical calculations

2.4 Simulation results for free fermion fields

Using the QITE algorithm



(a) $T \gg m$ case



(b) $m \gg T$ case

Qian & Wu, 2024 [arXiv:2404.07912]

Analytical result: Fermi-Dirac distribution $f_p \equiv \langle \hat{a}_p^\dagger \hat{a}_p \rangle_\beta$ → $f_p = \frac{1}{e^{\beta E_p} + 1}$

2.5 Thermal states of interacting fermion fields on lattice

- Four-fermion interaction vanishes → we introduce one more Majorana field $\psi_B = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ i & -i\end{pmatrix}\begin{pmatrix}b\\ b^\dagger\end{pmatrix}$

$$L = \int dx \left[\frac{1}{2}\bar{\psi}(i\partial\!\!\!/ - m_0)\psi - \frac{g}{4}(\bar{\psi}\psi)(\bar{\psi}_B\psi_B)\right] + \frac{1}{2}\bar{\psi}_B(i\gamma^0\partial_t - M)\psi_B \qquad \hat{H}_I = \frac{M}{2}\bar{\psi}_B\psi_B + \frac{g}{4}\int dx\bar{\psi}\psi\bar{\psi}_B\psi_B$$

- There exist two types of quasiparticles with two phase-space distributions:

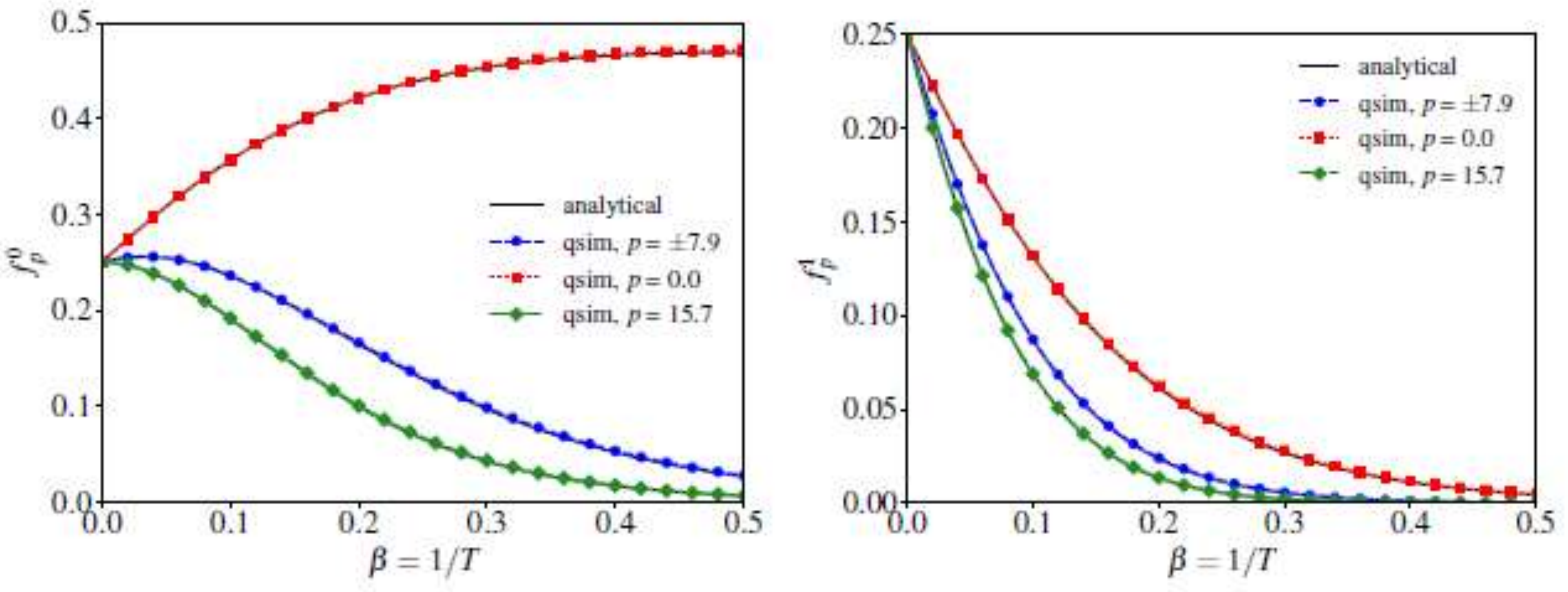
$$f_p^0 \equiv \langle \hat{a}_p^\dagger \hat{a}_p\rangle_\beta = \frac{Z_\beta^0}{Z_\beta}\frac{1}{1+e^{\beta E_p(\bar{m})}}, \qquad f_p^1 \equiv \langle \hat{a}_p'^\dagger \hat{a}_p'\rangle_\beta = \frac{Z_\beta^1}{Z_\beta}\frac{1}{1+e^{\beta E_p(\bar{m}+g)}}$$

where $$Z_\beta = Z_\beta^0 + Z_\beta^1$$

$$\bar{m} = E_0 - E_\Omega$$

$$Z_\beta^0 \equiv e^{-\beta E_\Omega}\prod_p\left(1+e^{-\beta E_p(\bar{m})}\right), \qquad Z_\beta^1 \equiv e^{-\beta E_\Omega^1}\prod_p\left(1+e^{-\beta E_p(\bar{m}+g)}\right)$$

2.6 Simulation results for interacting fermion fields



Qian & Wu, 2024 [arXiv:2404.07912]

3.1 SCALAR FIELD THEORY

IC, Qian & Wu [work in progress]

Lagrangian density for the ϕ^4 theory in d + 1

$$\mathcal{L} = \frac{1}{2}[\partial_\mu\phi\partial^\mu\phi - m\phi^2] - \frac{\lambda}{4!}\phi^4$$

Field and conjugate-field operators

$$[\phi(x),\phi(y)] = [\pi(x),\pi(y)] = 0, \qquad [\phi(x),\pi(y)] = i\delta(x-y)$$

- Step 1: Discretised hamiltonian

$$H_{\rm lat} = a^d \sum_{n=0}^{N-1}\left[\frac{1}{2}\pi_n^2 + \frac{1}{2}m^2\phi_n^2 + \frac{1}{2}(\nabla\phi)_n^2 + \frac{\lambda}{4!}\phi_n^4\right]$$

We use dimensionless hamiltonian in (1+1) spacetime

$$\bar{H} = \sum_{n=0}^{N-1}\left[\frac{1}{2}\bar{\Pi}_n^2 + \frac{1}{2}\bar{m}^2\bar{\Phi}_n^2 + \frac{1}{2}(\bar{\Phi}_{n+1} - \bar{\Phi}_n)^2 + \frac{\bar{\lambda}}{4!}\bar{\Phi}_n^4\right]$$

$$\bar{\Phi}_n = a^{\frac{d-1}{2}}\phi_n, \quad \bar{\Pi}_n = a^{\frac{d+1}{2}}\pi_n \qquad [\bar{\Phi}_n, \bar{\Pi}_{n'}] = i\delta_{nn'}$$

- Step 2: Map it onto qubits

One can use both coordinate and momentum space to represents on qubits

3.2 Field operator discretisation

Macridin et al., 2021 [arXiv:2108.10793]

- The lattice Hilbert space is a tensor product of local Hilbert space at each lattice site
- The local Hilbert space at a single lattice site is infinite dimensional because there are infinitely many bosons contributing to the local wave function

$$\phi_n = (-\infty, \infty)$$

- We truncate the number of bosons by a cutoff number N_b and then digitize the continuous field operators to discretized values

$$\phi_n = [-\phi_{\max}, \phi_{\max}]$$

Discrete field operators Φ_n acting on H_n

$$\Phi_n \left|\varphi_\alpha\right\rangle_n = \varphi_\alpha \left|\varphi_\alpha\right\rangle_n, \qquad \alpha = 0, 1, \ldots, N_\varphi - 1$$

$$\varphi_\alpha = \Delta_\varphi\left(\alpha - \frac{N_\varphi - 1}{2}\right), \qquad \Delta_\varphi = \sqrt{\frac{2\pi}{N_\varphi \bar{m}}}$$

Discrete conjugate field operators Π_n acting on H_n

$$\Pi_n = \bar{m}\mathcal{F}_n \Phi_n \mathcal{F}_n^{-1}$$

$$\Pi_n \left|\kappa_\beta\right\rangle_n = \kappa_\beta \left|\kappa_\beta\right\rangle_n, \qquad \beta = 0, 1, \ldots, N_\varphi - 1$$

$$\kappa_\beta = \Delta_\kappa\left(\beta - \frac{N_\varphi - 1}{2}\right), \qquad \Delta_\kappa = \sqrt{\frac{2\pi\bar{m}}{N_\varphi}}$$

$$[\Phi_n, \Pi_n] \left|n\right\rangle_n = i \left|n\right\rangle_n + \mathcal{O}(\epsilon)$$

3.3 Scalar field theory on the qubit

$N_\varphi = 2^{n_Q}$
$n_T = N n_Q$

- We use a 1D lattice of N quantum registers to represent N lattice points. In each register, we use n_Q qubits

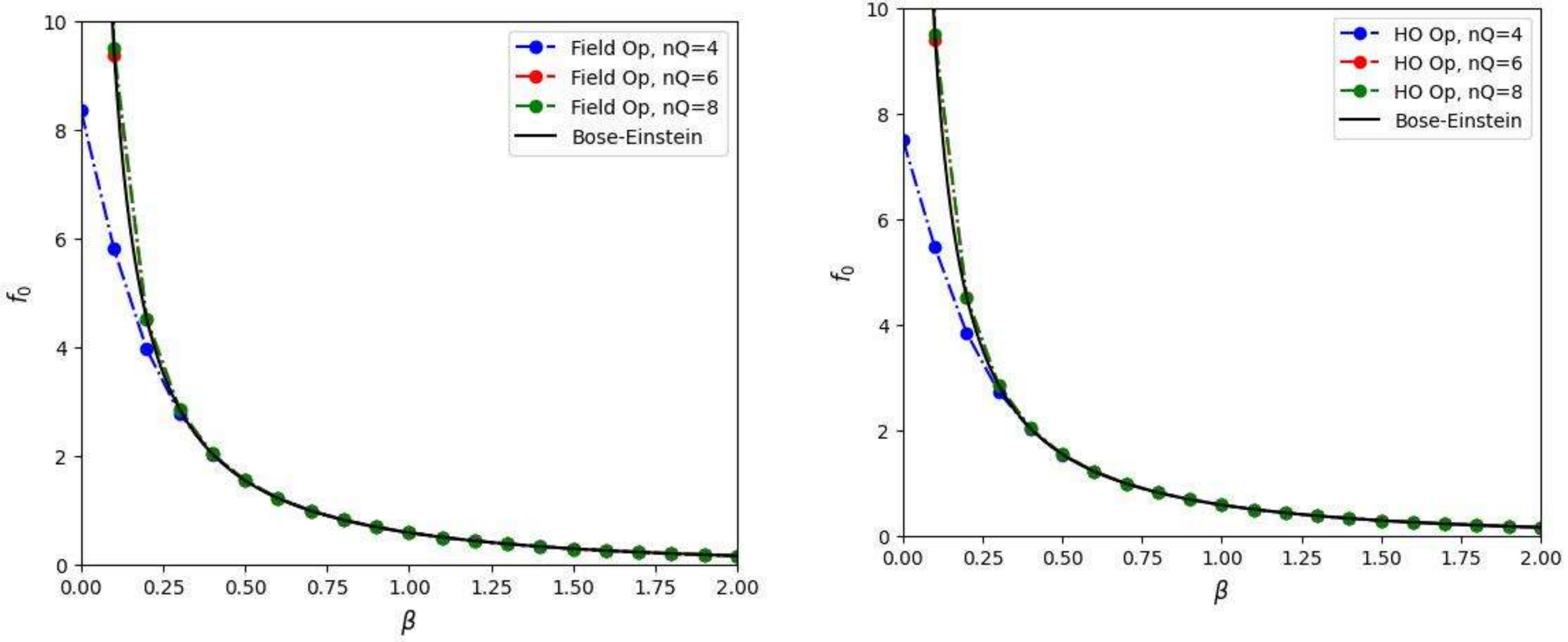
- We represent the $\{|\varphi_\alpha\rangle\}_n$ on the n^th quantum register using binary representation of the label α. The generic state |k⟩ in coordinate space is

$$
\begin{aligned}
|k\rangle &= |k\rangle_0 |k\rangle_1 \dots |k\rangle_{N-1} \\
&= \big(|q_{n_Q-1}\rangle |q_{n_Q-2}\rangle \dots |q_0\rangle\big)_0 \big(|q_{n_Q-1}\rangle |q_{n_Q-2}\rangle \dots |q_0\rangle\big)_1 \dots \big(|q_{n_Q-1}\rangle |q_{n_Q-2}\rangle \dots |q_0\rangle\big)_{N-1}
\end{aligned}
$$

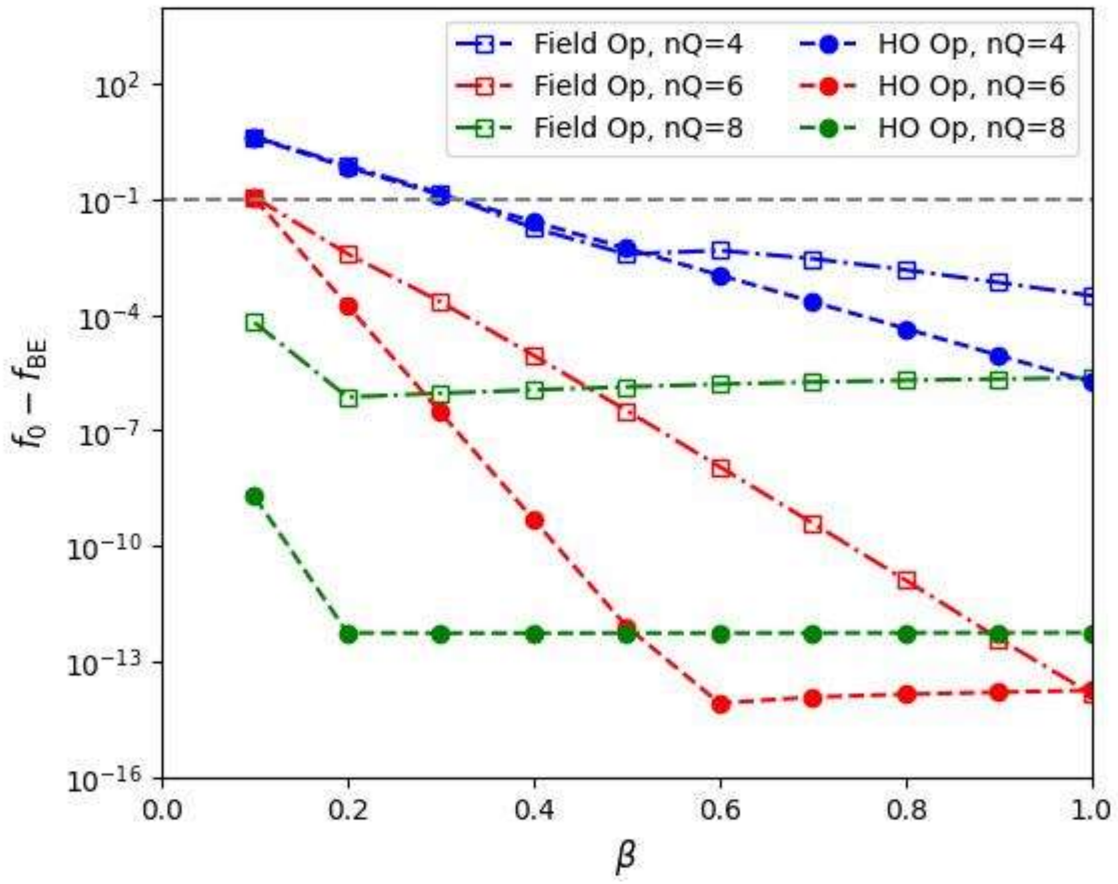
- Again, we can do the mapping onto qubits using eigenstates of $a_p^\dagger a_p$ as the computation basis, but now $a_p^\dagger a_p$ must be truncated

3.5 Simulation results for scalar fields

IC, Qian & Wu [work in progress]



Analytical results: Bose-Einstein distribution $f_p \equiv \langle \hat{a}_p^\dagger \hat{a}_p \rangle_\beta$ → $f_p = \dfrac{1}{e^{\beta E_p} - 1}$



Field Op, nQ=4
Field Op, nQ=6
Field Op, nQ=8
HO Op, nQ=4
HO Op, nQ=6
HO Op, nQ=8
10^{2}
10^{-1}
10^{-4}
10^{-7}
10^{-10}
10^{-13}
10^{-16}
$f_0 - f_{BE}$
0.0
0.2
0.4
0.6
0.8
1.0
β

Summary

- We formulated the quantum field theory for Majorana fermions and scalar fields in 1+1 dimensions on the qubits and studied its various thermal properties at finite temperature using quantum simulation algorithms

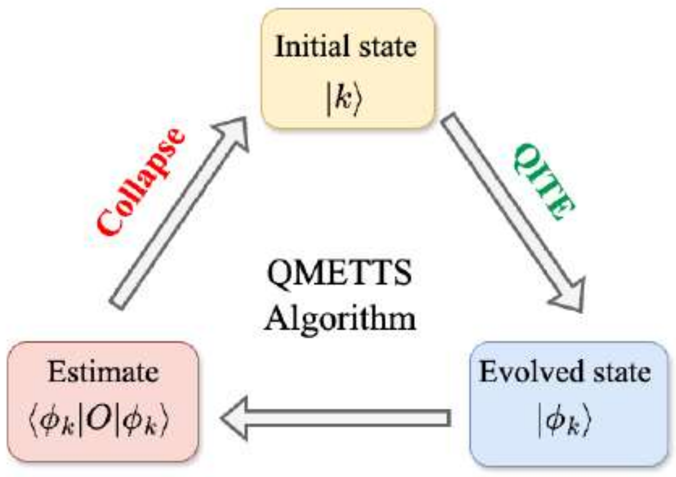
- We showed that the QITE algorithm can be used to study thermal observables such as the distribution function at finite temperature.

- Our numerical results using quantum simulation are compared to analytical calculations and exact diagonalization methods, showing good agreement

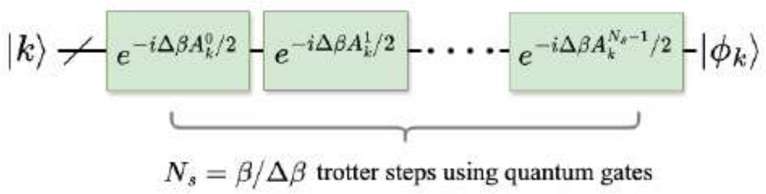
Quantum imaginary time evolution

Motta, 2019 [arXiv:1901.07653]

Trotter formula: $|\psi_k(\beta/2)\rangle = e^{-\beta \hat{H}/2}|k\rangle = \prod_{i=1}^{N_s} e^{-\Delta\beta \hat{H}/2}|k\rangle$



(a) QMETTS algorithm



(b) QITE algorithm

Figure 1. Skematic diagram of the workflow for the QMETTS and QITE algorithms [24] used in this work. Note the QITE is a subroutine in the QMETTS.

$$|\psi_k^{i+1}\rangle = e^{-\Delta\beta \hat{H}/2}|\psi_k^i\rangle = \sqrt{c_k^i(\Delta\beta)}\, e^{-i\Delta\beta \hat{A}_k^i/2}|\psi_k^i\rangle + \mathcal{O}(\Delta\beta^2)$$

Real-time Hamiltonian operator

$$\hat{A}_k^i = \sum_I a_I \sigma_I$$

determined by solving the linear matrix equation

$$(\boldsymbol{S} + \boldsymbol{S}^T)\boldsymbol{a}_i = \boldsymbol{b}$$

whose matrix elements are evaluated as expectation values on the quantum circuit

$$b_I = -i\,\langle\psi_k^i|(\hat{H}\sigma_I - \sigma_I^\dagger \hat{H})|\psi_k^i\rangle / \sqrt{c_k^i(\Delta\beta)}$$

$$S_{IJ} = \langle\psi_k^i|\sigma_I^\dagger \sigma_J|\psi_k^i\rangle$$

Thermal expectation on the circuit

White, 2009 [arXiv:0902.4475]

Minimally entangled typical thermal state method (METTS)

Redefined quantum state $|\phi_k\rangle = P_k^{-1/2} e^{-\beta \hat{H}/2} |k\rangle \,, \quad P_k = \langle k| e^{-\beta \hat{H}} |k\rangle$

in QITE: $|\phi_k\rangle \equiv \prod_{i=1}^{N_s} e^{-i\Delta\beta \hat{A}_k^i/2} |k\rangle \,, \qquad P_k \equiv \prod_{i=1}^{N_s} c_k^i(\Delta\beta)$

Thermal observables $\langle \hat{O} \rangle_\beta = \sum_{k \in \mathcal{S}} \frac{P_k}{Z} \langle \hat{O}_k \rangle_\beta \,, \qquad \langle \hat{O}_k \rangle_\beta = \langle \phi_k | \hat{O} | \phi_k \rangle \,, \qquad Z = \sum_{k \in \mathcal{S}} P_k$

Equivalent to sampling $|\phi_k\rangle$ with probability P_k/Z and summing its expectations $\langle O_k \rangle_\beta$

Thermal states of free fermion fields on lattice

$$\hat{H}_0|p\rangle_p = (E_p + E_{\Omega_F})|p\rangle_p.$$

Vacuum energy E_{Ω_F} satisfies

$$\hat{H}_0|0\rangle_p = E_{\Omega_F}|0\rangle_p \equiv -\frac{1}{2}\sum_p E_p|0\rangle_p$$

$$\psi_n(t) = e^{i\hat{H}_0 t}\psi_n e^{-i\hat{H}_0 t} = \sum_n \frac{1}{n!}\underbrace{[i\hat{H}_0,[i\hat{H}_0,[\cdots,[i\hat{H}_0}_{n},\psi_n]\cdots]]]$$
$$= \sum_p \frac{1}{\sqrt{2NE_p}}[\hat{a}_p u_p e^{-iE_p t+ipan} + \hat{a}_p^\dagger u_p^* e^{iE_p t-ipan}].$$

Phase-space distribution function $f_p \equiv \langle \hat{a}_p^\dagger \hat{a}_p\rangle_\beta$ → $f_p = \dfrac{1}{e^{\beta E_p}+1}$

$$f_p = \frac{1}{2E_p}\sum_n [\gamma^0 u_p]_{\alpha'}[\bar{u}_p\gamma^0]_\alpha e^{ipan}\langle\bar{\psi}_n^{\alpha'}\psi_0^\alpha\rangle_\beta$$

Diagonalization of the discrete Hamiltonian

Discretizing ψ and expressing ψ_B in terms of $b^\dagger$ and b:

$$\hat{H} = \hat{H}_0 + M\left(b^\dagger b - \frac{1}{2}\right) + g\sum_n \left(a_n^\dagger a_n - \frac{1}{2}\right)\left(b^\dagger b - \frac{1}{2}\right)$$

- H is a hermitian $2^{N+1} \times 2^{N+1}$ matrix
- All its off-diagonal matrix elements vanish between the eigenstates of $b^\dagger\, b$

$$\hat{H} = \begin{pmatrix} \hat{H}_\psi^0 & 0 \\ 0 & \hat{H}_\psi^1 \end{pmatrix}$$

$$\hat{H}_\psi^0 = \hat{H}_0 - \frac{M}{2} - \frac{g}{2}\left(a_n^\dagger a_n - \frac{1}{2}\right) = \sum_p E_p(\bar{m})\left(\hat{a}_p^\dagger \hat{a}_p - \frac{1}{2}\right) - \frac{M}{2}$$

$$\hat{H}_\psi^1 = \hat{H}_0 + \frac{M}{2} + \frac{g}{2}\left(a_n^\dagger a_n - \frac{1}{2}\right) = \sum_p E_p(\bar{m} + g)\left(\hat{a}_p'^\dagger \hat{a}_p' - \frac{1}{2}\right) + \frac{M}{2}$$

Field operator representation

$$\hat{\Phi}_n = -\frac{\Delta_\varphi}{2}\sum_{j=0}^{n_Q-1} 2^j \sigma_z^j = -\frac{\varphi_{\max}}{N_\varphi - 1}\sum_{j=0}^{n_Q-1} 2^j \sigma_z^j.$$

$$\hat{\Pi}_n = \mathcal{F}_n \Phi_n \mathcal{F}_n^{-1}$$

$$\mathcal{F}_n = e^{-i\frac{n_\phi \delta^2}{2\pi}} \left(\prod_{j=0}^{n_Q-1} R_Z^j(-2^j \delta) \right) \mathcal{QFT}_n \left(\prod_{j=0}^{n_Q-1} R_Z^j(-2^j \delta) \right)$$