Quantum Simulation of Chiral Phase Transitions

Journal Club 2024/6/5(Wed)

Harunobu Fujimura

Reference : arXiv:2112.03944 [hep-ph]

Author : Alexander M. Czajka , Zhong-Bo Kang , Henry Ma , Fanyi Zhao

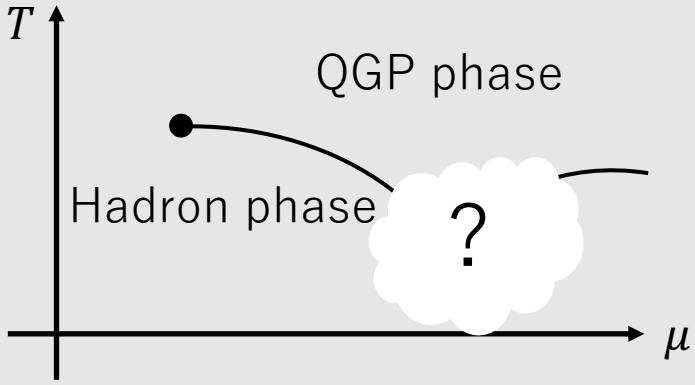
1. Introduction

One way to analyse non-perturbative system of quantum field theory (e.g. QCD)

→ **Lattice simulation**

Lattice field theory

One of the major research interests is to draw QCD phase diagrams.

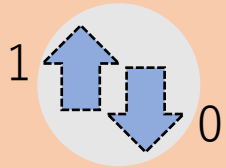


One key concept is chiral phase transitions.

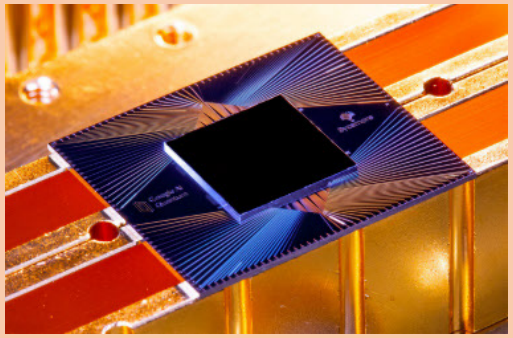
Apply

Quantum computer

Unit of information:
→Qubit



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



Google, Sycamore

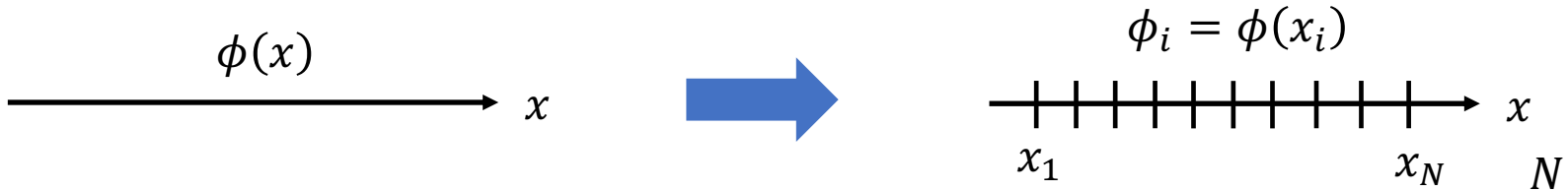
New computational methods that have been developed recently.

Why do we need quantum simulations ?

1. Introduction

Classical computer-based analysis methods in Lattice field theory

- Discretization of space-time :



N : the number of sites

- Path integral (Lagrangian formalism) :

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \, \mathcal{O}(\phi) \, e^{-S[\phi]} \quad \Rightarrow \quad \langle \mathcal{O} \rangle = \frac{1}{Z} \int d\phi_1 \cdots d\phi_N \, \mathcal{O}(\{\phi\}) \, e^{-S[\{\phi\}]}$$

$$Z = \int D\phi \, e^{-S[\phi]}$$

$$\{\phi\} = (\phi_1, \cdots, \phi_N)$$

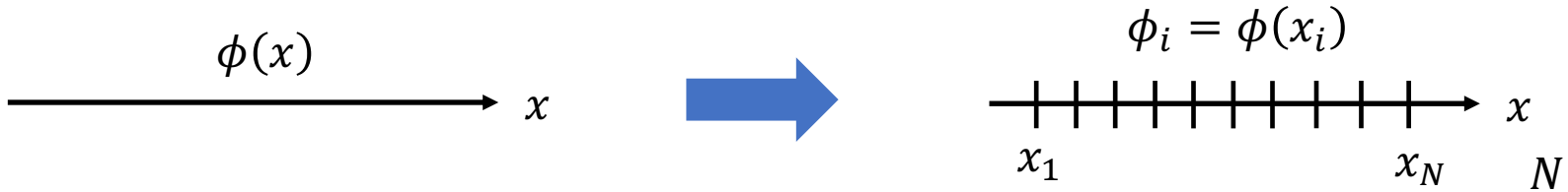
- **Monte Carlo method** :

$$\langle \mathcal{O} \rangle = \frac{1}{N_{sample}} \sum_{i=1}^{N_{sample}} \mathcal{O}(\{\phi^{(i)}\}) \text{ with probability } \propto e^{-S[\{\phi^{(i)}\}]}$$

1. Introduction

Classical computer-based analysis methods in Lattice field theory

・Discretization of space-time :



N : the number of sites

・Path integral (Lagrangian formalism) :

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \, \mathcal{O}(\phi) \, e^{-S[\phi]} \quad \Rightarrow \quad \langle \mathcal{O} \rangle = \frac{1}{Z} \int d\phi_1 \cdots d\phi_N \, \mathcal{O}(\{\phi\}) \, e^{-S[\{\phi\}]}$$

$$Z = \int D\phi \, e^{-S[\phi]}$$

$$\{\phi\} = (\phi_1, \cdots, \phi_N)$$

・**Monte Carlo method** :

$$\langle \mathcal{O} \rangle = \frac{1}{N_{sample}} \sum_{i=1}^{N_{sample}} \mathcal{O}(\{\phi^{(i)}\}) \text{ with } \boxed{\text{probability} \propto e^{-S[\{\phi^{(i)}\}]}}$$

Must be positive number !

1. Introduction

However, when $e^{-S[\{\phi^{(i)}\}]}$ becomes a complex number, the infamous sign problem appears.

→ We cannot use probability interpretation.

Situations where sign problems appear ;

- Topological term
- real time evolution e^{iHt}
- chemical potential μ

etc.

$$Z_f(\mu) \equiv \int D\bar{\psi}D\psi \exp\left[-\int d^4x\, \bar{\psi}\left(iD_\mu\gamma^\mu + m + \mu\gamma^4\right)\psi\right]$$

$$\vdots$$

$$= \left(Z_f(-\mu)\right)^*$$

$$\neq \left(Z_f(\mu)\right)^*$$

$Z_f(\mu)$ is not real

➡ Monte Carlo method cannot handle (large values of) chemical potentials.

1. Introduction

A promising way to solve these problems is Quantum simulation.

Quantum simulation is simulation using a quantum computer.

Quantum computers are computers composed of quantum mechanical elements that obey quantum mechanical laws.

=Qubits

Quantum simulation can compute physical quantities without sign problems.

We can also deal with chemical potentials μ with arbitrary values, as a example.

Introduction

Quantum simulation

Qubit = Quantum bit ;

Super position

1-qubit : $|\psi\rangle = \alpha_1|0\rangle + \alpha_2|1\rangle$

2-qubits : $\alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$

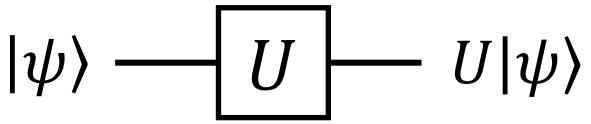
⋮

Basic quantum gate operators ;

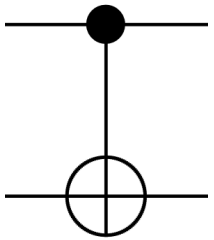
$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}, X = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, Y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \dots$$

$$CNOT = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}, \dots$$

Circuitous notation ;



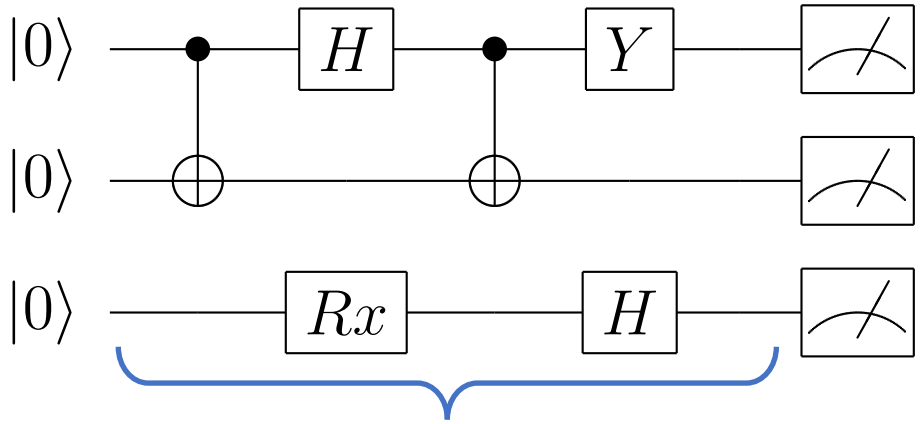
$U = H, X, Y$ … etc

$CNOT =$ 

Introduction

Quantum simulation

1. Initial state



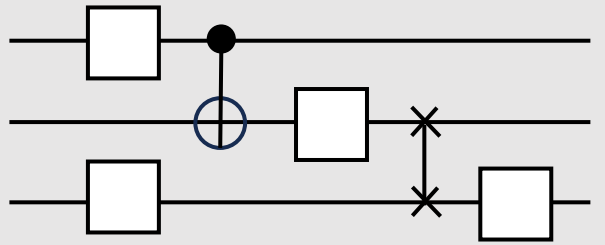
2. Quantum gate operations

3. Measurement

$$\langle \mathcal{O} \rangle = \langle \psi | \mathcal{O} | \psi \rangle$$

Theorem :
Arbitrary unitary operators can be written in terms of basic quantum gates.

$^{\forall}U$: unitary, $U =$



...

We can calculate (measure) expectation values of arbitrary unitary operators

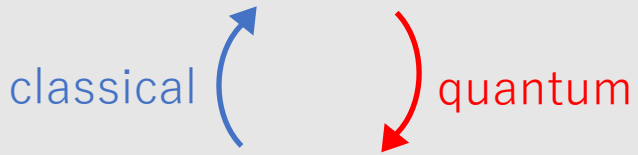
Introduction

Quantum algorithm for preparing the ground state $|\Psi\rangle$

VQE

θ : optimization parameters

Ansatz : $|\psi(\theta)\rangle$



$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$$

$$\min_{\theta} E(\theta) = E(\theta_0) \quad \rightarrow |\Psi\rangle = |\psi(\theta_0)\rangle$$

Adiabatic preparation

$H_A(t)$: adiabatic Hamiltonian

$$H_A(T) = H, \qquad H_A(0) = H_0$$

$$|\Psi\rangle = \lim_{T\to\infty} \mathcal{T} \exp\left(-i \int_0^T H_A(t)\right) |\Psi_0\rangle$$

Well-known state

etc…

Through recent research, the algorithms for zero temperature are known to some extent.

Individual states (such as the ground state) can be prepared by quantum circuits in some way.

Introduction

The main question of this paper:

Can quantum simulation handle phenomena such as chiral phase transitions ?

We have to consider finite temperature and chemical potential

→ △ mixed state　　→no problem

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\left[\mathcal{O} e^{-\beta H} \right]$$

non-unitary operator

How to treat it in quantum simulation ? ➡ QITE and QMETTS algorithms

Introduction

Short summary

- In order to deal with finite temperature system in quantum simulation, they focus on quantum algorithms called QITE and QMETTS.
- As a example, they consider Gross-Neveu model with chemical potential at (1+1) dim and calculate chiral condensation $\langle\bar{\psi}\psi\rangle$ by quantum simulation.
- They compared quantum simulation result, analytical result and naïve classical simulation
- They showed that quantum simulations could potentially handle chiral phase transitions..

Gross-Neveu model ;

$$S = \int d^2x \left[\bar{\psi}\left(i\,\gamma^\mu\partial_\mu - m\right)\psi + g(\bar{\psi}\psi)^2 + \mu\,\bar{\psi}\gamma^0\psi\right]$$

Quantum simulation

$\langle\bar{\psi}\psi\rangle$ for various T and μ

Outline

1. Introduction
2. The Gross-Neveu model with chemical potential
3. Quantum algorithm (QITE, QMETTS)
4. Numerical results
5. Summary

Outline

1. Introduction
2. The Gross-Neveu model with chemical potential
3. Quantum algorithm (QITE, QMETTS)
4. Numerical results
5. Summary

2. The Gross-Neveu model

Gross-Neveu model (1+1 dim, finite temperature T, 1-flavor); [D. J. Gross, A. Neveu. 1974]

$$\mathcal{L} = \bar{\psi}\left(i\,\gamma^{\mu}\partial_{\mu} - m\right)\psi + g(\bar{\psi}\psi)^2$$

$\gamma^0 = \sigma_Z$, $\gamma^1 = -i\sigma_Y$, σ_Z, σ_Y : Pauli matrices

ψ : Dirac fermion, m : fermion mass,

g : coupling constant (dimensionless)

Grand canonical ensemble

$$e^{-\beta H} \longrightarrow e^{-\beta H + \beta\mu Q} \qquad Q = \int d^2x \bar{\psi}\gamma^0\psi$$

Target : $\mathcal{L} = \bar{\psi}\left(i\,\gamma^{\mu}\partial_{\mu} - m\right)\psi + g\,(\bar{\psi}\psi)^2 + \mu\,\bar{\psi}\gamma^0\psi$

μ : chemical potential

2. The Gross-Neveu model

Gross-Neveu model (1+1 dim, finite temperature T, 1-flavor); [D. J. Gross, A. Neveu. 1974]

$$\mathcal{L} = \bar{\psi}\left(i\,\gamma^{\mu}\partial_{\mu} - m\right)\psi + g\,(\bar{\psi}\psi)^2$$

$\gamma^0 = \sigma_Z$, $\gamma^1 = -i\sigma_Y$, σ_Z, σ_Y : Pauli matrices

ψ : Dirac fermion, m : fermion mass,

g : coupling constant (dimensionless)

Grand canonical ensemble

$$e^{-\beta H} \longrightarrow e^{-\beta H + \beta\mu Q} \qquad Q = \int d^2x \bar{\psi}\gamma^0\psi$$

Target : $\mathcal{L} = \bar{\psi}\left(i\,\gamma^{\mu}\partial_{\mu} - m\right)\psi + g\,(\bar{\psi}\psi)^2 + \mu\,\bar{\psi}\gamma^0\psi$

μ : chemical potential

Sign problem appear in Monte Carlo
but Quantum simulation can deal with it

2. The Gross-Neveu model

Gross-Neveu model with chemical potential :

$$\mathcal{L} = \bar{\psi}\left(i\,\gamma^{\mu}\partial_{\mu} - m\right)\psi + g\,(\bar{\psi}\psi)^2 + \mu\,\bar{\psi}\gamma^{0}\psi$$

☆This model shows chiral phase transition-like behavior.

Discrete chiral transformation ; $\psi \to \gamma^5\psi \quad , \gamma^5 \equiv \gamma^0\gamma^1$

$$\bar{\psi}\, i\,\gamma^{\mu}\partial_{\mu}\psi \to \bar{\psi}\, i\,\gamma^{\mu}\partial_{\mu}\psi,$$

$$\bar{\psi}\gamma^{0}\psi \to \bar{\psi}\gamma^{0}\psi$$

$\bar{\psi}\psi \to -\bar{\psi}\psi$

$\underline{m = 0}$ The Lagrangian has discrete chiral sym, but it break dynamically,

Order parameter : chiral condensate $\langle\bar{\psi}\psi\rangle$

- $\langle\bar{\psi}\psi\rangle = 0$ (sym preserved phase) ,
- $\langle\bar{\psi}\psi\rangle \neq 0$ (sym broken phase)

$\underline{m \neq 0}$ We treat $\langle\bar{\psi}\psi\rangle$ as “quasi-order parameter”

2. The Gross-Neveu model

First, we analyse GN model using mean-field approximation as a cross-check of the quantum simulation;

Mean field approximation;

$$\bar{\psi}\psi = \langle\bar{\psi}\psi\rangle + \sigma, \quad \text{where } \left|\frac{\sigma}{\langle\bar{\psi}\psi\rangle}\right| \ll 1$$

We assume $\langle\bar{\psi}\psi\rangle$ is constant

i.e global chiral condensation : $\langle\bar{\psi}\psi(x)\rangle = \langle\bar{\psi}\psi\rangle = \text{cost}$

$$\mathcal{L} = \bar{\psi}\left(i\,\gamma^{\mu}\partial_{\mu} - m\right)\psi + g\,(\bar{\psi}\psi)^2 + \mu\,\bar{\psi}\gamma^{0}\psi$$

↓ Substitute $\bar{\psi}\psi = \langle\bar{\psi}\psi\rangle + \sigma$ and neglect $\mathcal{O}(\sigma^2)$

$$\mathcal{L}_{eff} = \bar{\psi}\left(i\,\gamma^{\mu}\partial_{\mu} - m + 2g\langle\bar{\psi}\psi\rangle + \mu\gamma^{0}\right)\psi - g\langle\bar{\psi}\psi\rangle^2$$

$$= \mathcal{L}_{\text{Dirac}}(M,\mu) - V$$

where, $M \equiv m - 2g\langle\bar{\psi}\psi\rangle$, $V \equiv \frac{(M-m)^2}{4g}$

2. The Gross-Neveu model

Let's calculate grand partition function;

$$Z \equiv \int D\bar{\psi}D\psi \exp\left[\int d^2x \mathcal{L}_{eff}\right]$$
$$= \int D\bar{\psi}D\psi \exp\left[\int d^2x (\mathcal{L}_{\text{Dirac}}(M,\mu) - V)\right]$$
$$= e^{-\frac{L}{T}(\Omega_{\text{Dirac}}+V)}$$

$$V = \frac{(M-m)^2}{4g}$$

L : total special distance

Known results [N. Kapusta, C. Gale, 2006]

$$\Omega_{\text{Dirac}}(\mu, T; M) = -\frac{2}{\pi}\int_0^\infty dk \left[\omega_k + T\ln(1+e^{-\beta(\omega_k+\mu)}) + T\ln(1+e^{-\beta(\omega_k-\mu)})\right]$$

where $\omega_k = \sqrt{k^2+M^2}$.

➡ We can get grand partition function of GN model analytically

2. The Gross-Neveu model

Grand partition function of GN model :

$$Z = e^{-\frac{L}{T}\Omega(\mu,T;M)} \qquad \text{where } \omega_k = \sqrt{k^2 + M^2}.\ \ M \equiv m - 2g\langle\bar{\psi}\psi\rangle$$

$$\Omega(\mu,T;M) = \frac{(M-m)^2}{4g} - \frac{2}{\pi}\int_0^\infty dk\left[\omega_k + T\ln(1+e^{-\beta(\omega_k+\mu)}) + T\ln(1+e^{-\beta(\omega_k-\mu)})\right]$$

How to get $\langle\bar{\psi}\psi\rangle$? → Self consistency equation

$$\langle\bar{\psi}\psi\rangle = \frac{1}{Z}\int \mathcal{D}\psi\mathcal{D}\bar{\psi}\ \psi\bar{\psi}\ \exp\left[\int d^2x\,\mathcal{L}_{eff}\right] \qquad , \mathcal{L}_{eff} = \bar{\psi}\left(i\gamma^\mu\partial_\mu - M + \mu\gamma^0\right)\psi - \frac{(M-m)^2}{4g}$$

$$= \frac{1}{Z}\int \mathcal{D}\psi\mathcal{D}\bar{\psi}\left(-\frac{T}{L}\frac{\partial}{\partial M} + \frac{m-M}{2g}\right)\exp\left[\int d^2x\,\mathcal{L}_{eff}\right]$$

$$= -\frac{T}{L}\frac{\partial}{\partial M}\log Z + \frac{m-M}{2g}$$

$$= \frac{\partial\Omega}{\partial M} + \frac{m-M}{2g}$$

Should be zero

Solve $\frac{\partial\Omega}{\partial M} = 0$ (gap equation)

→ We get $\langle\bar{\psi}\psi\rangle$

2. The Gross-Neveu model

They numerically solve $\frac{\partial \Omega}{\partial M} = 0$ and get M

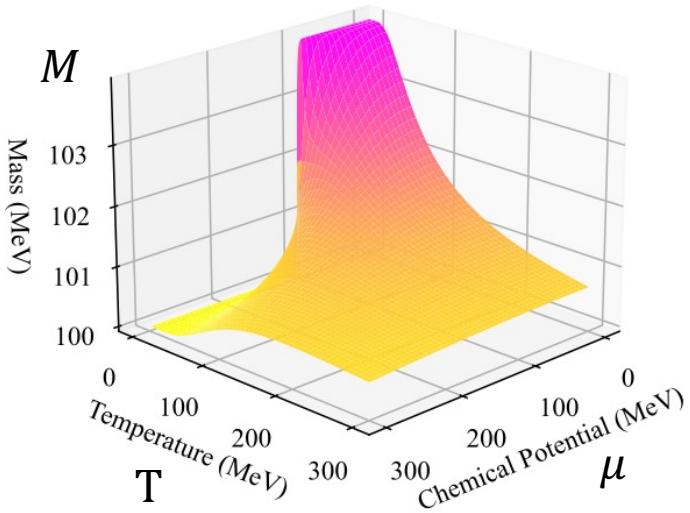
Introduce momentum cutoff :

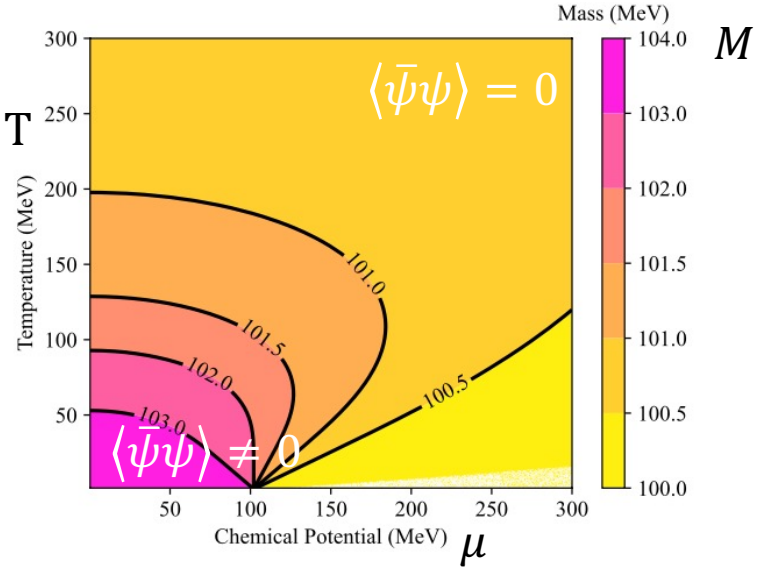
$$\Omega(\mu, T; M) = \frac{(M-m)^2}{4g} - \frac{2}{\pi}\int_0^{\infty} dk \left[\omega_k + T\ln(1+e^{-\beta(\omega_k+\mu)}) + T\ln(1+e^{-\beta(\omega_k-\mu)})\right]$$

$\int_0^{\Lambda} dk$, $\Lambda = \frac{\pi}{a}$, a : Lattice spacing

Mass generation;

$\Delta m = M - m$





$m = 100$ MeV
$a = 1\ \mathrm{MeV}^{-1}$
$\mathrm{g} = 1$ MeV,
$\mathrm{T}, \mu \in [0, 300\mathrm{MeV}]$

This is an analytical result. It will be compared with quantum simulations later.

Outline

1. Introduction
2. The Gross-Neveu model with chemical potential
3. Quantum algorithm (QITE, QMETTS)
4. Numerical results
5. Summary

3. Quantum Imaginary Time Evolution (QITE)

In order to simulate thermal system, we have to deal with $e^{-\beta H}$ which is not unitary.

How to prepare $e^{-\beta H}$ in quantum simulation ?

➡ Quantum Imaginary Time Evolution (QITE) [M. Motta , et al. 2019]

Strategy :

1. Trotterization : $e^{-\beta H} = \left(e^{-\Delta\beta H}\right)^M + \mathcal{O}(\Delta\beta^2)$, $\Delta\beta \equiv \frac{\beta}{M}$

2. Approximating the non-unitary operation with a unitary operation :

$$e^{-\Delta\beta H} = e^{-\Delta\beta \hat{h}_1} e^{-\Delta\beta \hat{h}_2} \ldots$$

$$e^{-\Delta\beta \hat{h}_i} = \underline{e^{-i\Delta\beta \hat{A}}} + \mathcal{O}(\Delta\beta^2), \quad \hat{A}^\dagger = \hat{A}$$

Unitary (implementable in quantum simulation)

3. Quantum Imaginary Time Evolution (QITE)

2. Approximating the non-unitary operation with a unitary operation :

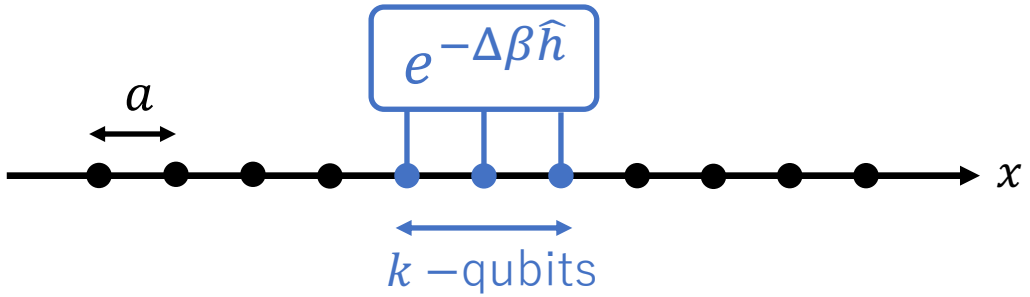
Let‘s consider N-qubits Hilbert space

In general, the Lattice Hamiltonian can be decomposed into k-local parts.

$$e^{-\Delta\beta H} = e^{-\Delta\beta\hat{h}_1} e^{-\Delta\beta\hat{h}_2} \ldots$$

Let $\hat{h} =$ k-local Hamiltonian $(k \ll N)$

Act on k neighboring qubits

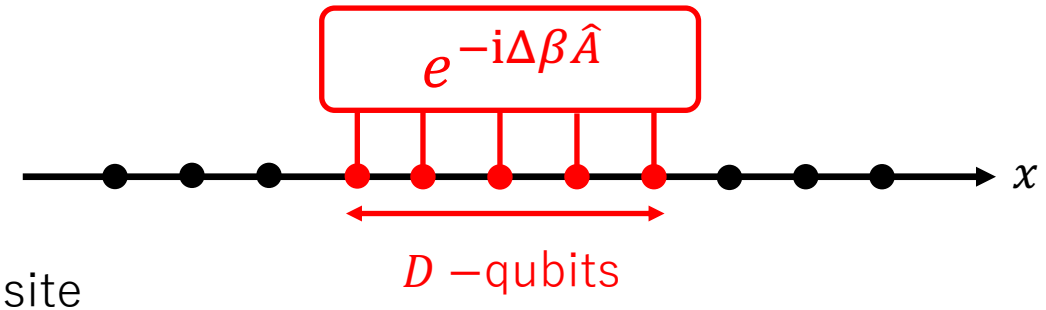


Expand Hermite op $\hat{A}$ in term of Pauli matrices on D qubits $(k< D)$;

$$\hat{A} = \sum_{\mu} a_\mu \hat{\sigma}_\mu \ , \qquad \hat{\sigma}_\mu = \prod_{l=1}^{D} \hat{\sigma}^{(l)}{}_{\mu_l}$$

Pauli matrix on l-th site

$$\mu = \mu_1, \ldots, \mu_D, \qquad \mu_l \in \{I, X, Y, Z\}$$



3. Quantum Imaginary Time Evolution (QITE)

The construction of Hermite op $\hat{A}$

Compare the difference of state induced by two time evolutions

$$|\Delta\Psi_h(\beta)\rangle \equiv \left(\frac{1}{\sqrt{c(\Delta\beta)}} e^{-\Delta\beta\hat{h}} - 1\right)|\Psi(\beta)\rangle$$

$$|\Delta\Psi_A(\beta)\rangle \equiv \left(e^{-\mathrm{i}\Delta\beta\hat{A}} - 1\right)|\Psi(\beta)\rangle$$

Objective function : $F(a) \equiv \left||\Delta\Psi_h(\beta)\rangle - |\Delta\Psi_A(\beta)\rangle\right|^2$ $\quad a_\mu = (a_{\mu_1}, \dots, a_{\mu_D}),$ $\quad \hat{A} = \sum_\mu a_\mu \hat{\sigma}_\mu$

Minimize $F(a)$. $\rightarrow \frac{\partial F}{\partial a_\mu} = 0$ for all $\mu = \mu_1, \dots, \mu_D$,

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

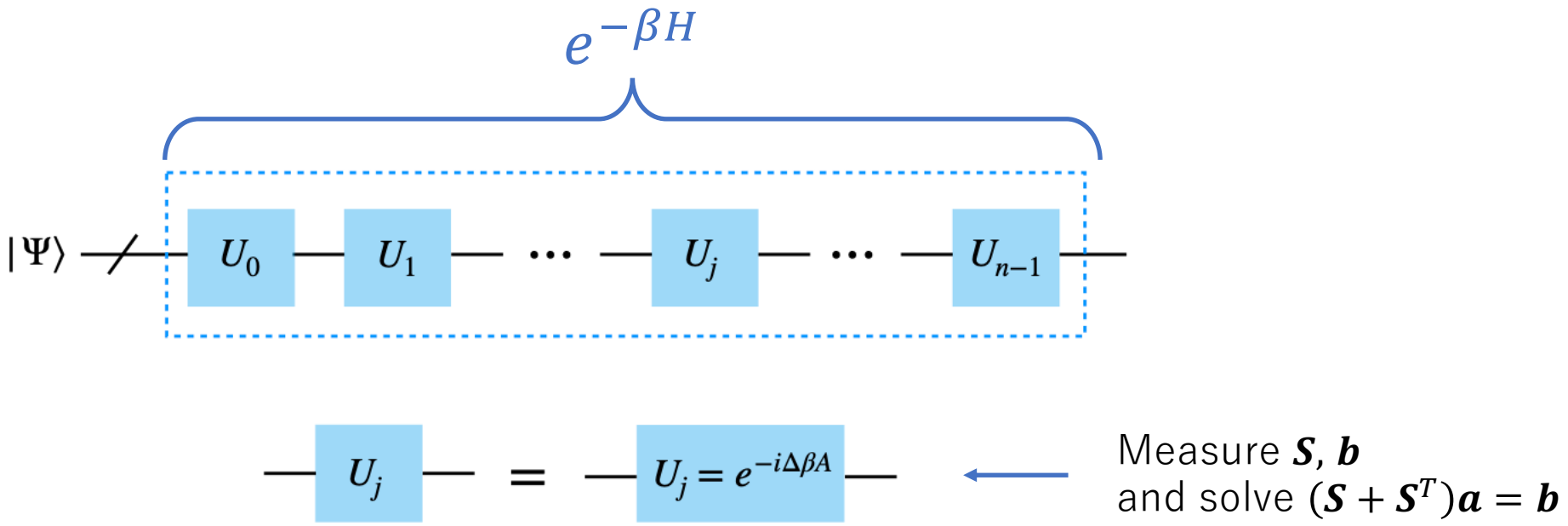
4^D equations , $(D < N)$

where, $S_{\mu\nu} \equiv \langle\Psi(\beta)|\, \hat{\sigma}^\dagger{}_\mu\, \hat{\sigma}_\nu\, |\Psi(\beta)\rangle,\ b_\mu \equiv -\frac{i}{\sqrt{c(\Delta\beta)}}\langle\Psi(\beta)|\left(H\hat{\sigma}_\mu - \hat{\sigma}^\dagger{}_\mu H\right)|\Psi(\beta)\rangle$

3. Quantum Imaginary Time Evolution (QITE)

Let me summarize the procedure of QITE

1. Measure $\boldsymbol{S}$ and $\boldsymbol{b}$ in quantum simulation
2. Solve equations $(\boldsymbol{S}+\boldsymbol{S}^T)\boldsymbol{a}=\boldsymbol{b}$ and get $\boldsymbol{a}$
3. Get $e^{-\Delta\beta H}$ in terms of $\hat{A}$

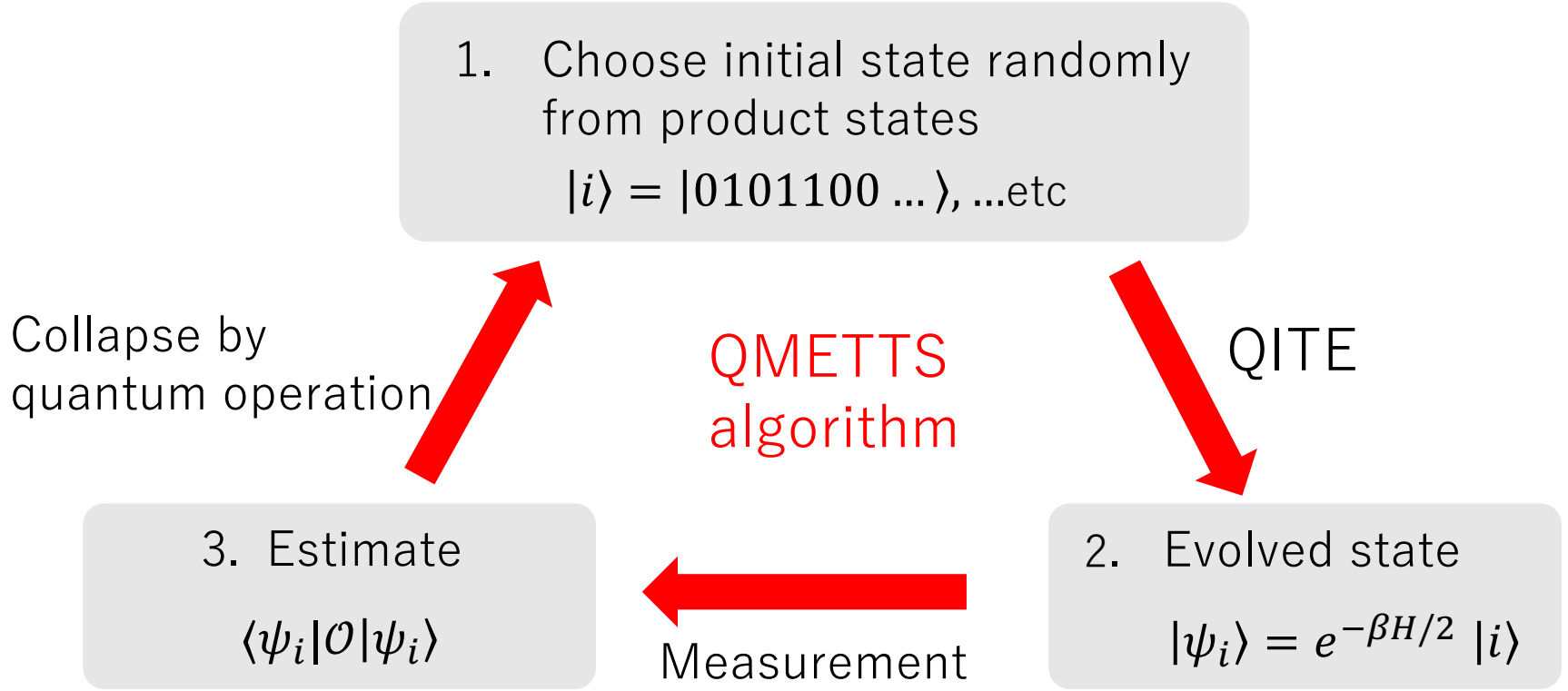


We can implement $e^{-\beta H}$ in quantum simulation

3. QITE and QMETTS

How to calculate thermal expectation value $\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\left[\mathcal{O}\, e^{-\beta H} \right]$ efficiently by quantum simulation?

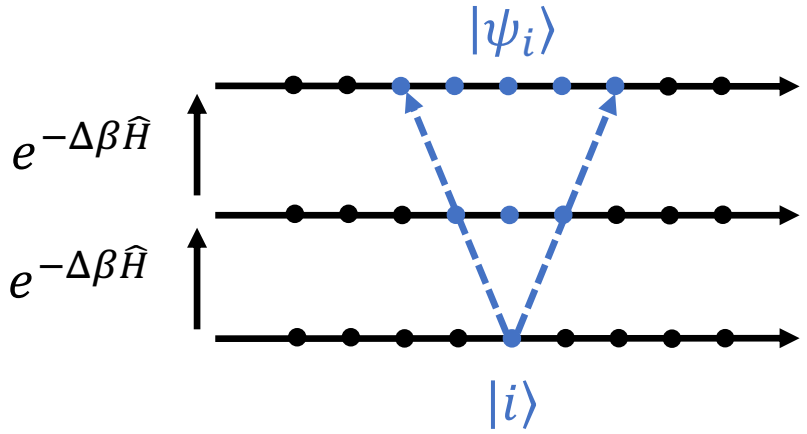
➡ Quantum Minimally Entangled Typical Thermal States (QMETTS) [SR. White 2009]



3. QITE and QMETTS

Continue QMETTS cycles N_S times, until convergence

QITE and QMETTS : $\langle \mathcal{O} \rangle \cong \frac{1}{N_S} \sum_{i=1}^{N_S} \langle \psi_i | \mathcal{O} | \psi_i \rangle$



Comments of QITE and QMETTS

- ✓ Inherently, this algorithm does not require ancilla qubit.
  → Small number of qubits
- ✓ No ansatz is needed.
  → There is no optimization issue ↔ VQE
- ✓ As the size of the system (or dimension of space time) increases, the $\frac{N_S}{2^N}$ tend to be small.
  → Promising methods for future quantum computers.
- △ Computation cost depends on correlation length.
  c.f. $(\boldsymbol{S} + \boldsymbol{S}^T)\boldsymbol{a} = \boldsymbol{b}$, 4^D equations , $(D < N)$

Outline

1. Introduction
2. The Gross-Neveu model with chemical potential
3. Quantum algorithm (QITE, QMETTS)
4. Numerical results
5. Summary

4. Numerical simulation

Let's implement a quantum simulation in Gross-Neveu model.

Hamiltonian : $H = \int dx\, \bar{\psi}(i\,\gamma^1\partial_1 + m)\psi - g\,(\bar{\psi}\psi)^2 - \mu\,\bar{\psi}\gamma^0\psi$

1. Divide the space into $N/2$ points with lattice spacing a.
2. Represent Dirac fermion ψ as staggered fermion

staggered fermion

$$\psi(x = ia) = \begin{pmatrix} \psi_u(x = ia) \\ \psi_d(x = ia) \end{pmatrix} = \frac{1}{\sqrt{a}} \begin{pmatrix} \chi_{2i} \\ \chi_{2i+1} \end{pmatrix} \quad , i = 0, 1, \ldots N/2 - 1.$$

Lattice Hamiltonian :

$$H = -\frac{i}{2a}\left[\sum_{n=0}^{N-2}\left(\chi_n^\dagger\chi_{n+1} - \chi_{n+1}^\dagger\chi_n\right) + m\sum_{n=0}^{N-1}(-1)^n\,\chi_n^\dagger\chi_n + (\text{interaction term})\right]$$

4. Numerical simulation

In order to implement the quantum simulation, we have to rewrite everything in terms of Pauli matrices

Lattice Hamiltonian : $$H = -\frac{i}{2a}\left[\sum_{n=0}^{N-2}\left(\chi_n^\dagger \chi_{n+1} - \chi_{n+1}^\dagger \chi_n\right) + m\sum_{n=0}^{N-1}(-1)^n \chi_n^\dagger \chi_n + (\text{interaction term})\right]$$

Jordan-Wigner transformation: [P. Jordan and E. Wigner. 1928]

$$\chi_n = \frac{\sigma_X^{(n)} - i\sigma_Y^{(n)}}{2}\prod_{j=0}^{n-1}\left(-i\sigma_Z^{(j)}\right)$$

$\sigma_X^{(n)}, \sigma_Y^{(n)}, \sigma_Z^{(n)}$: Pauli matrices on n-th site

Qubit Hamiltonian : $$H = \frac{1}{4a}\sum_{n=0}^{N-1}\left(\sigma_X^{(2n)}\sigma_X^{(2n+1)} + \sigma_Y^{(2n)}\sigma_Y^{(2n+1)}\right) + \frac{m}{2}\sum_{n=0}^{N-1}(-1)^n\sigma_Z^{(n)} + (\text{interaction term})$$

Everything are written in term of Pauli matrices.

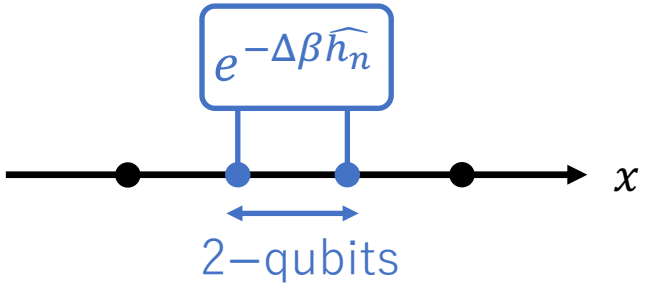
4. Numerical simulation

Qubit Hamiltonian : $$H = \frac{1}{4a}\sum_{n=0}^{N-1}\left(\sigma_X^{(2n)}\sigma_X^{(2n+1)} + \sigma_Y^{(2n)}\sigma_Y^{(2n+1)}\right) + \frac{m}{2}\sum_{n=0}^{N-1}(-1)^n\sigma_Z^{(n)} + (\text{interaction term})$$

For example,

$$\hat{h}_n = (-1)^n\sigma_Z^{(n)}$$

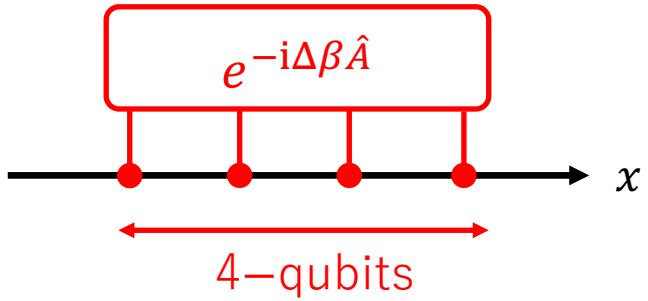
$\rightarrow e^{-\Delta\beta\hat{h}_n}$: 1-local operator



$$\hat{h'}_n = \sigma_X^{(2n)}\sigma_X^{(2n+1)} + \sigma_Y^{(2n)}\sigma_Y^{(2n+1)}$$

$\rightarrow e^{-\Delta\beta\hat{h'}_n}$: 2-local operator

etc…



Other terms can be written in the same way.

They set $N = 4$, and prepare Hermite op $\hat{A}$ by using 4 qubits for simplicity.

4. Numerical simulation

We compare the following three methods

1. Quantum simulation results by QITE and QMETTS.

2. Analytical calculation by mean field approximation.

$$\bar{\psi}\psi = \langle\bar{\psi}\psi\rangle + \sigma, \quad \text{where} \left|\frac{\sigma}{\langle\bar{\psi}\psi\rangle}\right| \ll 1$$

3. Exact diagonalization

↓

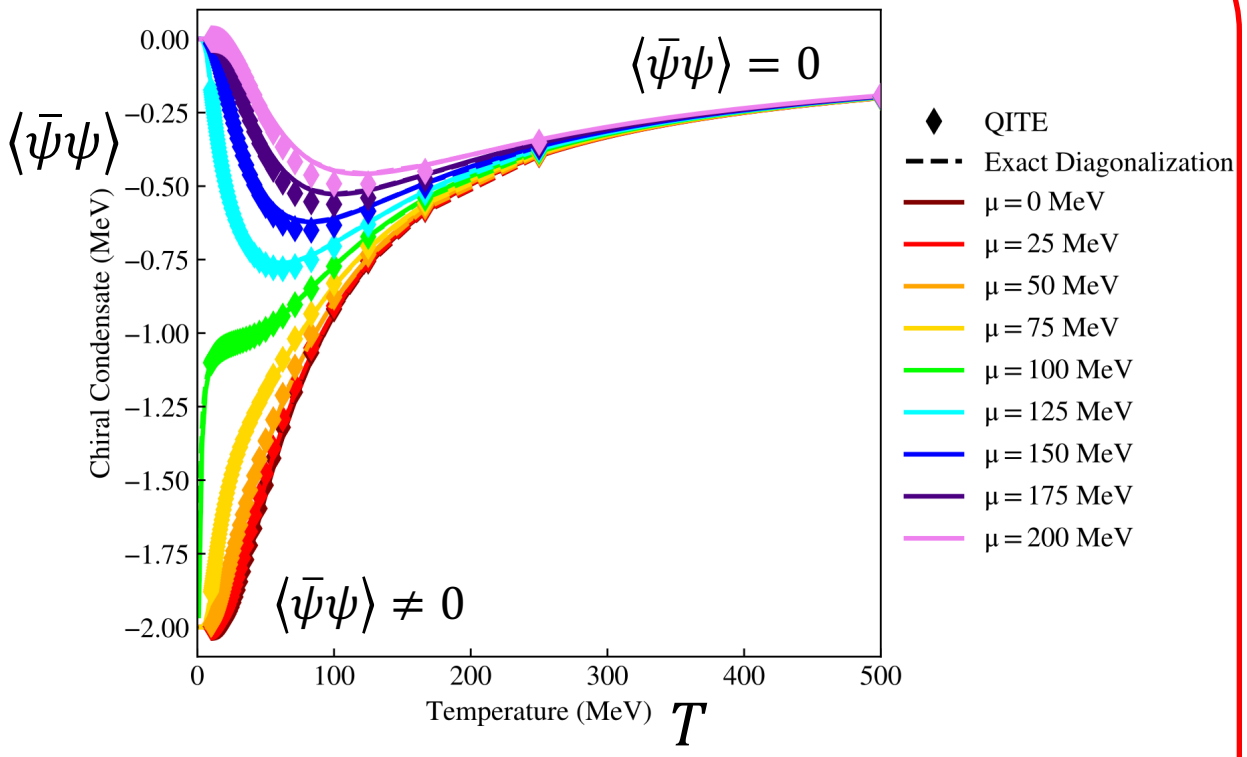
This is a naïve matrix calculation using a classical computer
(precise Hamilton simulation but very costly)

4. Numerical simulation

Temperature dependence

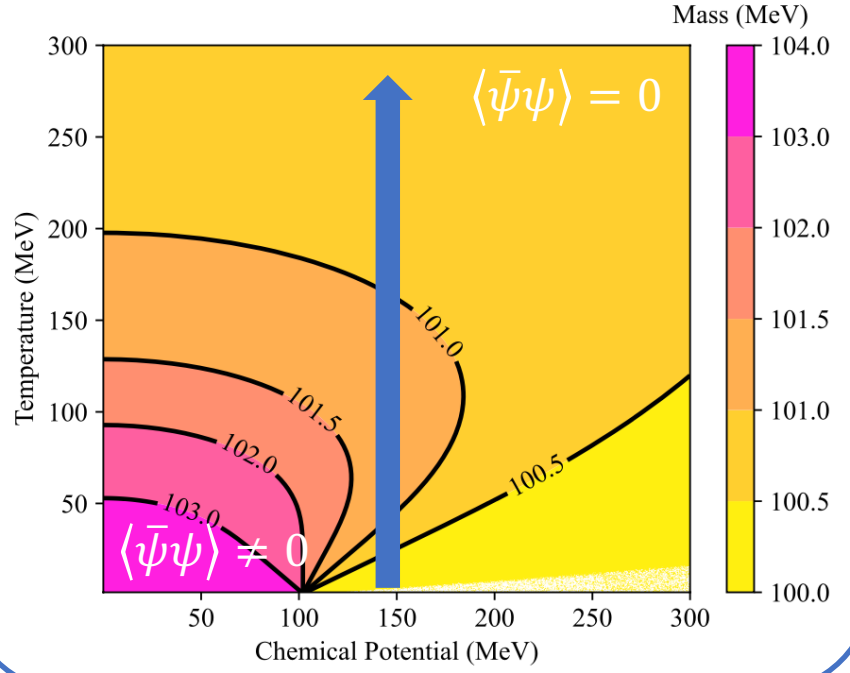
$N = 4,\ m = 100\ \text{MeV},\ a = 1\ \text{MeV}^{-1},\ \text{g} = 1\ \text{MeV},\ \text{T}, \mu \in [0, 300\text{MeV}]$

Quantum Simulation results;



◆ : QITE and QMETTS, —— : analytical results,
- - - : exact diagonalization

Analytical calculation by mean field approximation

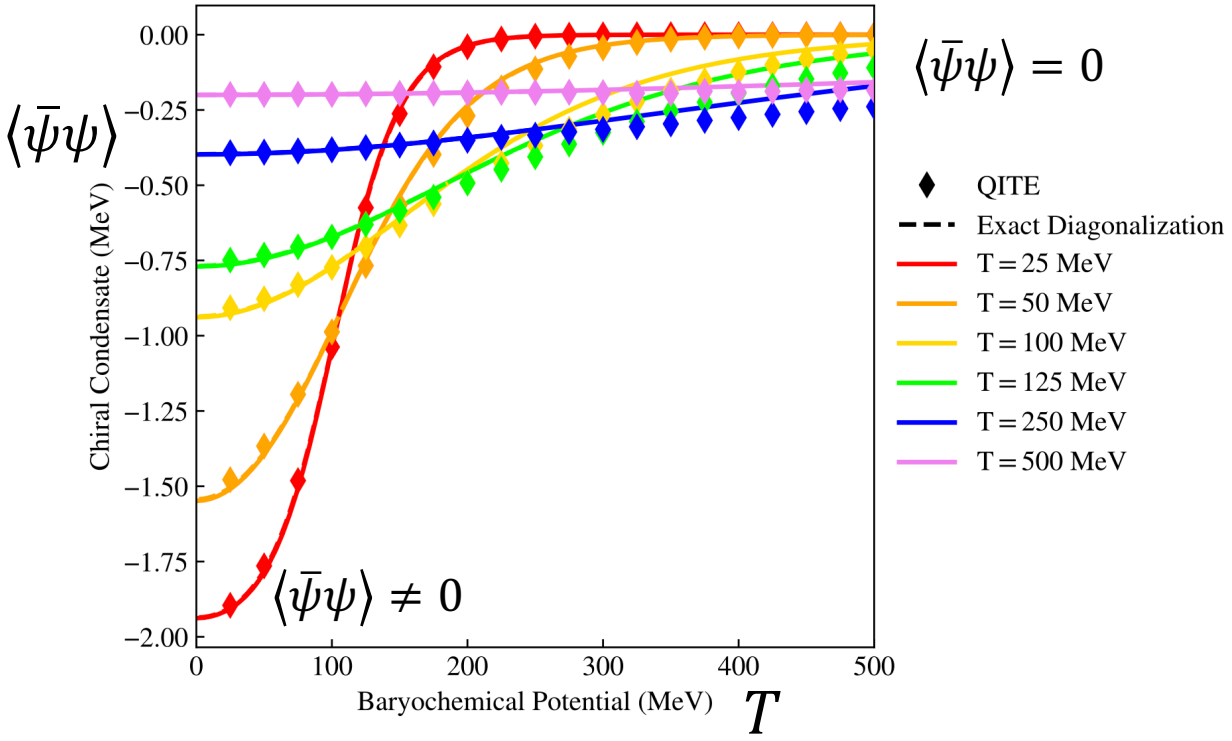


Quantum simulations gave consisitent results.

4. Numerical simulation

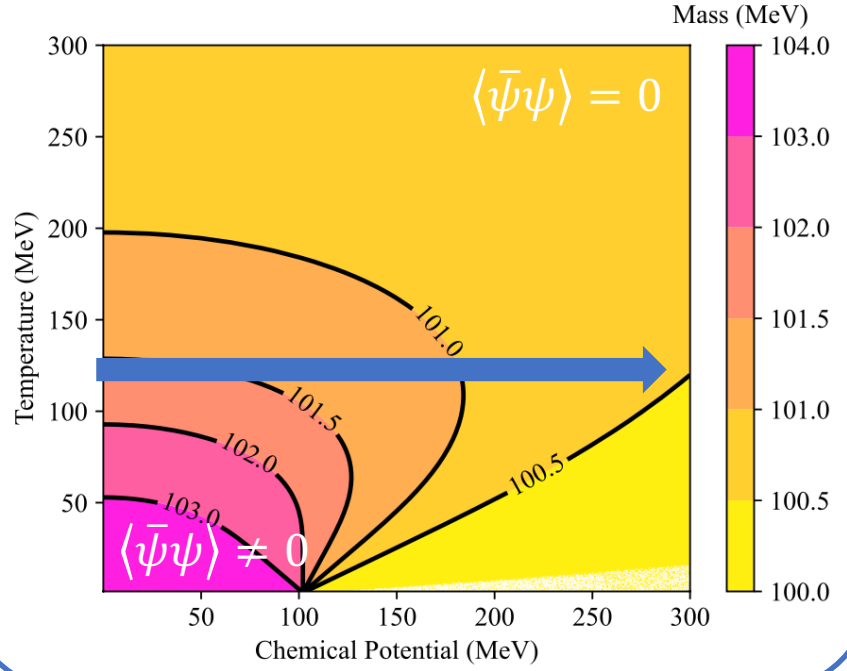
Chemical potential dependence $N = 4,\ m = 100\ \mathrm{MeV},\ a = 1\ \mathrm{MeV}^{-1},\ \mathrm{g} = 1\ \mathrm{MeV},\ \mathrm{T}, \mu \in [0, 300\mathrm{MeV}]$

Quantum Simulation results;



◆ : QITE and QMETTS, —— : analytical results,
- - - : exact diagonalization

Analytical calculation by mean field approximation



Quantum simulation is valid even for finite chemical potentials where sign problems occur.

Outline

1. Introduction
2. The Gross-Neveu model with chemical potential
3. Quantum algorithm (QITE, QMETTS)
4. Numerical results
5. Summary

5. Summary

- The conventional method (Monte Carlo) has difficulty in dealing with finite chemical potential due to infamous sign problem
- They performed quantum simulations on the Gross-Neveu model and showed that quantum simulations work successfully even with finite chemical potential.
- The QMETTS algorithm which used in this study, is expected to be advantageous when dealing with large system.
- This could be a first step towards dealing with phenomena such as chiral phase transitions in quantum computers developed in the future.

Thank you for attention !

Appendix

Appendix

Computational cost of exact diagonalization

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\left[\mathcal{O}\, e^{-\beta H} \right] = \frac{1}{Z} \sum_{k=0}^{2^N - 1} e^{-\beta E_k} \langle k | \mathcal{O} | k \rangle$$

Diagonalization cost : $\mathcal{O}(2^{3N})$
Trace cost :$\mathcal{O}(2^{4N})$

$N = 4 \quad \rightarrow 2^{3N} + 2^{4N} = 69{,}632$

$N = 5 \quad \rightarrow 2^{4N} = 1081{,}344$

Appendix

$$Z_f(\mu) \equiv \int D\bar{\psi} D\psi \exp\left[-\int d^4x\, \bar{\psi}\left(iD_\mu\gamma^\mu + m + \mu\gamma^4\right)\psi\right]$$

$$= \det\left[iD_\mu\gamma^\mu + m + \mu\gamma^4\right]$$

$$= \det\left[\gamma^5(iD_\mu\gamma^\mu + m + \mu\gamma^4)\gamma^5\right] \quad \gamma^5\gamma^\mu\gamma^5 = -\gamma^\mu$$

$$= \det\left[-iD_\mu\gamma^\mu + m - \mu\gamma^4\right]$$

$$= \det\left[\left(iD_\mu\gamma^\mu + m - \mu\gamma^4\right)^\dagger\right] \quad (\gamma^\mu)^\dagger = \gamma^\mu$$

$$= \left(Z_f(-\mu)\right)^* \neq \left(Z_f(\mu)\right)^*$$

$Z_f(\mu)$ is not real

Appendix

Some applications to QFT ;

- ✓ ϕ^4 theory (algorithm only) [SP. Jordan, et al. 1111.3633]
- ✓ Fermionic field theory (Gross-Nuveu model, algorithm only) [SP. Jordan, et al. 1404. 7115]
- ✓ Schwinger model (ground state & energy simulation) [M. Honda et al. 2105.03276]

Appendix

Let's calculate grand partition function;

$$\mathcal{Z} = \int \mathcal{D}\psi \int \mathcal{D}\bar{\psi} \exp\left[\int_0^\beta d\tau \int dx\, \mathcal{L}_{\mathrm{eff},E}\right]$$

$$= \int \mathcal{D}\psi \int \mathcal{D}\bar{\psi} \exp\left[\int_0^\beta d\tau \int dx\, (\mathcal{L}_{\mathrm{Dirac},E} - \mathcal{V})\right]$$

$$= e^{-\beta L \mathcal{V}} \int \mathcal{D}\psi \int \mathcal{D}\bar{\psi} \exp\left[\int_0^\beta d\tau \int dx\, \mathcal{L}_{\mathrm{Dirac},E}\right]$$

$$= e^{-L\mathcal{V}/T} \mathcal{Z}_{\mathrm{Dirac}}$$

$$= e^{-\frac{L}{T}(\Omega_{\mathrm{Dirac}} + \mathcal{V})} .$$

$\mathcal{V} = (M-m)^2/4g$

L : total special distance

Known results [N. Kapusta, C. Gale, 2006]

$$\Omega_{\mathrm{Dirac}}(\mu, T; M) = -\frac{2}{\pi}\int_0^\infty dk \left[\omega_k + T\ln(1+e^{-\beta(\omega_k+\mu)}) + T\ln(1+e^{-\beta(\omega_k-\mu)})\right]$$

where $\omega_k = \sqrt{k^2+M^2}$.

➡ We can calculate grand partition function of GN model