Digital quantum simulation for screening and confinement in gauge theory with a topological term

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arXiv: 2105.03276 collaboration with M.Honda (YITP, Kyoto U.), Y.Kikuchi(BNL), L.Nagano, T.Okuda(U. of Tokyo)

Work in progress with M.Honda (YITP, Kyoto U.), Y.Kikuchi(BNL), Y.Tanizaki (YITP, Kyoto U.)

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Introduction
(my research interests)

- I am a high energy theorist. Mainly working on numerical simulations using supercomputer.
- In high energy theory, we would like to study nonperturbative property of quantum field theories.
  (ex. Phase transition, thermodynamics, correlation of observables)
- In particular, theory of elementary particles is described by gauge theory.
  (For instance, quantum chromodynamics (QCD) is given by SU(3) gauge theory)
- Lattice QCD simulation based on Markov-Chain-Monte-Carlo method has been a standard method in this subject, but it suffers from the sign problem if we consider some parameter regime.
- Implementation of quantum computing for QCD with such a regime is my long goal.

Today's talk

- We consider the simple gauge theory
  1+1 dimensional U(1) gauge theory + topological θ term coupled with fermion, Schwinger model
  (e.g. QCD is 3+1 dimensional SU(3) gauge theory coupled with fermions)

- We use a simulator (not real quantum device) to see if our strategy works well
  even in the parameter regime where the sign problem appears in conventional Monte Carlo

- State preparation here is adiabatic state preparation

- See the systematic error from adiabatic state preparation and adiabatic schedule function

Schwinger model

Schwinger model

M.Honda, E.I., Y.Kikuchi, L.Nagano, T.Okuda, arXiv: 2105.03276

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

$$\mathscr{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{g\theta_0}{4\pi}\epsilon_{\mu\nu}F^{\mu\nu} + i\bar{\psi}\gamma^{\mu}(\partial_{\mu} + igA_{\mu})\psi - m\bar{\psi}\psi$$

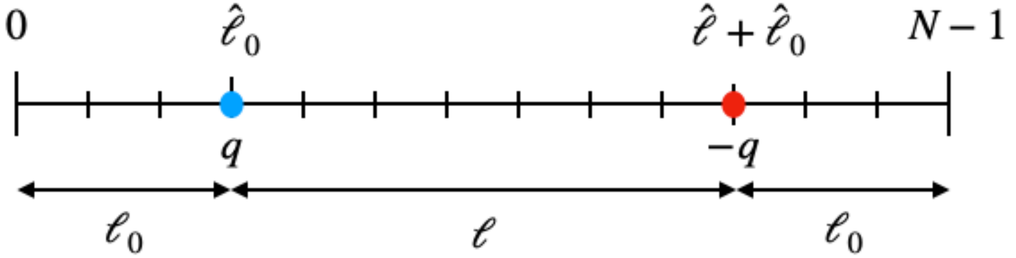
- θ term induces the sign problem in Monte Carlo simulation

- In this work, we numerically obtain the potential between two probe charges with the distance ℓ

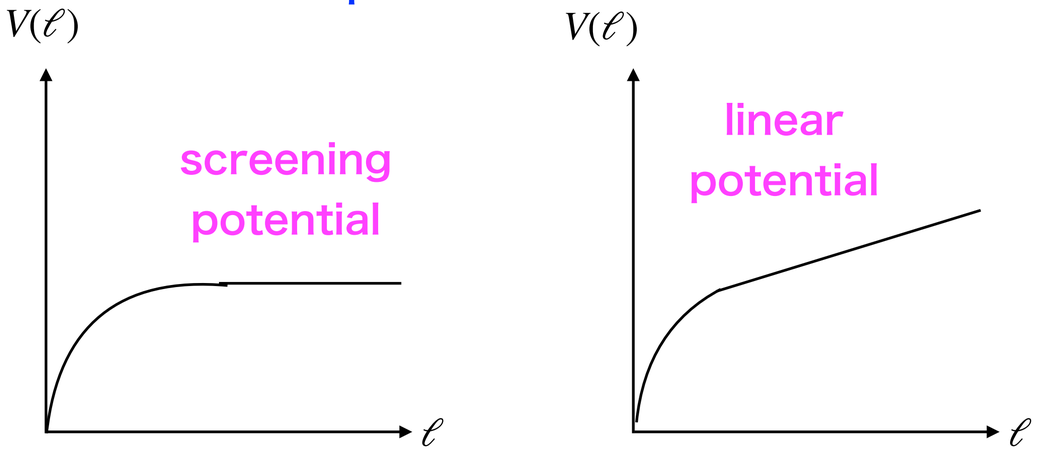
- Analytical calculation predicts the potential between two probe depends on m and q.

  S. Iso and H. Murayama Prog.Theor.Phys.84(1990)142
  D. J. Gross et al., NPB461 (1996)

- We compare the results with analytic results in both infinite vol. and finite vol. using the mass perturbation



theoretical predictions in infinite vol. limit



integer q in $m = 0,\ m \neq 0$

fractional q in $m = 0$

fractional q in $m \neq 0$

From $\mathscr{L}$ to $\mathscr{H}$ for Quantum computer

Ex) Schwinger model with open b.c.

- Lagrangian in continuum

PBC: Shaw et al. Quantum 4, 306 (2020)
arXiv:2002.11146

$$\mathscr{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{g\theta_0}{4\pi}\epsilon_{\mu\nu}F^{\mu\nu} + i\bar{\psi}\gamma^{\mu}(\partial_{\mu} + igA_{\mu})\psi - m\bar{\psi}\psi$$

Map the Lagrangian to the Spin Hamiltonian

- Spin Hamiltonian using Pauli matrices(Jordan-Wigner trans.)

$$H = J\sum_{n=0}^{N-2}\left[\sum_{i=0}^{n}\frac{Z_i + (-1)^i}{2} + \frac{\vartheta_n}{2\pi}\right]^2 + \frac{w}{2}\sum_{n=0}^{N-2}\left[X_nX_{n+1} + Y_nY_{n+1}\right] + \frac{m}{2}\sum_{n=0}^{N-1}(-1)^nZ_n$$

Jordan-Wigner trans.: $\chi_n = \frac{X_n - Y_n}{2}\prod_{i=0}^{n-1}(-iZ_i)$

Apply quantum algorithms to this spin hamiltonian.

From $\mathscr{L}$ to $\mathscr{H}$ for Quantum computer

Ex) Schwinger model with open b.c.

- Lagrangian in continuum

$$\mathscr{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{g\theta_0}{4\pi}\epsilon_{\mu\nu}F^{\mu\nu} + i\bar{\psi}\gamma^{\mu}(\partial_{\mu} + igA_{\mu})\psi - m\bar{\psi}\psi$$

PBC: Shaw et al. Quantum 4, 306 (2020)
arXiv:2002.11146

- Hamiltonian in continuum

$$H_{\text{con}} = \int dx \left[\frac{1}{2}\left(\Pi - \frac{g\theta_0}{2\pi}\right)^2 - i\bar{\psi}\gamma^1(\partial_1 + igA_1)\psi + m\bar{\psi}\psi\right]$$

Canonical momentum: $\Pi = \partial_0 A^1 + \frac{g\theta}{2\pi}$

- Hamiltonian on lattice (staggered fermion, link variable)

$$H = J\sum_{n=0}^{N-2}\left(L_n + \frac{\vartheta_n}{2\pi}\right)^2 - iw\sum_{n=0}^{N-2}\left(\chi_n^{\dagger}U_n\chi_{n+1} - \chi_{n+1}^{\dagger}U_n^{\dagger}\chi_n\right) + m\sum_{n=0}^{N-1}(-1)^n\chi_n^{\dagger}\chi_n$$

Link variable: $L_n \leftrightarrow -\Pi(x)/g, \quad U_n \leftrightarrow e^{-iagA^1(x)},$

Staggered fermion: $\frac{\chi_n}{\sqrt{a}} \leftrightarrow \begin{cases}\psi_u(x) & n : \text{even} \\ \psi_d(x) & n : \text{odd}\end{cases}$

- Remove gauge d.o.f. (OBC and Gauss law constraint)

$$H = J\sum_{n=0}^{N-2}\left(\epsilon_{-1} + \sum_{i=0}^{n}\left(\chi_i^{\dagger}\chi_i - \frac{1-(-1)^i}{2}\right) + \frac{\vartheta_n}{2\pi}\right)^2 - iw\sum_{n=0}^{N-2}\left(\chi_n^{\dagger}\chi_{n+1} - \chi_{n+1}^{\dagger}\chi_n\right) + m\sum_{n=0}^{N-1}(-1)^n\chi_n^{\dagger}\chi_n$$

Gauss law:
$0 = \partial_1\Pi + g\psi^{\dagger}\psi \rightarrow L_n - L_{n-1} = \chi_n^{\dagger}\chi_n - \frac{1-(-1)^n}{2}$

- Spin Hamiltonian using Pauli matrices(Jordan-Wigner trans.)

$$H = J\sum_{n=0}^{N-2}\left[\sum_{i=0}^{n}\frac{Z_i + (-1)^i}{2} + \frac{\vartheta_n}{2\pi}\right]^2 + \frac{w}{2}\sum_{n=0}^{N-2}\left[X_nX_{n+1} + Y_nY_{n+1}\right] + \frac{m}{2}\sum_{n=0}^{N-1}(-1)^nZ_n$$

Jordan-Wigner trans.: $\chi_n = \frac{X_n - Y_n}{2}\prod_{i=0}^{n-1}(-iZ_i)$

Apply quantum algorithms to this spin hamiltonian.

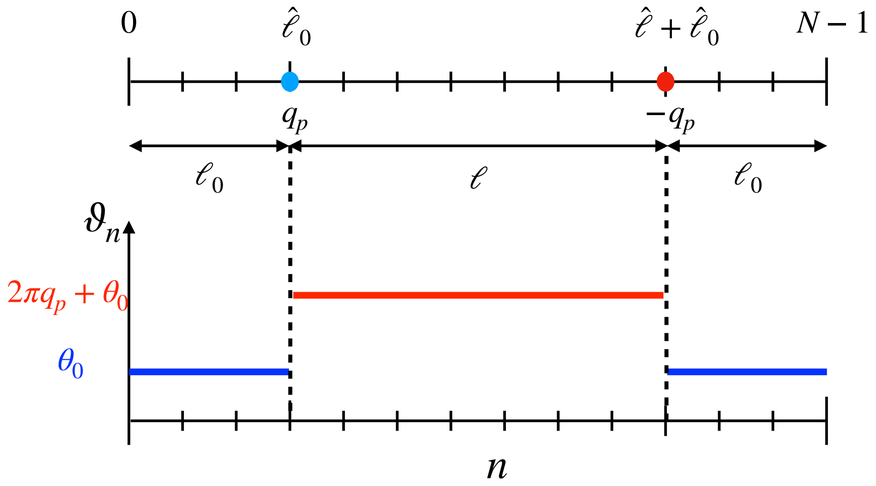
Summary of simulation strategy

- Spin Hamiltonian:

$$H = J\sum_{n=0}^{N-2}\left[\sum_{i=0}^{n}\frac{Z_i+(-1)^i}{2}+\frac{\vartheta_n}{2\pi}\right]^2+\frac{w}{2}\sum_{n=0}^{N-2}\left[X_nX_{n+1}+Y_nY_{n+1}\right]+\frac{m}{2}\sum_{n=0}^{N-1}(-1)^nZ_n$$

- Theta-term can be expressed as a background electric field (link variable) in Hamiltonian formalism.
  Probe charge shift the value of theta

$$\vartheta_n=\begin{cases}2\pi q+\theta_0, & \hat{\ell}_0\le n<\hat{\ell}_0+\hat{\ell},\\ \theta_0, & \text{otherwise.}\end{cases}$$



- Generate the ground state ($|\Omega\rangle$) using adiabatic state preparation with 2nd order Suzuki-Trotter decomposition

- Directly measure the energy $E(\ell)=\langle\Omega|H(\ell)|\Omega\rangle$, and $V(\ell)=E(\ell)-E(0)$

  Cf.) In Lattice QCD, we calculate the Wilson loop and extract the potential from its exponent.

  $\langle W(R,T)\rangle\sim\exp(-V(R)/T)$ with $V(R)\sim\sigma R+\alpha/R$

Simulation results

Simulation Setup

- IBM Qiskit library, Simulator (not real quantum device)
- lattice size: N=15,21, open b.c.(remove d.o.f. of gauge field)
- # of shots = 100,000 - 400,000
- a=0.4, g=1.0, mass= 0.00 - 0.25
  cf) 1st order phase transition emerges at $m_c/g \approx 0.33$ with $\theta_0 = \pi, q = 0$ in infinite limit

Result(1): integer charge ($\theta_0 = 0$)

- $a \to 0,\ N \to \infty$ screening potential

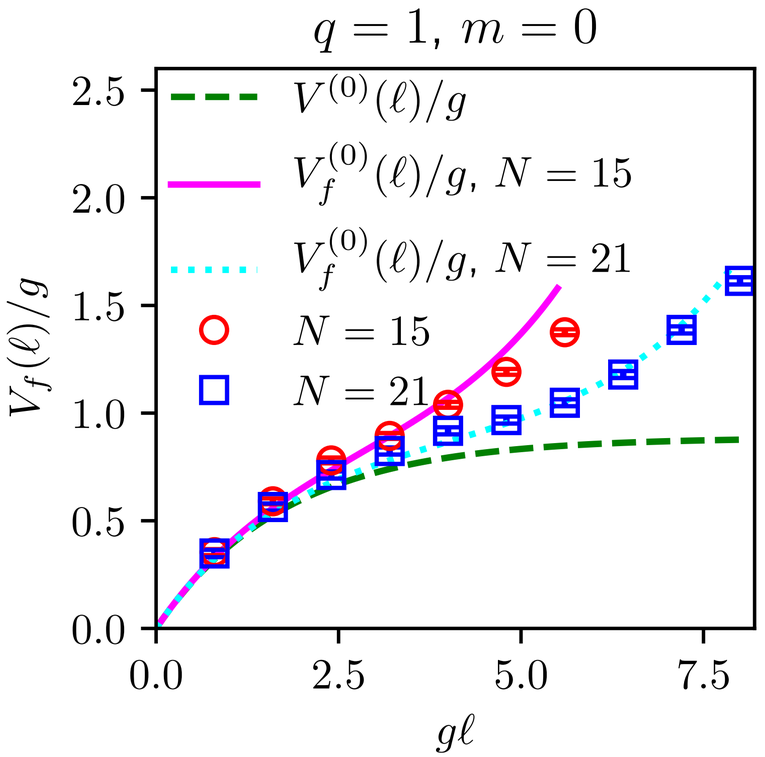
  - - - - denotes $V^{(0)}$

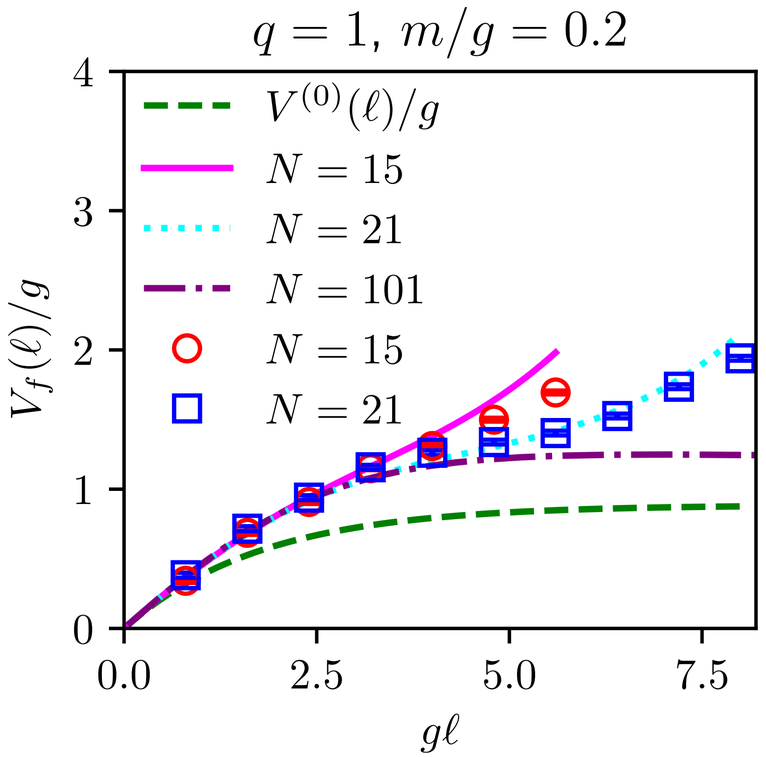
- In $a \to 0$ and finite N is given by

$$V_f^{(0)}(\ell) = \frac{q^2 g^2}{2\mu} \frac{(1 - e^{-\mu\ell})(1 + e^{-\mu(L-\ell)})}{1 + e^{-\mu L}},$$

- const. term remains in $\mathcal{O}(m)$

  - ・ - ・ (roughly) denotes $V^0 + V^{(1)}$



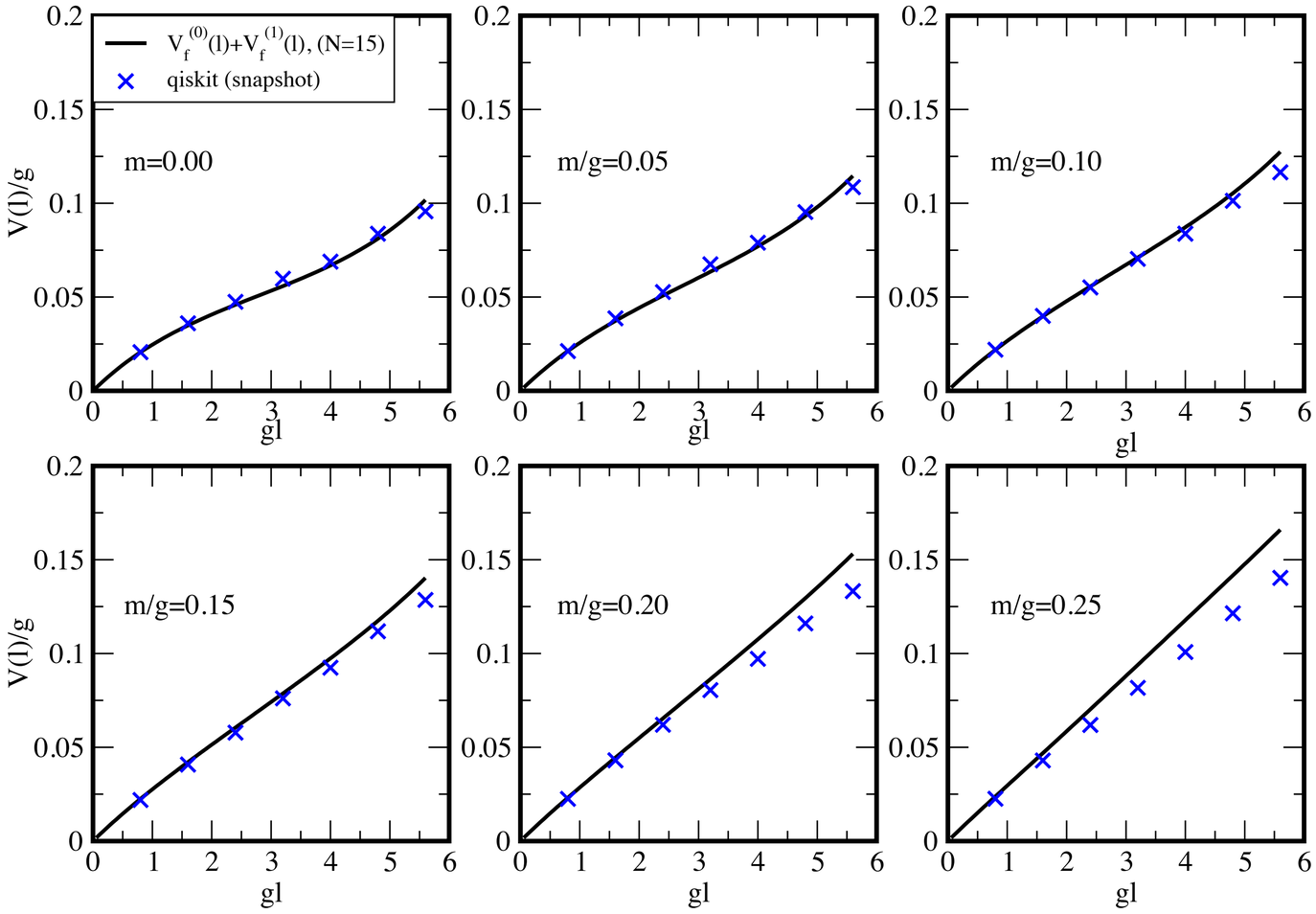


- Our results are consistent with the theoretical predictions in the finite N
  We expect the discrepancy comes from finite a effect

Result(2): fractional charge ($\theta_0 = 0$)

Potential shape as a function of mass

- If Q is fractional, in $a \to 0, N \to \infty$
  $V(\ell)$ is screening for massless case
  $V(\ell)$ is confinement in large ℓ for nonzero masses
- In $a \to 0$ and finite N, potential shape gradually changes (see black curve)
- Around $0.20 \lesssim m/g \lesssim 0.25$, black curve depicts linear behavior



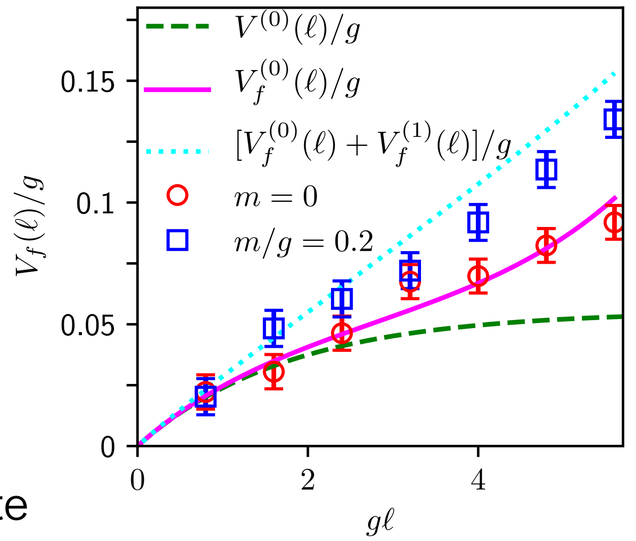
Result(2): fractional charge ($\theta_0 = 0$)

- string tension is calculated by fitting long ℓ data
- It shows the large discrepancy from Coulomb potential (pure U(1) gauge theory)
- Our data are consistent with the **analytical prediction of 1st order mass perturbation in finite vol.**
- Around $q = 0.5$ $(\theta = \pi)$, string tension in finite vol. is quite different from result in infinite volume:

  $V^{(1)}(\ell) = m\Sigma(1 - \cos(2\pi q))\ell$

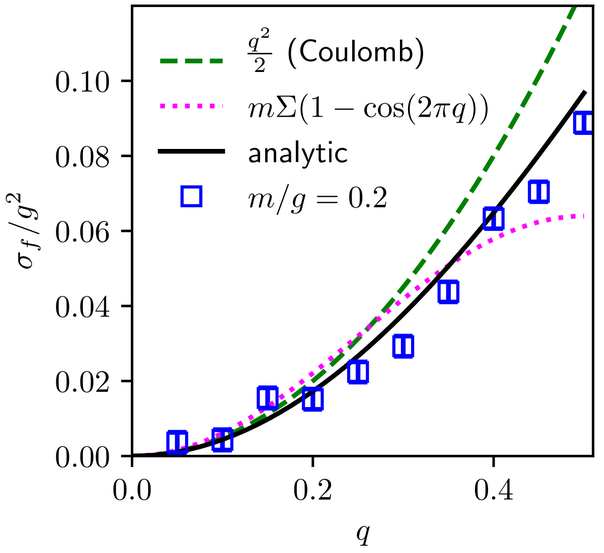
  because of open boundary condition
  (We will show the restoration of the periodicity
  Work in progress w/ Honda, Kikuchi and Tanizaki)

Potential
N=15, q=0.25



String tension (σ)

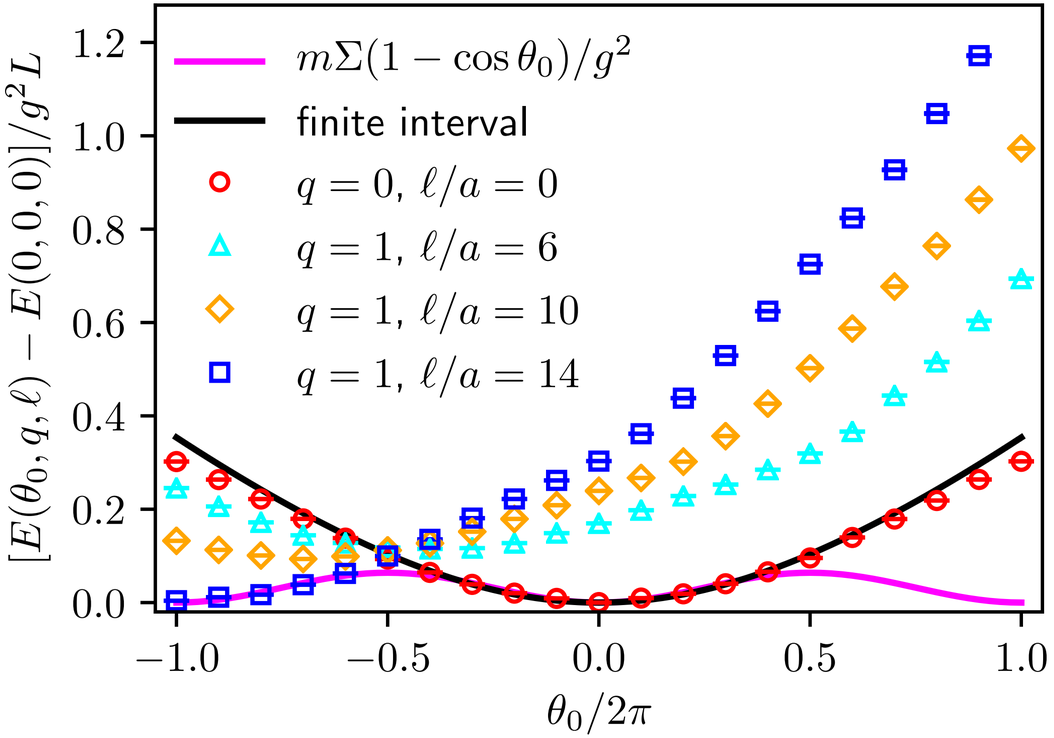
$V(\ell) = \sigma\ell + c_0$



Result(3): non-zero θ_0 case

- non-zero θ_0 simulation is doable
- 2π periodicity is broken because of open b.c.
  Infinite volume limit: $E(\theta) = m\Sigma(1-\cos\theta)\ell)$
- $q = 1,\ \ell/a = 14$ is a 2π shift of boundary charge (θ_0)
  for $q = 0,\ \ell/a = 0$

Energy density



Systematic error

Systematic errors from adiabatic state preparation

Generate (approximate) ground state based on adiabatic theorem

Work in progress with M.Honda, Y.Kikuchi, Y.Tanizaki

$$|\Omega\rangle = \lim_{T\to\infty} \mathcal{T} \exp\left(-i\int_0^T dt\ H_A(t)\right)|\Omega\rangle_0$$

Here, $H_A(t)$ is adiabatic Hamiltonian $H_A(0) = H_0 \quad H_A(T) = H$

- Systematic errors: Adiabatic error (T)
  Trotter error (δt)
  (initial mass ($m_{init.} \approx m + 0.5$))

In finite T, an approximate ground state is obtained.

In the adiabatic Hamiltonian, the parameters of model depend on the time (t/T),
(e.g. $\theta_0 f(t/T)$ where $f(x)$ with $f(0) = 0 \quad , f(1) = 1$)

If we take a linear fn, $w \to w\frac{t}{T},\ \theta_0 \to \theta_0\frac{t}{T},\ q \to q\frac{t}{T}, m \to m_0\left(1 - \frac{t}{T}\right) + m\frac{t}{T}$

Adiabatic error and adiabatic schedule

Theorem. *Suppose $H(s)$ has a nondegenerate ground state for all $s \in [0,1]$, and suppose that the total evolution time satisfies*

$$T \geq \frac{2}{\epsilon}\left[c_1 \frac{\|\dot{H}(0)\|}{\Delta(0)^2} + c_1 \frac{\|\dot{H}(1)\|}{\Delta(1)^2} + \int_0^1 \mathrm{d}s \left((3c_1^2 + c_1 + c_3)\frac{\|\dot{H}\|^2}{\Delta^3} + c_2 \frac{\|\ddot{H}\|}{\Delta^2}\right)\right]. \qquad (49)$$

Lecture note by A. Childs

$\dot{H}(t/T)$ denotes the first derivative of adiabatic Hamiltonian at t=0 and t=T

$\Delta(t)$ denotes the gap energy

Adiabatic error (ϵ) scales $\mathcal{O}(1/T^{m+1})$ if the first m derivatives of the Hamiltonian is zero at the beginning and end of the evolution.

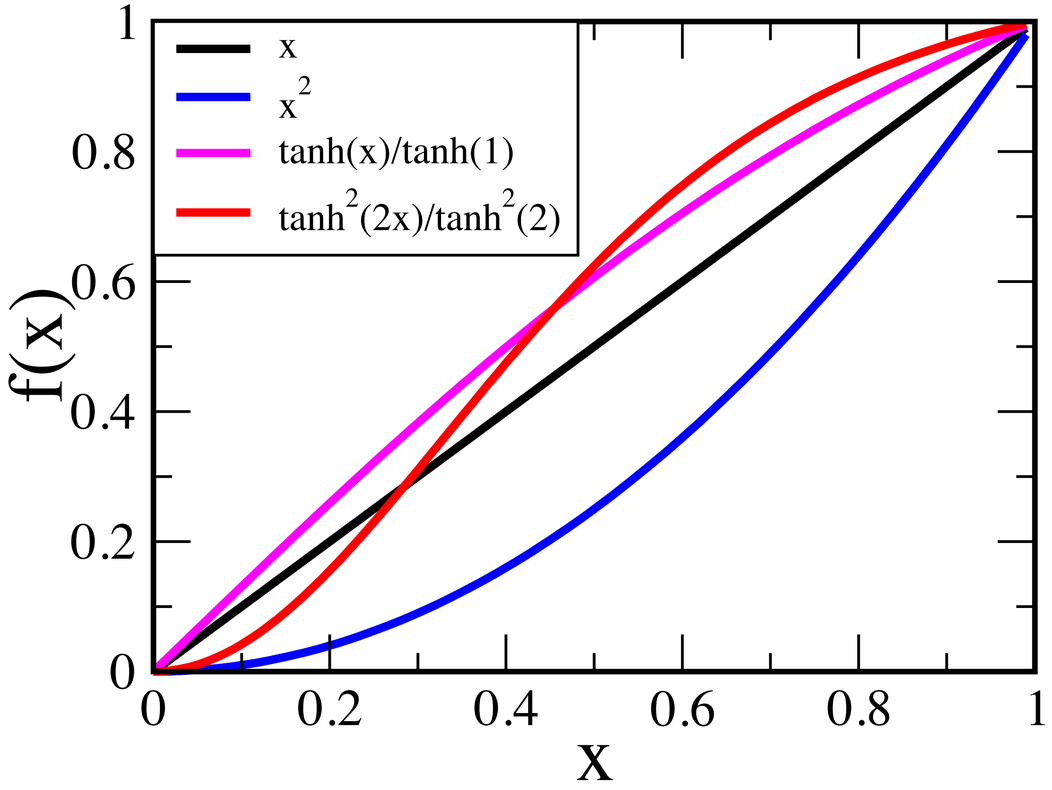
Rezakhani A T, Pimachev A K and Lidar D A 2010 Phys. Rev. A 82 052305
Lidar D A, Rezakhani A T and Hamma A 2009 J. Math. Phys. 50 102106

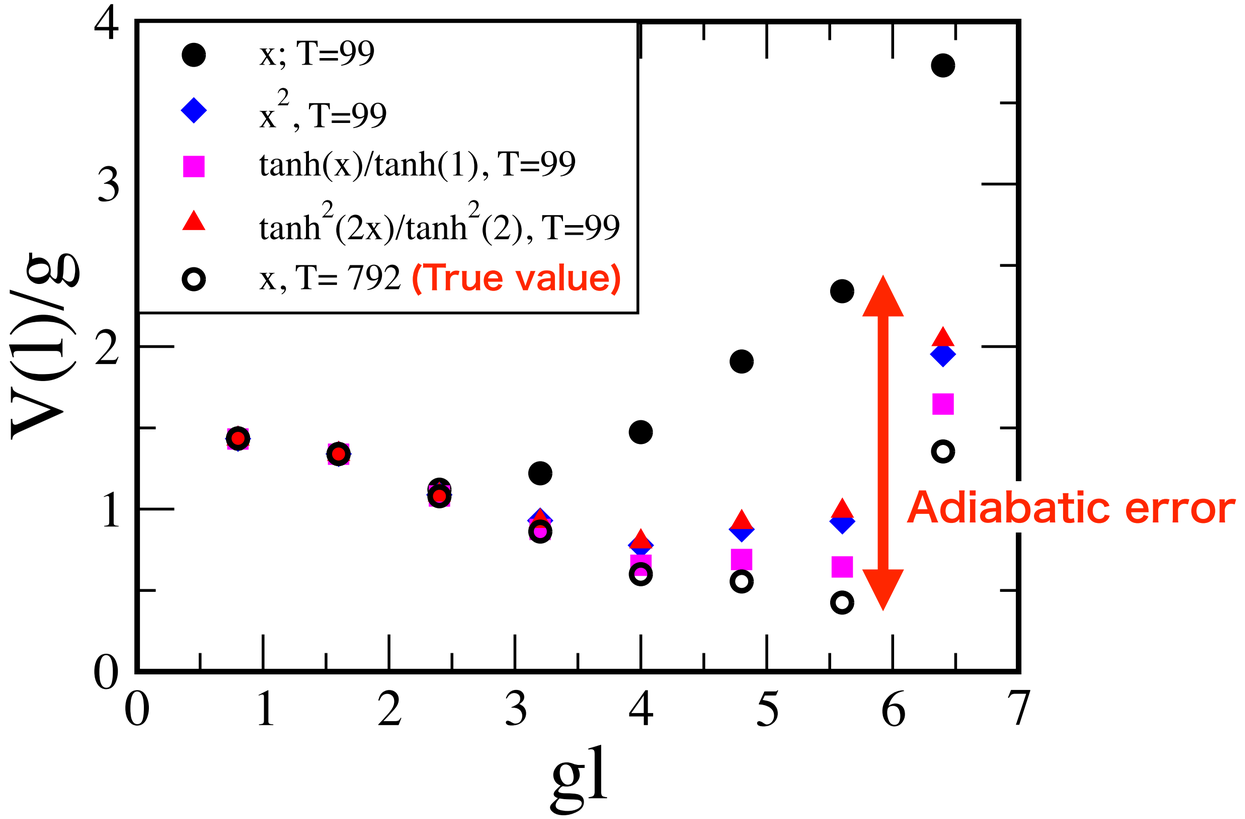
Thus, naively if the adiabatic schedule fn. has a mild slope at both edges of time evolution, then we expect that adiabatic error becomes small.

Adiabatic schedule function

Work in progress with M.Honda, Y.Kikuchi, Y.Tanizaki

- It is difficult to estimate where the gap energy is small in quantum field theory





We practically find that $\tanh(x)/\tanh(1)$ is good schedule fn if we take a parameter set of this model.

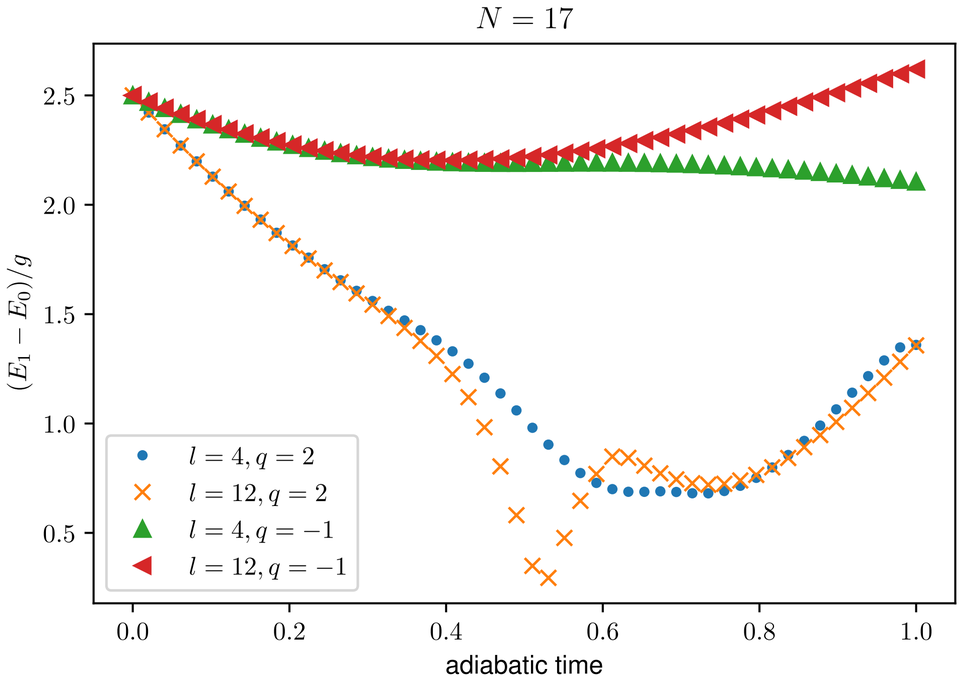
Why ?? Around x=0, and 1, $\tanh^2(2x)/\tanh^2(2)$ or x^2 has more gentle slop.

Adiabatic schedule function

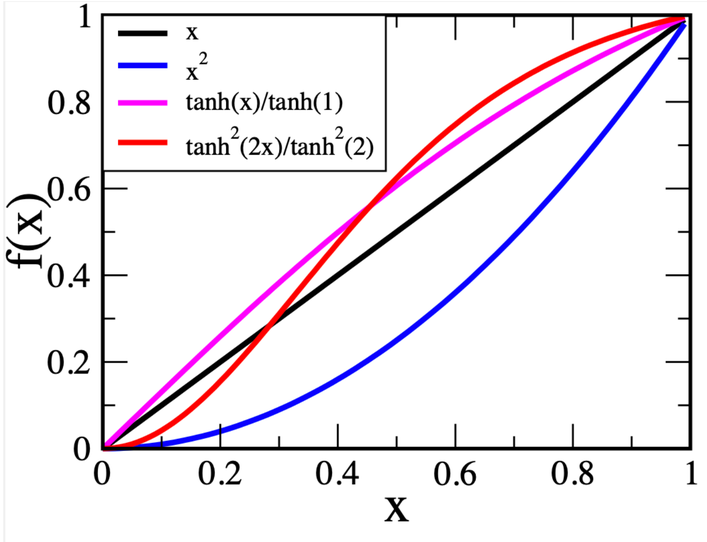
Work in progress with M.Honda, Y.Kikuchi, Y.Tanizaki

- It is difficult to estimate where the gap energy is small in quantum field theory

Gap energy between ground and 1st excited states in adiabatic process (exact diagonalization calculation)



Orange data has a rapid decreasing of gap energy around t/T =0.5.
It explains why $\tanh(x)/\tanh(1)$ is the best schedule fn,
since $\tanh(x)/\tanh(1)$ has the most gentle slope around t/T = 0.5.



Summary and outlook

- We carried out the numerical simulation for the screening-type and confinement potentials of Schwinger model using quantum algorithm
- Thanks to the Hamiltonian formalism, even in $\theta_0 \neq 0$ regime, we can perform the simulations
- The potential can be directly obtained from the vev of Hamiltonian.
- If we consider $a \to 0, N \to \infty$ limits, some improvements are necessary.
- Choice of adiabatic schedule is nontrivial in some QFT.
- Using quantum algorithm, we can investigate various QFTs which suffer from the sign problem in conventional Monte Carlo approach.

Confinement potential in Lattice QCD

M.Creutz, PRD21 (1980) 2308

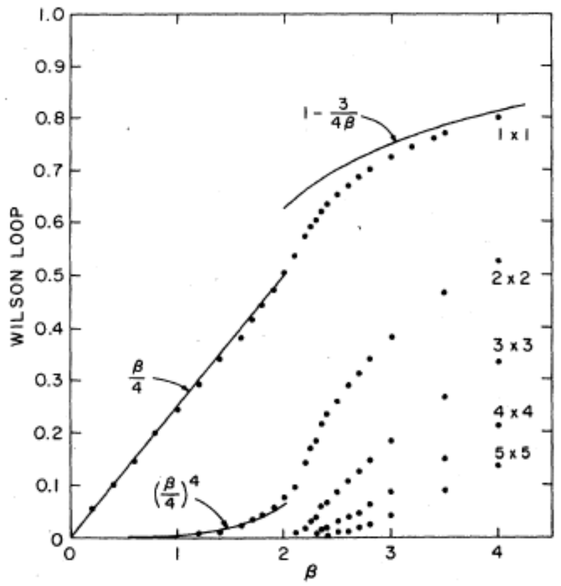


FIG. 4. Wilson loops as a function of β.

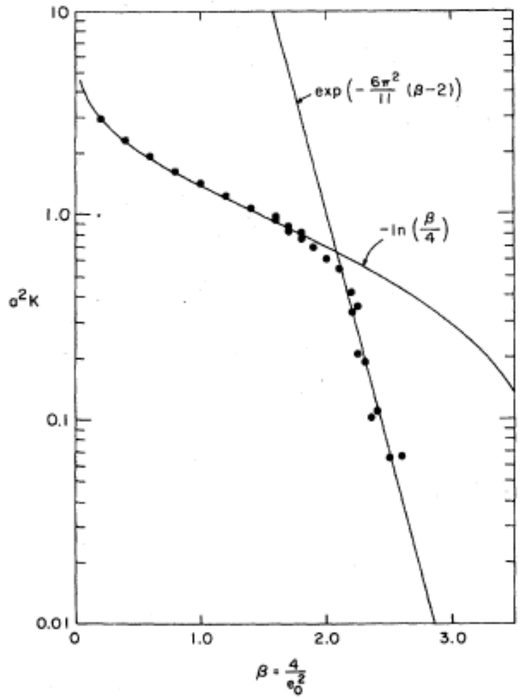


FIG. 6. The cutoff squared times the string tension as a function of β. The solid lines are the strong- and weak-coupling limits.

Lattice QCD simulations started the derivation of the confinement potential.

Now, QC for QFT (or QCD) have just started!