量子計算を用いた
(1+1)次元Schwinger模型における
実時間ダイナミクスの解析

Daisuke Inotani (RIKEN, Keio Univ.)

Collaborators
Etsuko Itou(RIKEN), Masazumi Honda(YITP),
Yuta Kikuchi(Cambridge Quantum), Bipasha Chakraborty(Cambridge U.)

Contents

Contents

Quantum computing and real time dynamics of physical system

<u>What can quantum computers do?</u>

$$|\phi\rangle = \prod_k U_k \, |\phi_{\mathrm{in}}\rangle$$

$$|\phi\rangle = \sum_{s_1, s_2 \ldots s_N} \alpha_{s_1, s_2 \ldots s_N} |s_1, s_2 \ldots s_N\rangle$$

$s_i = 0 \text{ or } 1$

Observable: $\langle \hat{O} \rangle = \langle \phi | O(s_1, s_2 \ldots s_N) | \phi \rangle$

<u>Real time dynamics of quantum systems</u>

$$|\psi(t)\rangle = \int_0^t dT \, e^{-iHT} \, |\psi(t=0)\rangle$$

$$\Downarrow$$

$$|\psi(t = M\Delta t)\rangle = \prod_{k=1}^{M} e^{-iH_{\mathrm{k}}\Delta t} \, |\psi(t=0)\rangle$$

$$O(t) = \langle \psi(t) | \hat{O} | \psi(t) \rangle$$

Unitary transformation & measurement

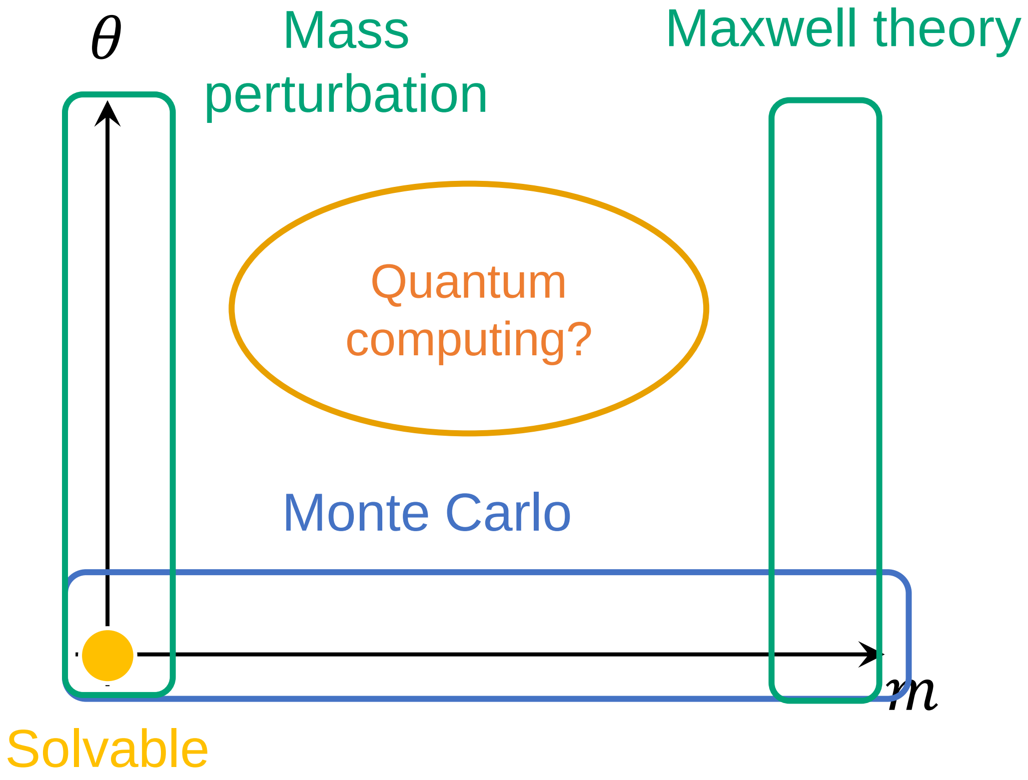
How to map physical system $|\psi(t)\rangle$ to N-qubit system $|\phi\rangle$?

(1+1) D Schwinger model with topological θ term

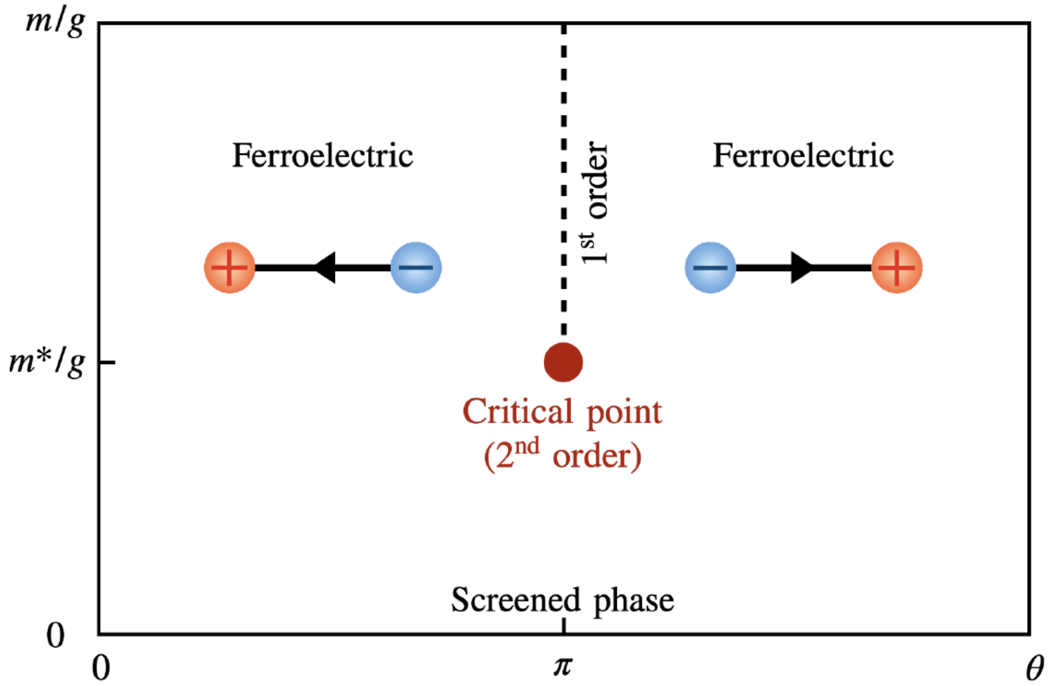
$$\mathcal{L} = \int dt dx \left[-\frac{1}{4g^2} F_{\mu\nu} F^{\mu\nu} + \frac{\theta}{4\pi} \epsilon_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\gamma^{\mu}(\partial_{\mu} + igA_{\mu})\psi - m\bar{\psi}\psi \right]$$

topological θ term

Difficulty



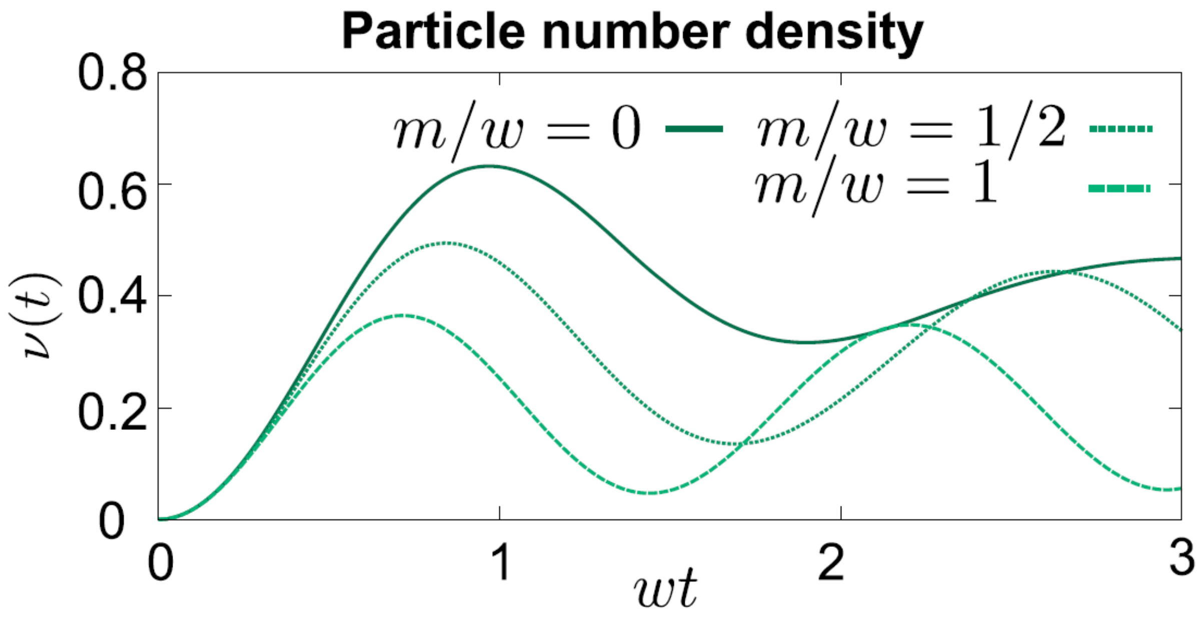
Phase diagram

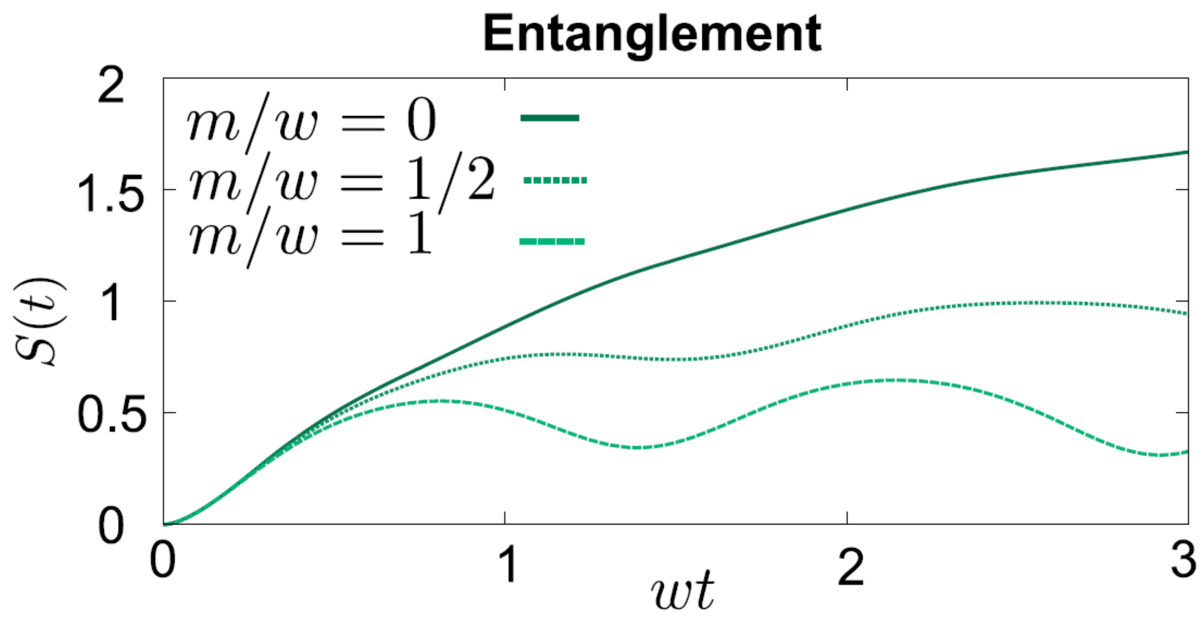


Coleman 1976, Ikeda, Kharzeev, Kikuchi (2021), etc

Real time dynamics of Schwinger model w/o θ term

Muschik *et al* 2017 *New J. Phys.* **19** 103020





$w = 1/(2a)$ a: lattice constant

- ✓ Real time dynamics of Schwinger model <u>w/o topological θ term</u> was investigated by quantum digital simulation.
- ✓ Initial state was simply taken to be vacuum state.

(1+1) D Schwinger model with topological θ term

$$\mathcal{L} = \int dtdx \left[-\frac{1}{4g^2} F_{\mu\nu}F^{\mu\nu} + \underline{\frac{\theta}{4\pi}\epsilon_{\mu\nu}F^{\mu\nu}} + i\bar{\psi}\gamma^{\mu}(\partial_{\mu} + \mathrm{i}gA_{\mu})\psi - m\bar{\psi}\psi \right]$$

topological θ term

Motivation

- ✓ We study **real-time dynamics** of the (1+1)-D Schwinger model by quantum digital simulation.
- ✓ From the time dependence of physical quantities, we obtain the information of excited states.
- ✓ Can we see the phase transition from real time dynamics?

Contents

Schwinger model with open boundary condition

$$\mathcal{L} = \int dtdx \left[-\frac{1}{4g^2} F_{\mu\nu} F^{\mu\nu} + \frac{\theta}{4\pi} \epsilon_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\gamma^{\mu}(\partial_{\mu} + \mathrm{i}gA_{\mu})\psi - m\bar{\psi}\psi \right]$$

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

Π: canonical momentum conjugate

g: coupling constant

A_1: vector potential

ψ: (spinless) Dirac fermion

m: fermion mass

θ: topological theta term

Mapping the Hamiltonian into spin system for quantum digital simulation

Mapping into spin system (= N-qubit system)

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

① Discretization

$$\psi(x) \to \psi_n = \psi(an)$$

$$\Pi(x) \to L_n = \Pi(an)/g$$

$$A_1(x) \to U_n = e^{-iaA_1(an)}$$

② Staggered fermion [Susskind, Kogut-Susskind '75]

$$\frac{\chi_n}{\sqrt{a}} \longleftrightarrow \psi_u(an) \quad \text{for even } n, \qquad \text{particle}$$

$$\frac{\chi_n}{\sqrt{a}} \longleftrightarrow \psi_d^\dagger(an) \quad \text{for odd } n. \qquad \text{antiparticle}$$

$$H = \frac{g^2 a}{2}\sum_{n=0}^{N-1}\left(L_n + \frac{\theta}{2\pi}\right)^2 - \frac{\mathrm{i}}{2a}\sum_{n=0}^{N-2}[\chi_{n+1}^\dagger U_n \chi_n - \chi_n^\dagger U_n^\dagger \chi_{n+1}] + m\sum_{n=0}^{N-1}(-1)^n \chi_n^\dagger \chi_n$$

③ Gauss law with open boundary condition
(eliminate (bosonic) gauge field L_n and U_n)

$$L_n - L_{n-1} = \chi_n^\dagger \chi_n - \frac{1-(-1)^n}{2}$$

$$H = \frac{g^2 a}{2}\sum_{n=0}^{N-1}\left[\sum_{i=1}^{n}\left(\chi_i^\dagger \chi_i - \frac{1-(-1)^i}{2}\right) + \epsilon_0 + \frac{\theta}{2\pi}\right]^2 - \frac{\mathrm{i}}{2a}\sum_{n=0}^{N-2}\left[\chi_{n+1}^\dagger \chi_n - \chi_n^\dagger \chi_{n+1}\right] + m\sum_{n=0}^{N-1}(-1)^n \chi_n^\dagger \chi_n$$

Mapping into spin system (= N-qubit system)

$$H=\frac{g^2a}{2}\sum_{n=0}^{N-1}\left[\sum_{i=1}^{n}\left(\chi_i^\dagger\chi_i-\frac{1-(-1)^i}{2}\right)+\epsilon_0+\frac{\theta}{2\pi}\right]^2-\frac{\mathrm{i}}{2a}\sum_{n=0}^{N-2}\left[\chi_{n+1}^\dagger\chi_n-\chi_n^\dagger\chi_{n+1}\right]+m\sum_{n=0}^{N-1}(-1)^n\chi_n^\dagger\chi_n$$

④ JW transformation
[Jordan-Wigner'28]

$$\chi_n=\frac{X_n-\mathrm{i}Y_n}{2}\prod_{i<n}(iZ_i)\quad \chi_n^\dagger=\frac{X_n+\mathrm{i}Y_n}{2}\prod_{i<n}(-\mathrm{i}Z_i)$$

X_n, Y_n, Z_n: spin operator

$$H=H_{XY}^{(0)}+H_{XY}^{(1)}+H_Z+C.$$

$$H_{XY}^{(0)}=\frac{1}{4a}\sum_{n=0}^{\lfloor\frac{N-2}{2}\rfloor}\left(X_{2n}X_{2n+1}+Y_{2n}Y_{2n+1}\right)$$

$$H_{XY}^{(1)}=\frac{1}{4a}\sum_{n=1}^{\lfloor\frac{N-1}{2}\rfloor}\left(X_{2n-1}X_{2n}+Y_{2n-1}Y_{2n}\right)$$

$$H_Z=\frac{g^2a}{4}\sum_{n=0}^{N-3}\sum_{l=n+1}^{N-2}(N-l-1)Z_nZ_l+\frac{g^2a}{4}\sum_{n=0}^{N-2}\frac{1+(-1)^n}{2}\sum_{l=0}^{n}Z_l$$
$$+\frac{\theta g^2a}{4\pi}\sum_{n=0}^{N-2}(N-n-1)Z_n+\frac{m}{2}\sum_{n=0}^{N-1}(-1)^nZ_n$$

$$C=\frac{\theta}{4\pi}\left(N-1+\frac{1+(-1)^N}{2}\right)+\left(\frac{\theta}{2\pi}\right)^2\frac{g^2a}{2}(N-1)$$

Quantum digital simulation for real-time dynamics

Initial state

Real time evolution

$$|\psi(t=0)\rangle = |\mathrm{GS}_0\rangle$$

$|\mathrm{GS}_0\rangle$: ground state of H_0

$$|\psi(t)\rangle = \exp(-iHt)\,|\psi(t=0)\rangle$$

(ii) Discretizing in time direction

(i) Preparation of an initial state

$$|\mathrm{GS}_0\rangle \simeq |\mathrm{GS}_V\rangle$$

Hamiltonian variational algorithm

(iii) measurement

- ✓ particle number density $\nu(t) = \frac{1}{2N}\sum_{n=0}^{N-1}\langle\Psi(t)|(-1)^n\hat{Z}_n + 1|\Psi(t)\rangle$
- ✓ vacuum persistent amplitude $\mathcal{G}(t) = \langle\psi(t=0)|e^{-\mathrm{i}\hat{H}t}|\psi(t=0)\rangle$

$$\lambda(t) = -N^{-1}\log(|\mathcal{G}(t)|^2)$$

Hamiltonian variational algorithm D. Wecker, M. B. Hastings, M. Troyer 2015

(i) Preparation of an initial state by Hamiltonian variational algorithm

$$|\psi_{\mathrm{V}}\rangle = \prod_{s=1}^{p}\left[e^{-iH_Z(t\leq 0)dt_Z(s)}e^{-iH_{XY}^{(1)}(t\leq 0)dt_{XY}^{(1)}(s)}e^{-iH_{XY}^{(0)}(t\leq 0)dt_{XY}^{(0)}(s)}\right]|\mathrm{vac}\rangle$$

$|\mathrm{vac}\rangle = |101010\ldots\rangle$: Neel state (vacuum state)

Variational parameters: $dt_{XY}^{(1)}(s), dt_Z(s), dt_{XY}^{(0)}(s)$

Determine the variational parameters to minimize $E_{\mathrm{V}} = \langle\psi_{\mathrm{V}}|H_0|\psi_{\mathrm{V}}\rangle$

Advantages

- ✓ The depth of quantum circuit becomes shallow.
- ✓ We keep the information of initial state in classical register.

Disadvantage

- ✓ Hamiltonian variational algorithm takes longer time than adiabatic state preparation.
- ✓ We don't know how to choose "good" variational function and initial condition.

Real-time evolution

(ii) Discretization in time (2nd order Suzuki-Trotter decomposition)

$$|\psi(t)\rangle = \exp(-iHt)\,|\psi(t=0)\rangle$$

$$\simeq \prod_{s=1}^{N_{\rm step}} e^{-\mathrm{i}H_{XY}^{(0)}\frac{\Delta t}{2}} e^{-\mathrm{i}H_{XY}^{(1)}\frac{\Delta t}{2}} e^{-\mathrm{i}H_Z\Delta t} e^{-\mathrm{i}H_{XY}^{(1)}\frac{\Delta t}{2}} e^{-\mathrm{i}H_{XY}^{(0)}\frac{\Delta t}{2}} \,|\psi(t=0)\rangle$$

$$\Delta t = t/N_{\rm step}$$

$$H_{XY}^{(0)} = \frac{1}{4a}\sum_{n=0}^{\lfloor\frac{N-2}{2}\rfloor}\left(X_{2n}X_{2n+1} + Y_{2n}Y_{2n+1}\right)$$

$$H_{XY}^{(1)} = \frac{1}{4a}\sum_{n=1}^{\lfloor\frac{N-1}{2}\rfloor}\left(X_{2n-1}X_{2n} + Y_{2n-1}Y_{2n}\right)$$

$$H_Z = \frac{g^2a}{4}\sum_{n=0}^{N-3}\sum_{l=n+1}^{N-2}(N-l-1)Z_nZ_l + \frac{g^2a}{4}\sum_{n=0}^{N-2}\frac{1+(-1)^n}{2}\sum_{l=0}^{n}Z_l + \frac{\theta g^2 a}{4\pi}\sum_{n=0}^{N-2}(N-n-1)Z_n + \frac{m}{2}\sum_{n=0}^{N-1}(-1)^nZ_n$$

$$C = \frac{\theta}{4\pi}\left(N-1+\frac{1+(-1)^N}{2}\right) + \left(\frac{\theta}{2\pi}\right)^2\frac{g^2a}{2}(N-1)$$

measurement

✓ particle number density

$$\rho_n = [(-1)^n \hat{Z}_n + 1]/2$$

$$\nu(t) = \frac{1}{N}\sum_{n=0}^{N-1}\langle\Psi(t)|\rho_n|\Psi(t)\rangle$$
$$= \frac{1}{N}\sum_{n=0}^{N-1}\sum_{i,j}\langle\phi_j|e^{iE_jt}C_j^*\rho_n C_i e^{-iE_it}|\phi_i\rangle$$

Expanding the initial state in terms of the energy eigenstate of H

$$|\psi(t=0)\rangle = \sum_i C_i|\phi_i\rangle$$
$$H|\phi_i\rangle = E_i|\phi_i\rangle$$

Fourier transformation $\nu(t) = \int e^{-i\omega t}\nu(\omega)$

$$\nu(\omega) = \sum_{i,j}\eta_{ij}\delta\left(\omega - E_i + E_j\right)$$
$$\eta_{ij} = \frac{1}{N}\sum_{n=0}^{N-1}\langle\phi_j|C_j^*\rho_n C_i|\phi_i\rangle$$

Information of excited states might be obtained from the real time dynamics of particle number density.

Parameters

$$H_{XY}^{(0)} = \frac{1}{4a} \sum_{n=0}^{\lfloor \frac{N-2}{2} \rfloor} \left(X_{2n} X_{2n+1} + Y_{2n} Y_{2n+1} \right)$$

$$H_{XY}^{(1)} = \frac{1}{4a} \sum_{n=1}^{\lfloor \frac{N-1}{2} \rfloor} \left(X_{2n-1} X_{2n} + Y_{2n-1} Y_{2n} \right)$$

$$H_Z = \frac{g^2 a}{4} \sum_{n=0}^{N-3} \sum_{l=n+1}^{N-2} (N-l-1) Z_n Z_l + \frac{g^2 a}{4} \sum_{n=0}^{N-2} \frac{1+(-1)^n}{2} \sum_{l=0}^{n} Z_l + \frac{\theta g^2 a}{4\pi} \sum_{n=0}^{N-2} (N-n-1) Z_n + \frac{m}{2} \sum_{n=0}^{N-1} (-1)^n Z_n$$

$$C = \frac{\theta}{4\pi} \left(N - 1 + \frac{1+(-1)^N}{2} \right) + \left(\frac{\theta}{2\pi} \right)^2 \frac{g^2 a}{2} (N-1)$$

a: lattice constant

g: coupling constant

m: fermion mass

θ: topological term

<u>Hamiltonian variational argorithm</u>

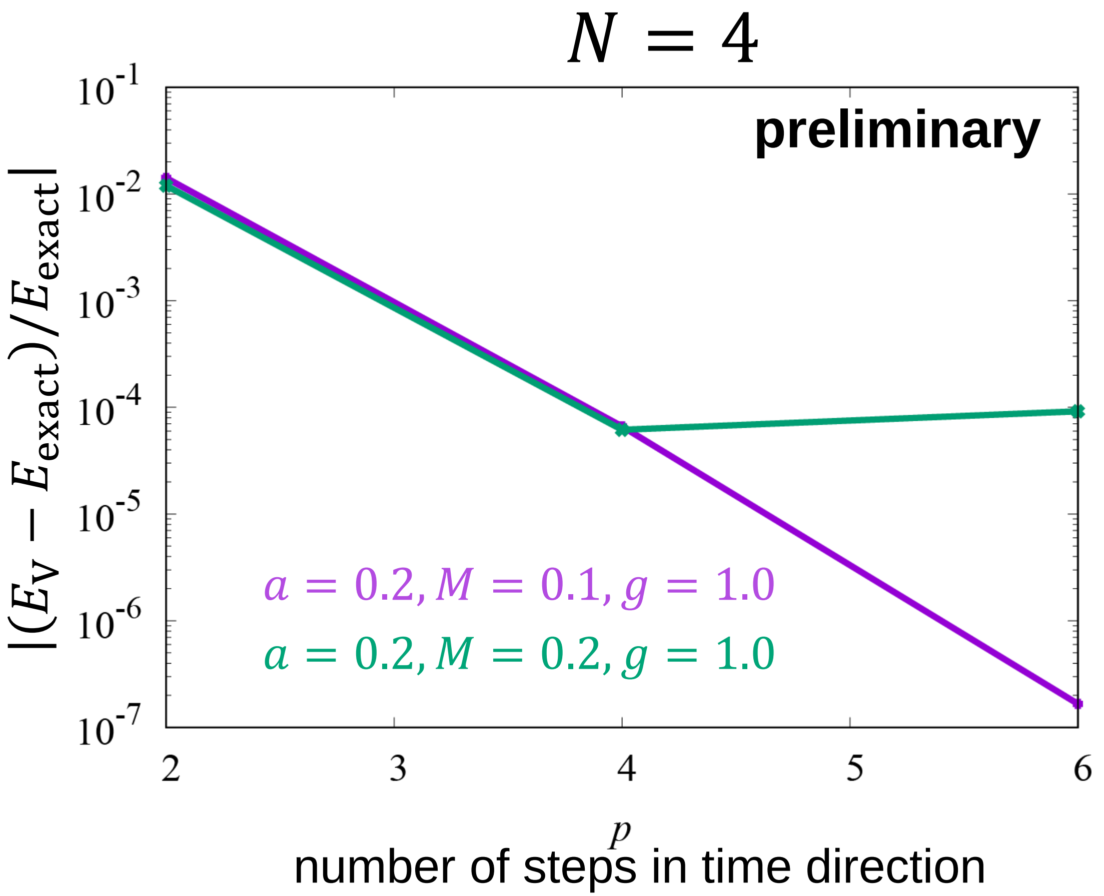
p: number of steps in time direction

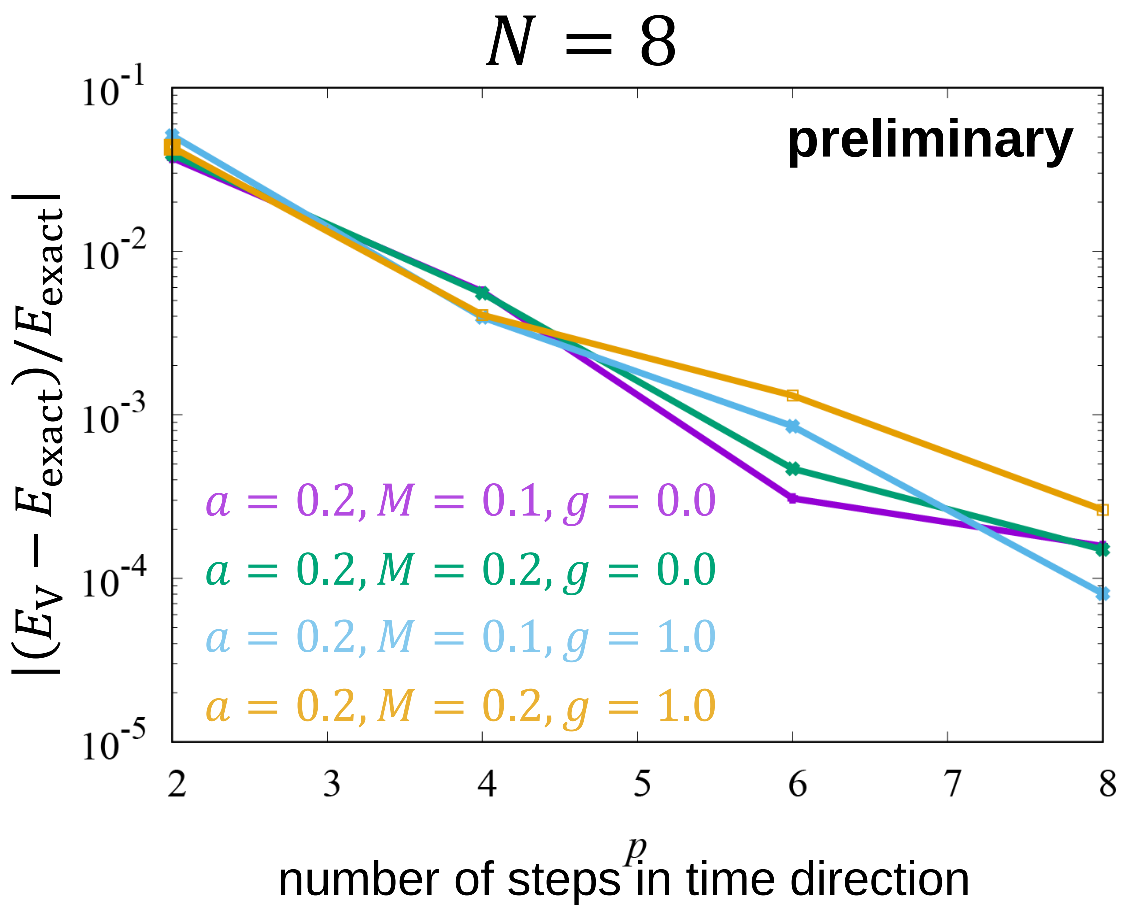
<u>Real-time evolution</u>

dt: step width of time

Contents

Prepare initial state by Hamiltonian variational algorithm





- ✓ Number of variational parameters $=3p$
- ✓ To accurately calculate the initial state with larger N, one needs to take larger p (number of variational parameters.)
- ✓ Accuracy of initial state also depends on other parameters (M and g).

Real time evolution (w/o theta-term) $N = 4, \theta = 0$

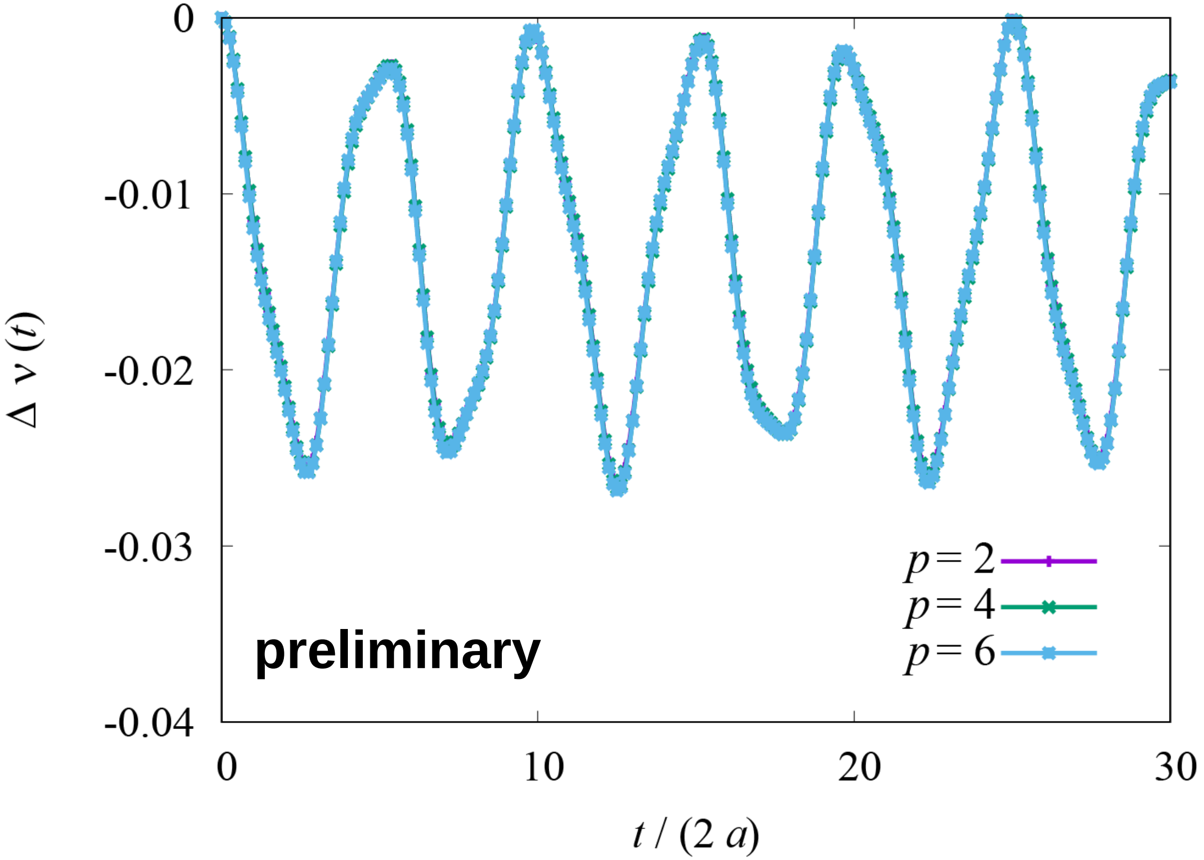
Initial state

$$a = 0.2, M = 0.1, g = 0$$

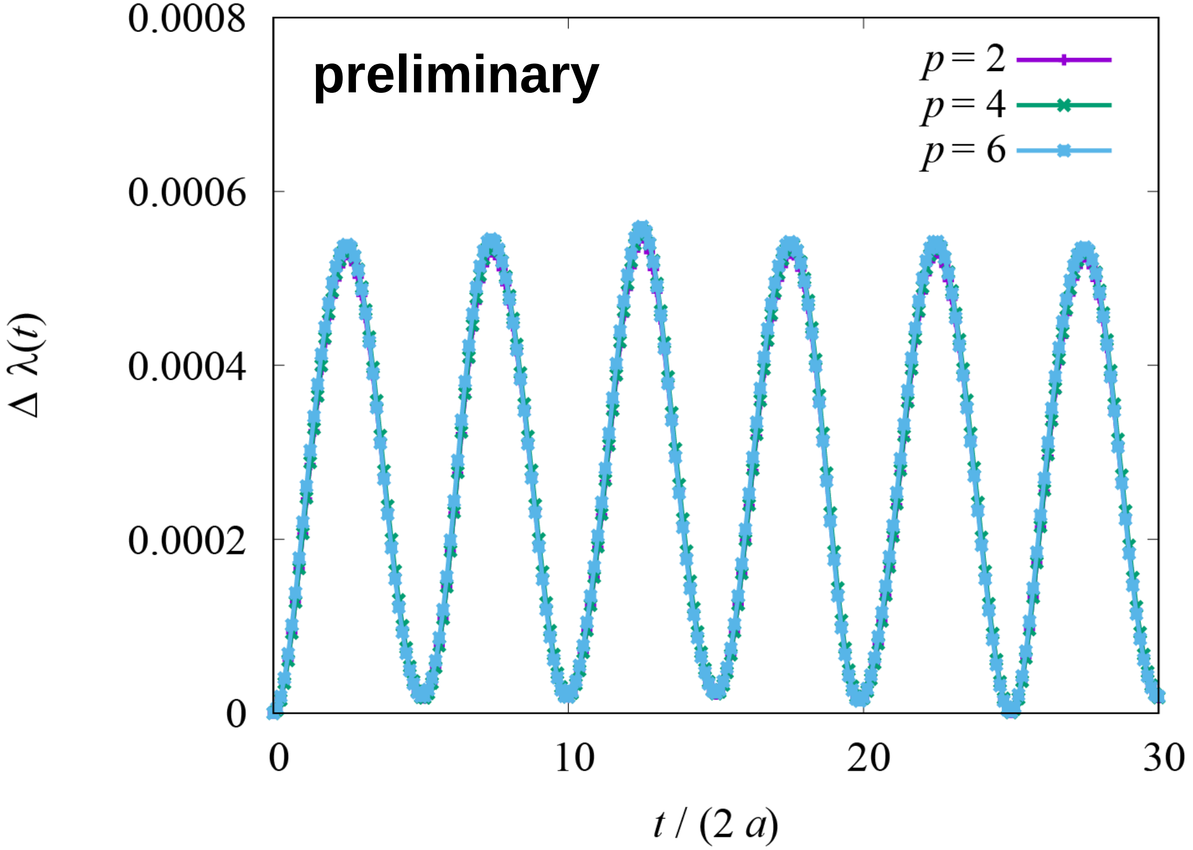
Real-time evolution

$$a = 0.2, M = 0.1, g = 1$$

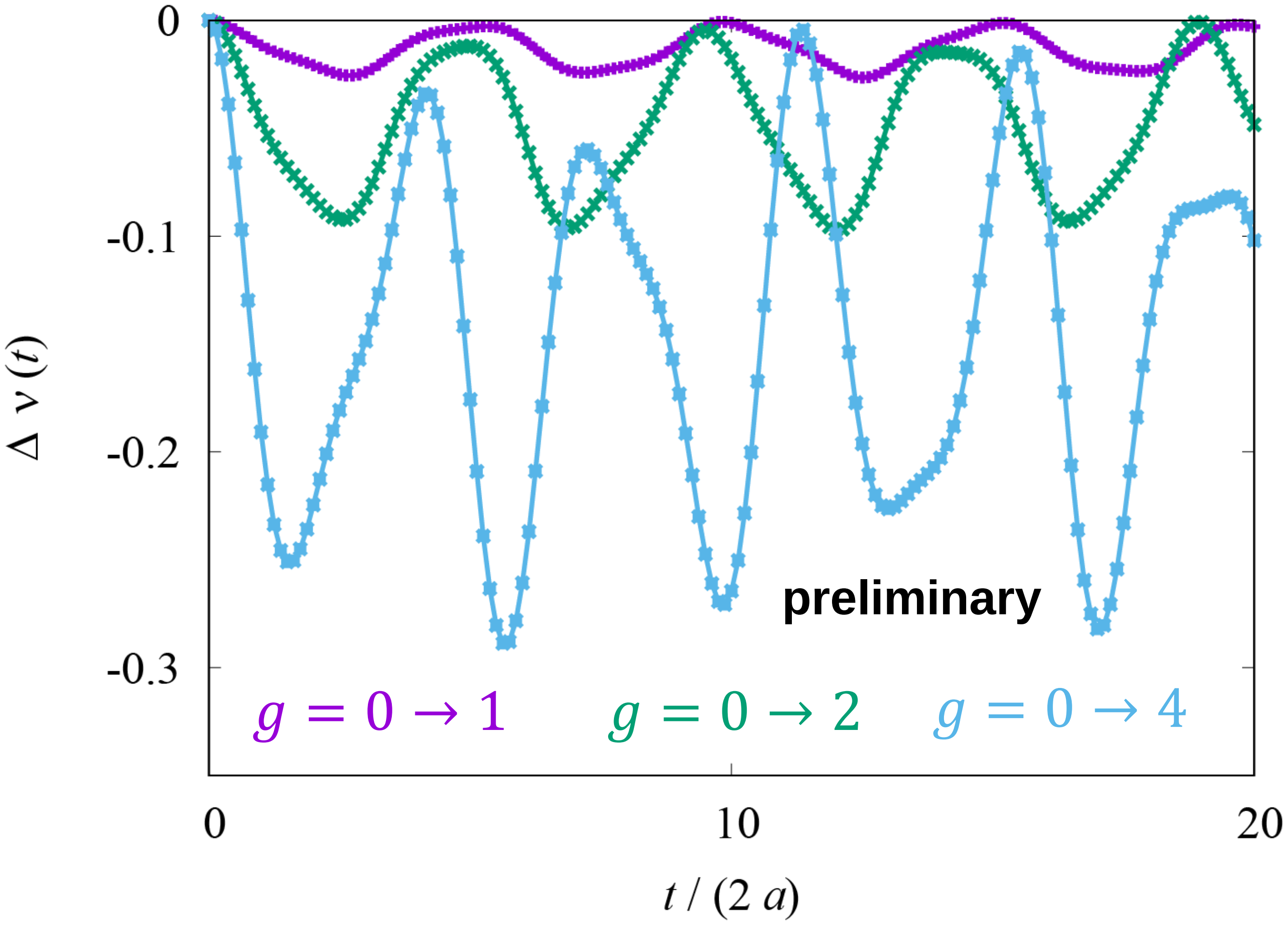
✓ particle number density



✓ vacuum persistent amplitude



Real time evolution (w/o theta-term) $N = 4, \theta = 0$



$a = 0.2, M = 0.1$

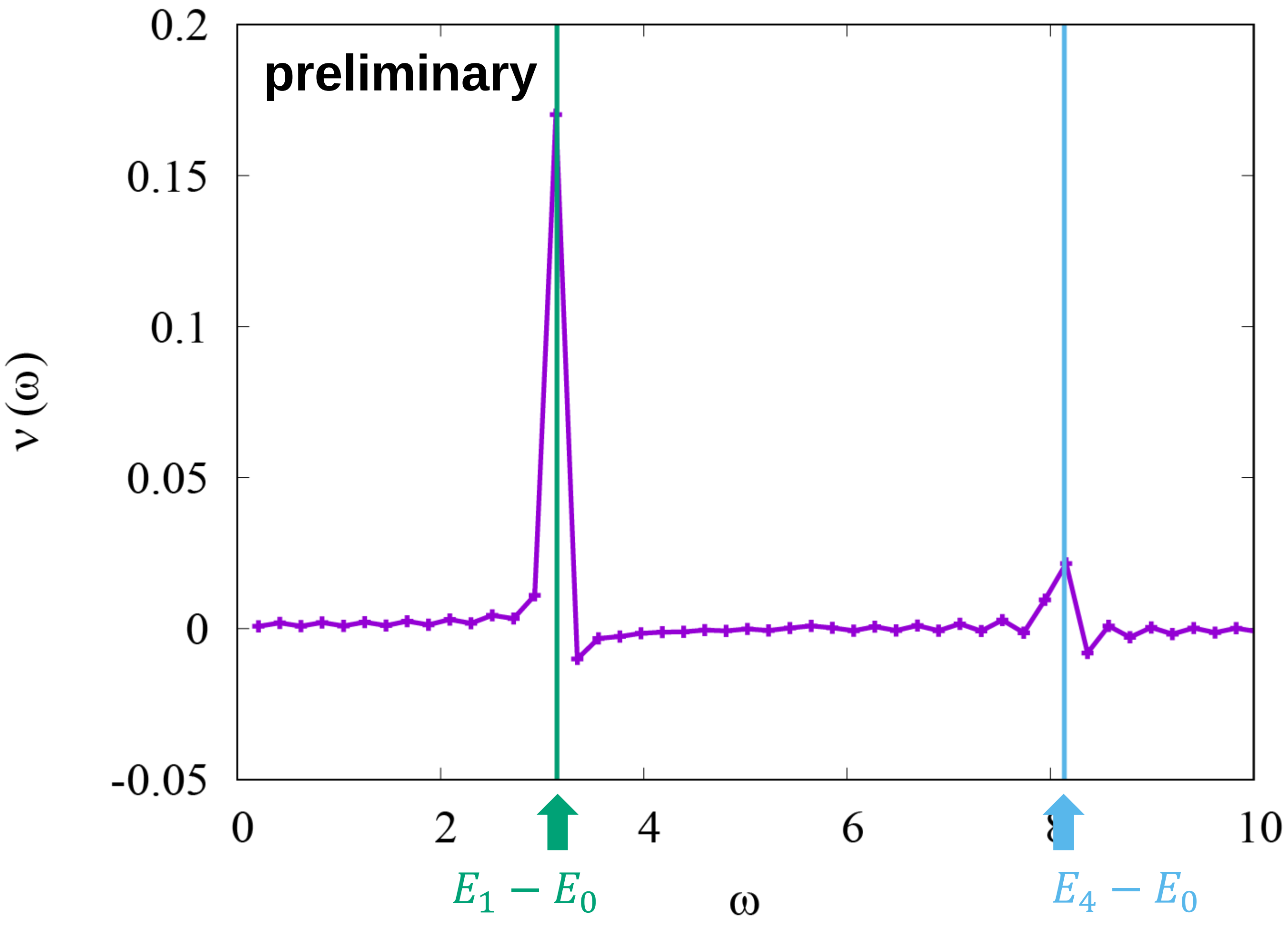
- ✓ Frequency of $\nu(t)$ depends on g of target Hamiltonian H.
- ✓ Amplitude of $\nu(t)$ increases as increasing g of target Hamiltonian H.
- ✓ Frequency should depend on the energy eigenvalue of H.

Particle number density: Fourier transformation

Initial state: $a = 0.2, M = 0.1, g = 0$

Real-time evolution: $a = 0.2, M = 0.1, g = 1$

$$N = 4, \theta = 0$$



step width of time: $dt = 0.05$

Number of steps: $M_{\mathrm{Time}} = 300$

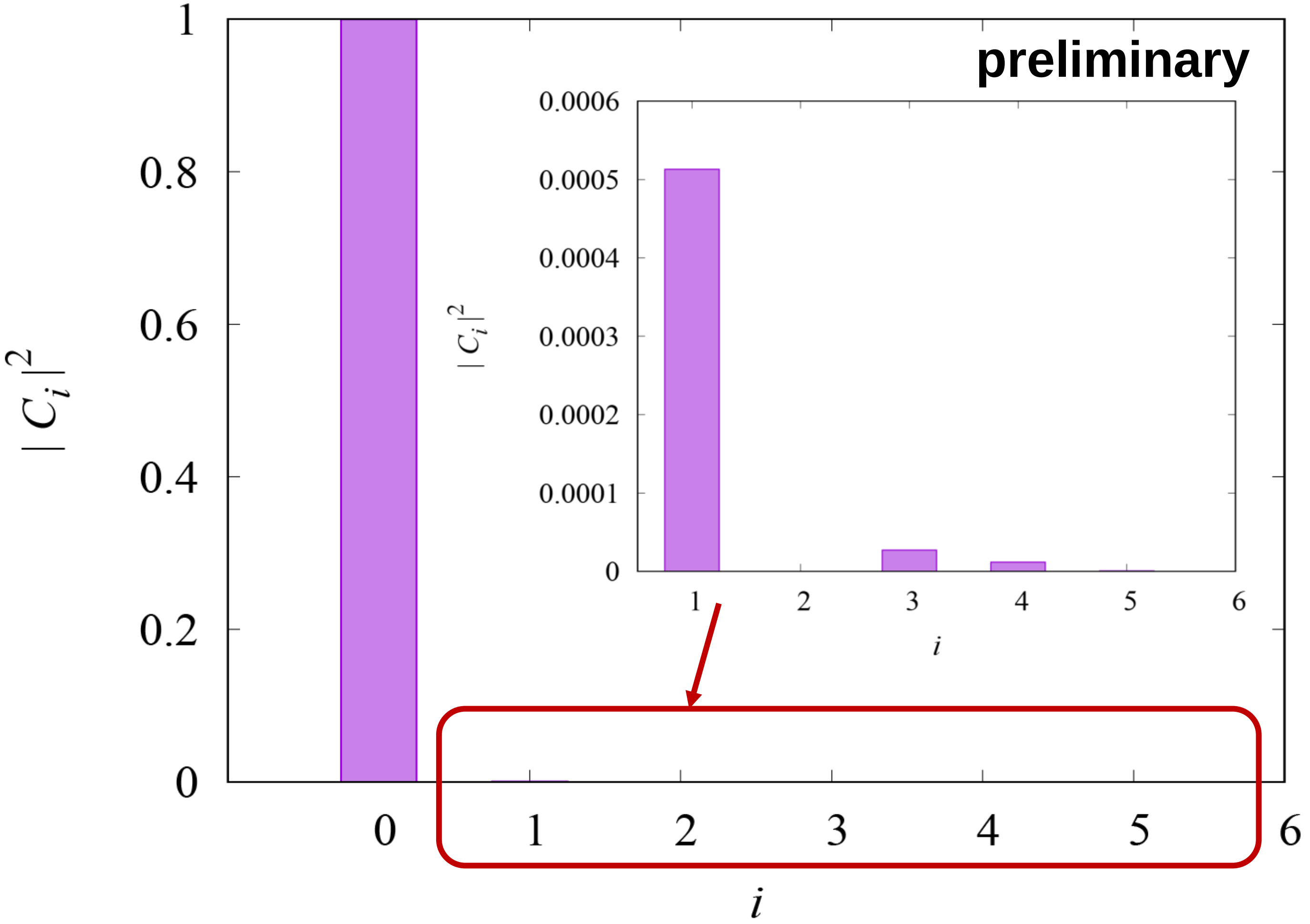
Simulation time : $t_{\max}/(2\mathrm{a}) = 37.5$

- ✓ To get high resolution of ω, one needs long-time simulation.
- ✓ $\omega = E_1 - E_0, E_4 - E_0$?
  →compare with the exact diagonalization

Exact diagonalization: initial state

Initial state: $a = 0.2, M = 0.1, g = 0$

Real-time evolution: $a = 0.2, M = 0.1, g = 1$



$$N = 4, \theta = 0$$

$$\nu(\omega) = \sum_{i,j} \eta_{ij} \delta\left(\omega - E_i + E_j\right)$$

$$\eta_{ij} = \frac{1}{N} \sum_{n=0}^{N-1} \langle \phi_j | C_j^* \rho_n C_i | \phi_i \rangle$$

$$|\psi(t=0)\rangle = \sum_i C_i |\phi_i\rangle$$

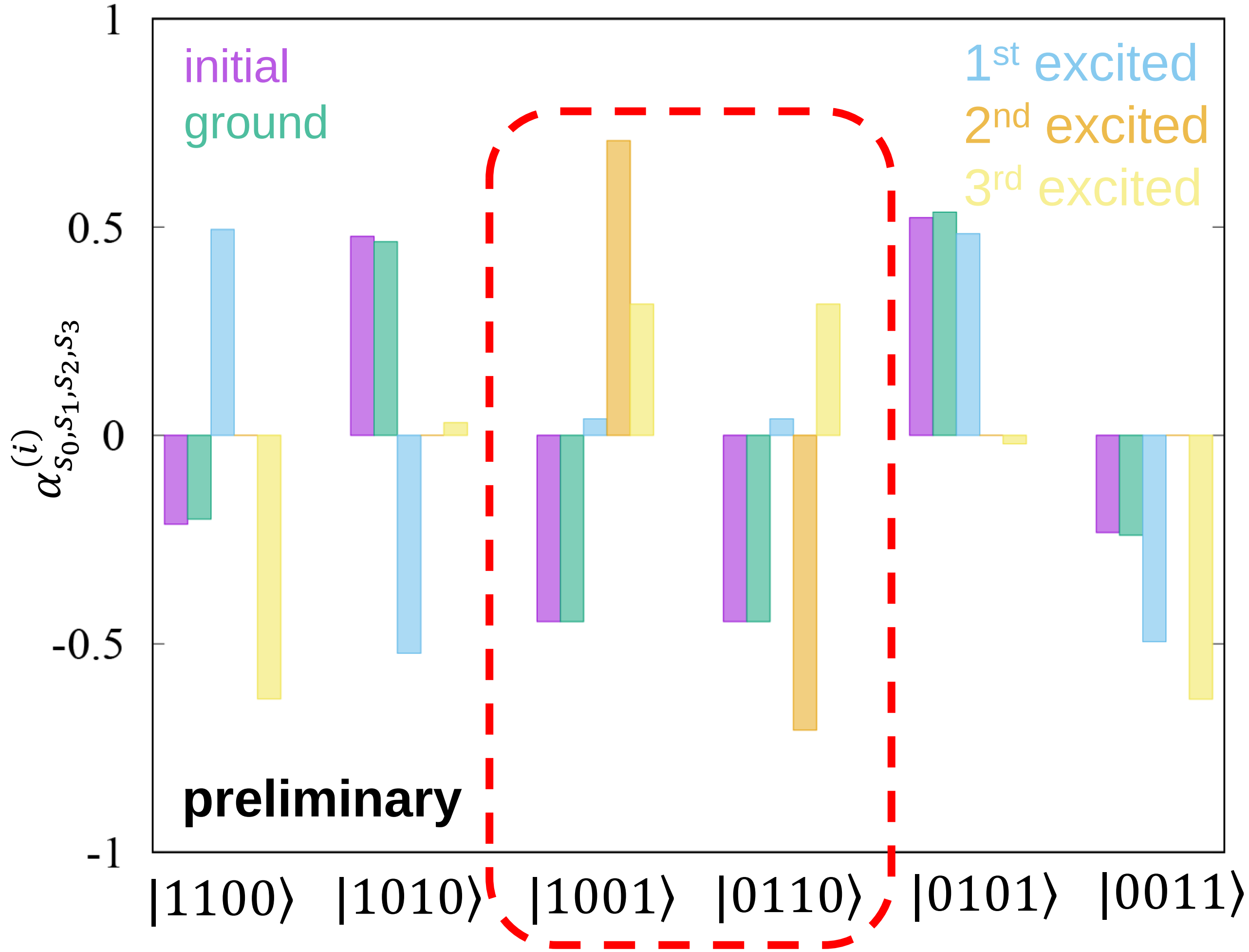
$$H|\phi_i\rangle = E_i |\phi_i\rangle$$

- ✓ Initial state consists of ground state, 1st , 3rd , and 4th excited states of H.
- ✓ Why is not the 2nd excited state included in initial state?

Exact diagonalization: state vector

Initial state: $a = 0.2, M = 0.1, g = 0$

Real-time evolution: $a = 0.2, M = 0.1, g = 1$

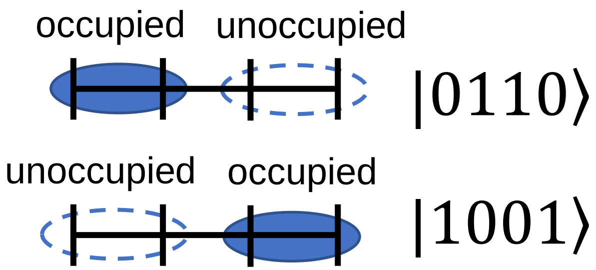


$$N = 4, \theta = 0$$

$$|\phi_i\rangle = \sum_{s_0,s_1,s_2,s_3} \alpha^{(i)}_{s_0,s_1,s_2,s_3} \, |s_3 s_2 s_1 s_0\rangle$$

$$|\phi_2\rangle \simeq \frac{1}{\sqrt{2}}(|1001\rangle - |0110\rangle)$$

$\alpha^{(i)}_{0110} \simeq \alpha^{(i)}_{1001}$ in other states



2nd excited state : CP odd

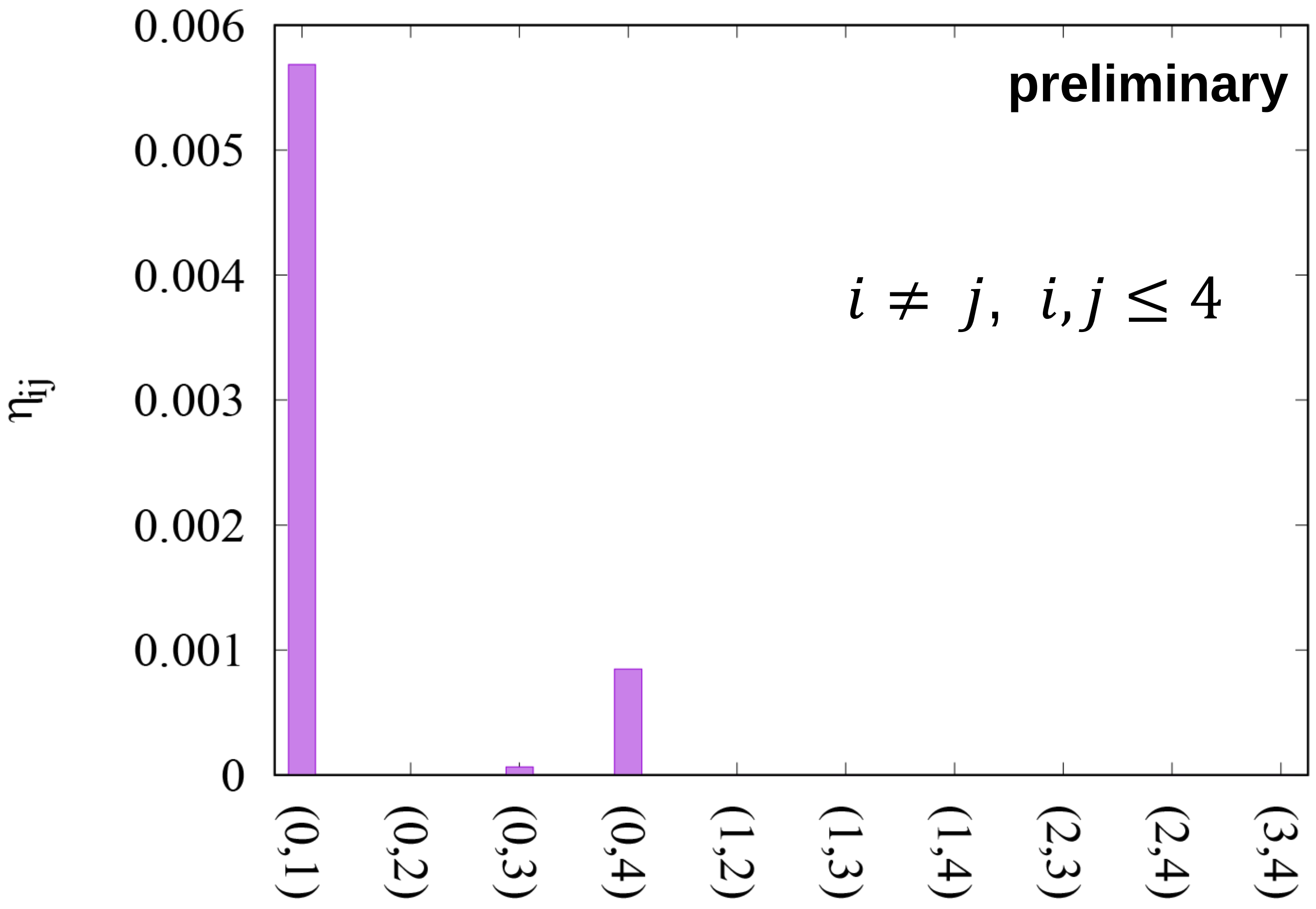
Other states : CP even

Exact diagonalization: η_{ij}

Initial state: $a = 0.2, M = 0.1, g = 0$

Real-time evolution: $a = 0.2, M = 0.1, g = 1$

$N = 4, \theta = 0$



$$\nu(\omega) = \sum_{i,j} \eta_{ij} \delta\left(\omega - E_i + E_j\right)$$

$$\eta_{ij} = \frac{1}{N} \sum_{n=0}^{N-1} \langle \phi_j | C_j^* \rho_n C_i | \phi_i \rangle$$

Contributions from

$|\phi_0\rangle \leftrightarrow |\phi_4\rangle$

$|\phi_0\rangle \leftrightarrow |\phi_1\rangle$

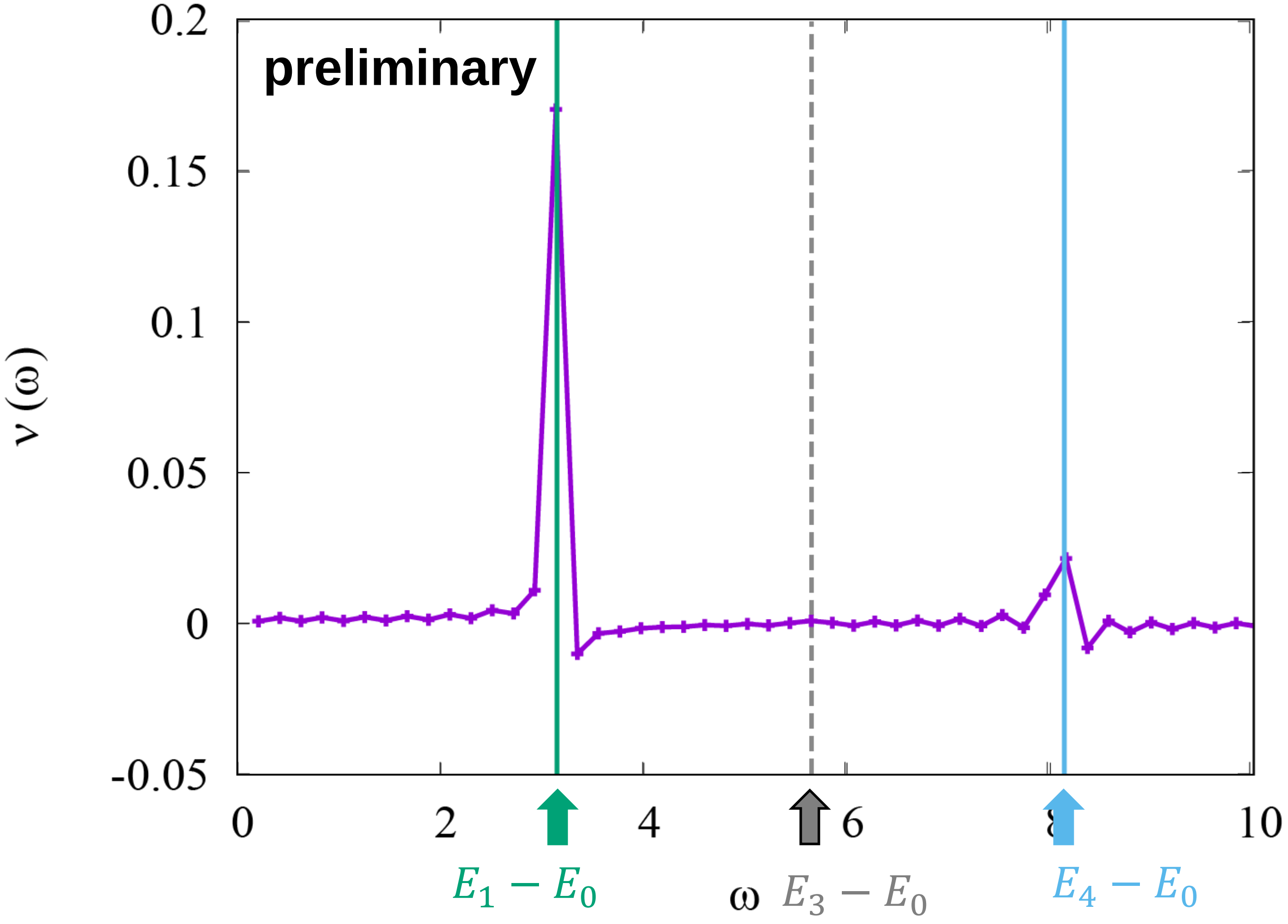
are dominant.

($|\phi_0\rangle \leftrightarrow |\phi_3\rangle$)

Exact diagonalization: η_{ij}

Initial state: $a = 0.2, M = 0.1, g = 0$

Real-time evolution: $a = 0.2, M = 0.1, g = 1$



$N = 4, \theta = 0$

$$\nu(\omega) = \sum_{i,j} \eta_{ij} \delta\left(\omega - E_i + E_j\right)$$

$$\eta_{ij} = \frac{1}{N} \sum_{n=0}^{N-1} \langle \phi_j | C_j^* \rho_n C_i | \phi_i \rangle$$

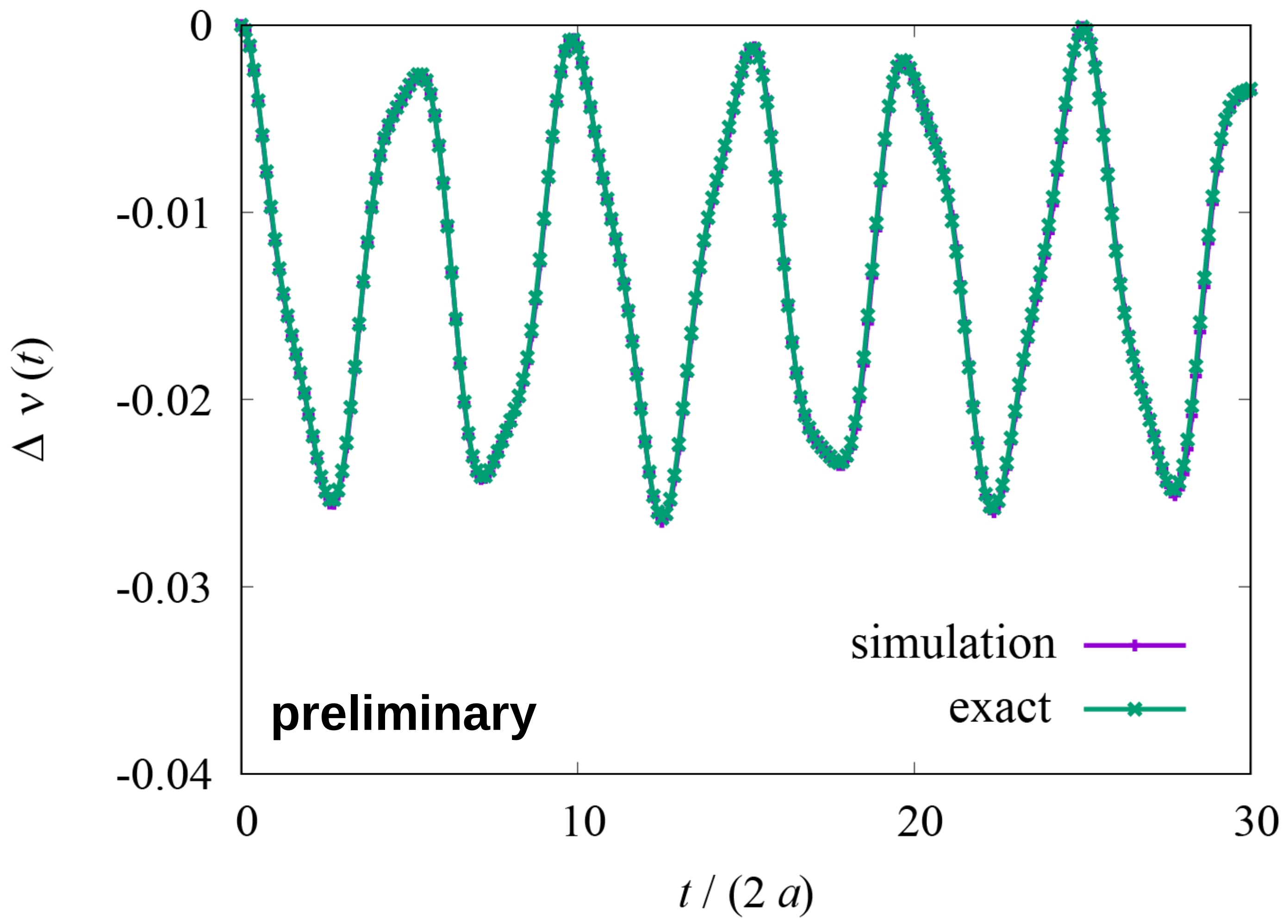
- ✓ $\omega = E_1 - E_0, E_4 - E_0$
- ✓ We can not see a peak structure corresponding to $\omega = E_3 - E_0$ in $\nu(\omega)$.

Comparison between quantum simulation and exact result

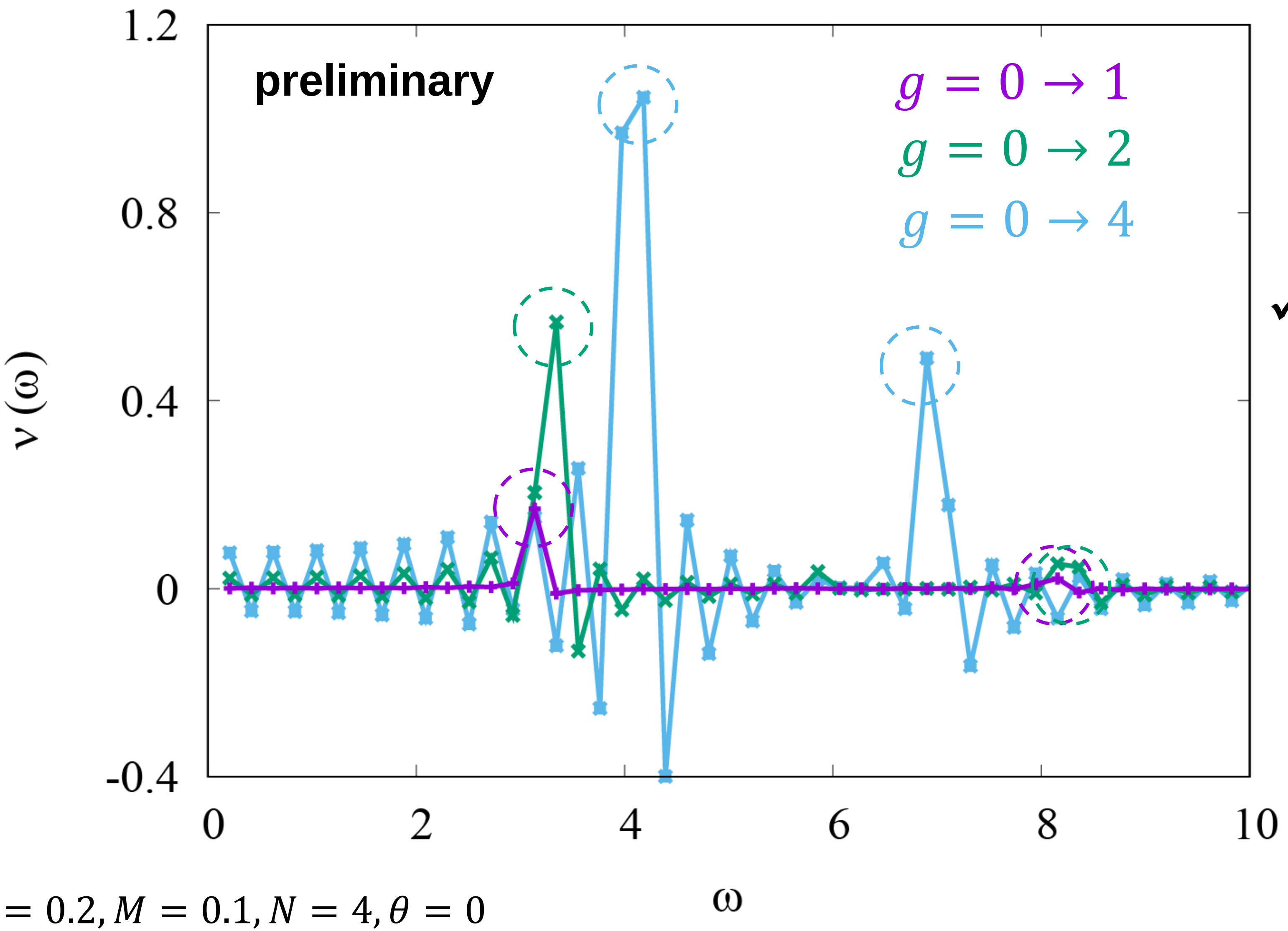
Initial state: $a = 0.2, M = 0.1, g = 0$

Real-time evolution: $a = 0.2, M = 0.1, g = 1$

$N = 4, \theta = 0$



g dependence of $\nu(t)$: Fourier component



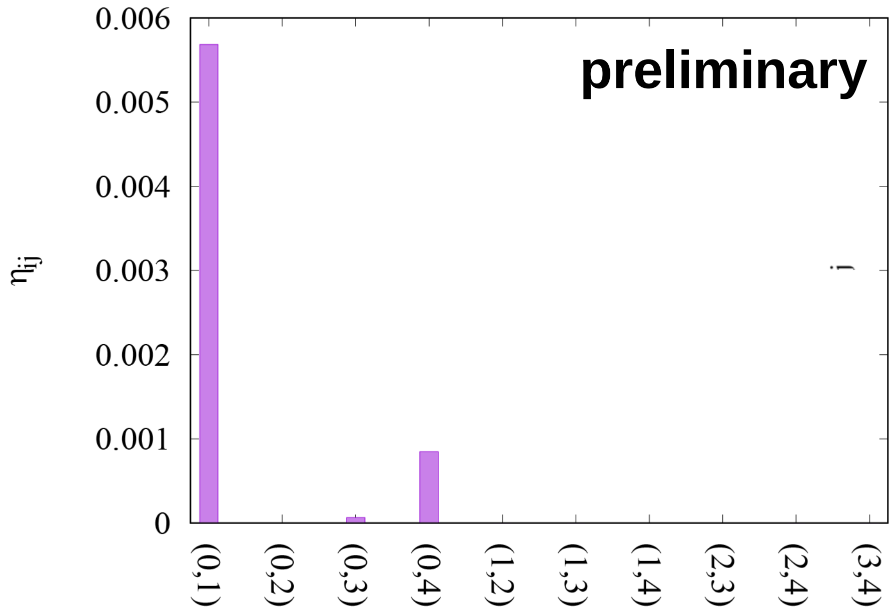
✓ position of peaks depend on g of target Hamiltonian.

$a = 0.2, M = 0.1, N = 4, \theta = 0$

g dependence of $\nu(t)$: η_{ij}

$$\nu(\omega) = \sum_{i,j} \eta_{ij} \delta(\omega - E_i + E_j) \qquad \eta_{ij} = \frac{1}{N} \sum_{n=0}^{N-1} \langle \phi_j | C_j^* \rho_n C_i | \phi_i \rangle$$

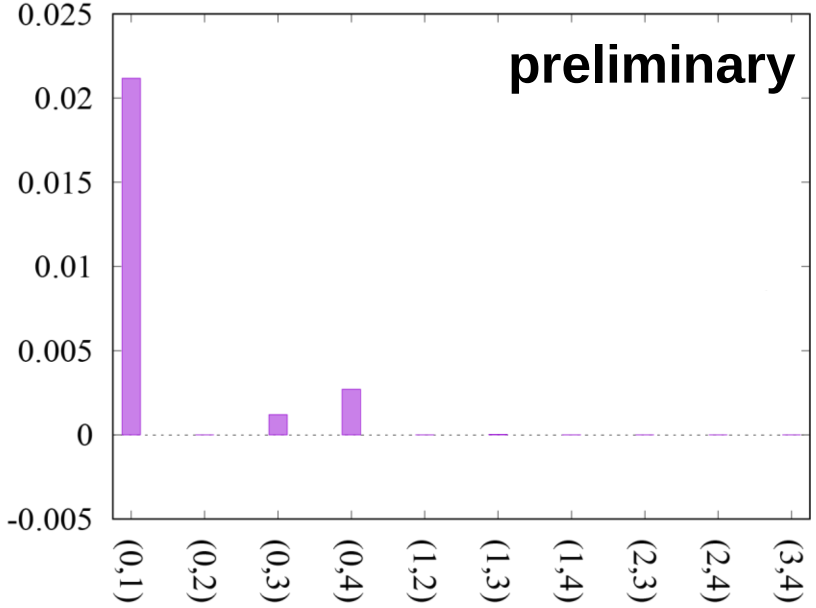
$g = 0 \to 1$



$|\phi_0\rangle \leftrightarrow |\phi_1\rangle$

$|\phi_0\rangle \leftrightarrow |\phi_4\rangle$

$g = 0 \to 2$

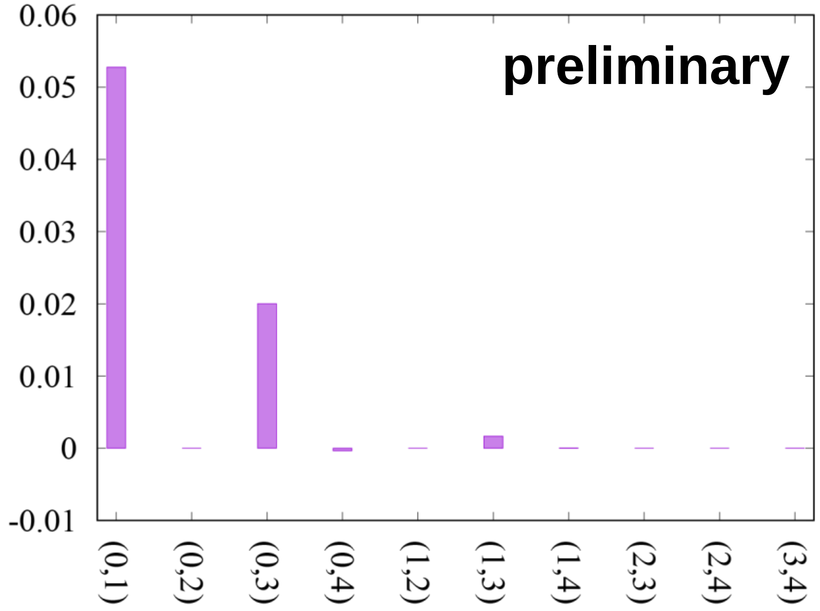


$|\phi_0\rangle \leftrightarrow |\phi_1\rangle$

$|\phi_0\rangle \leftrightarrow |\phi_4\rangle$

$(|\phi_0\rangle \leftrightarrow |\phi_3\rangle)$

$g = 0 \to 4$



$|\phi_0\rangle \leftrightarrow |\phi_1\rangle$

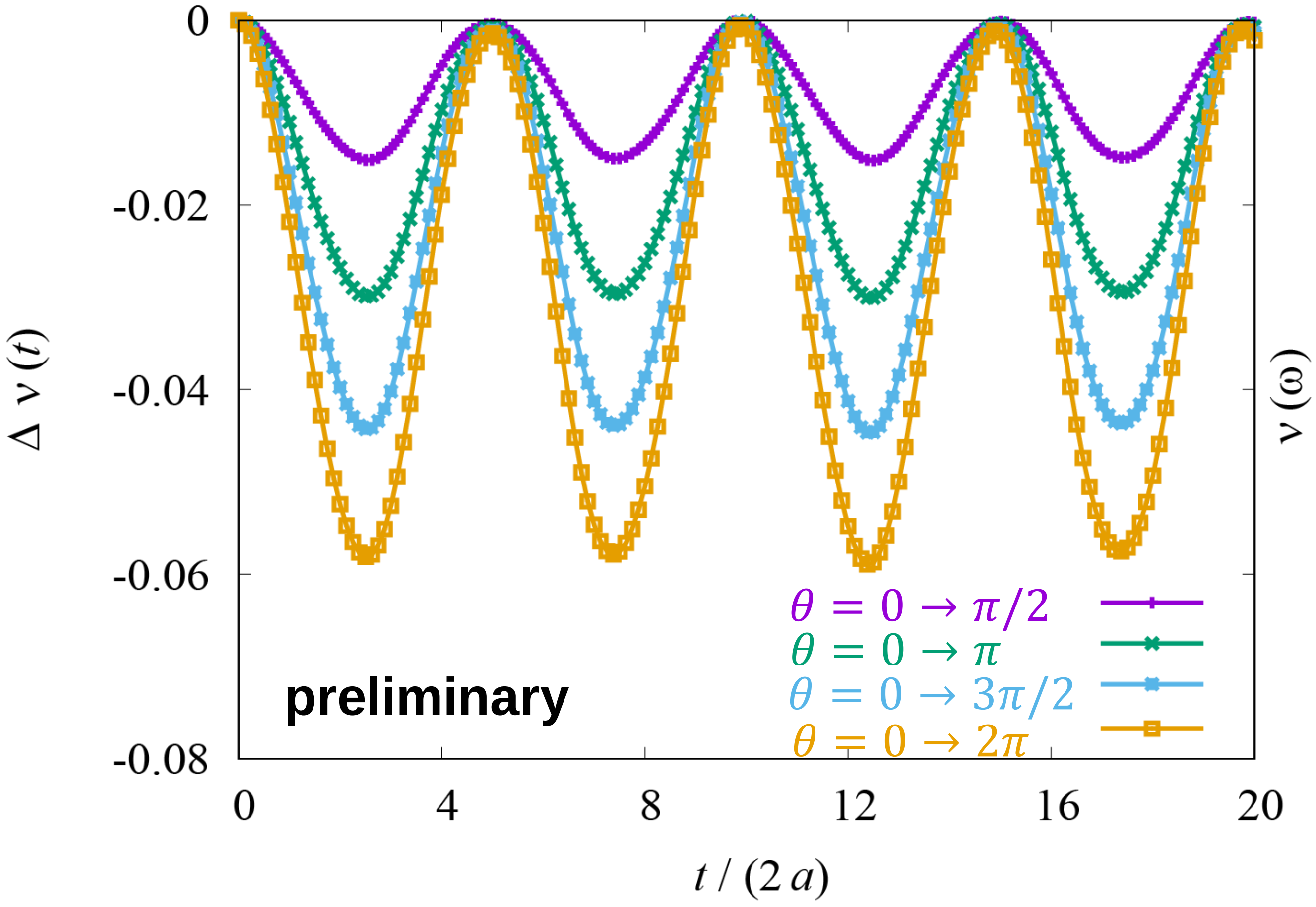
$|\phi_0\rangle \leftrightarrow |\phi_3\rangle$

$(|\phi_1\rangle \leftrightarrow |\phi_3\rangle)$

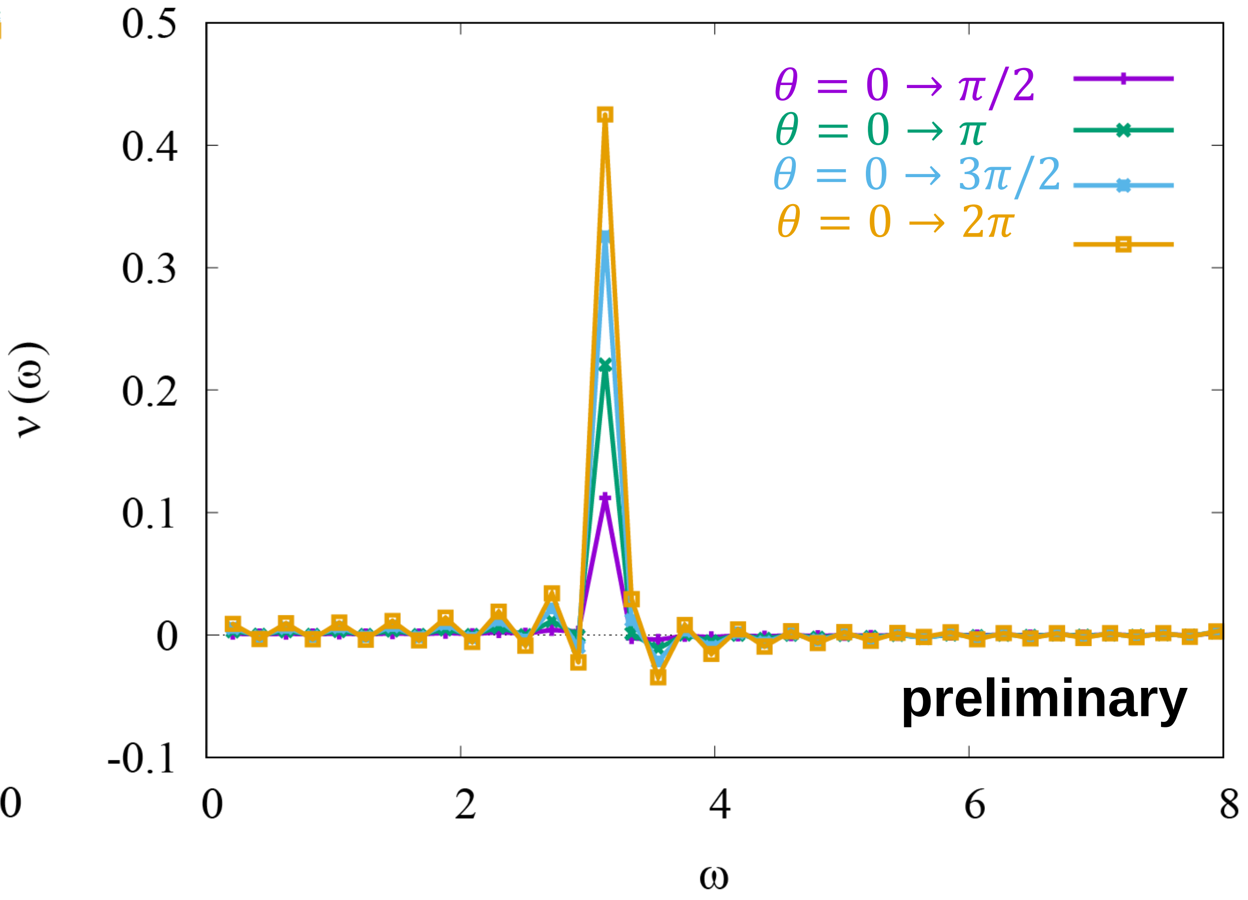
$a = 0.2, M = 0.1, N = 4, \theta = 0$

“Chiral quench” ($\theta = 0 \to$ finite) $a = 0.2, M = 0.1, g = 1, N = 4$

✓ $\nu(t)$



✓ $\nu(\omega)$

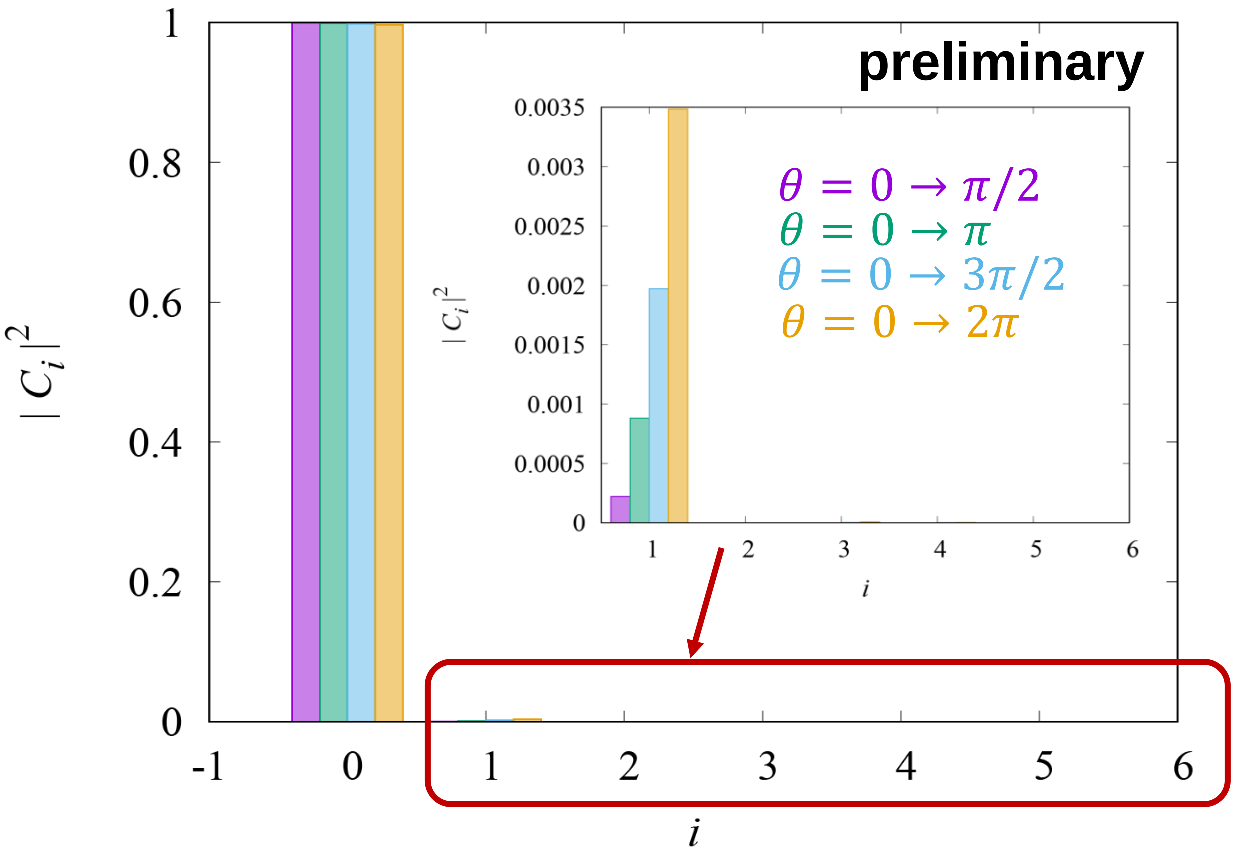


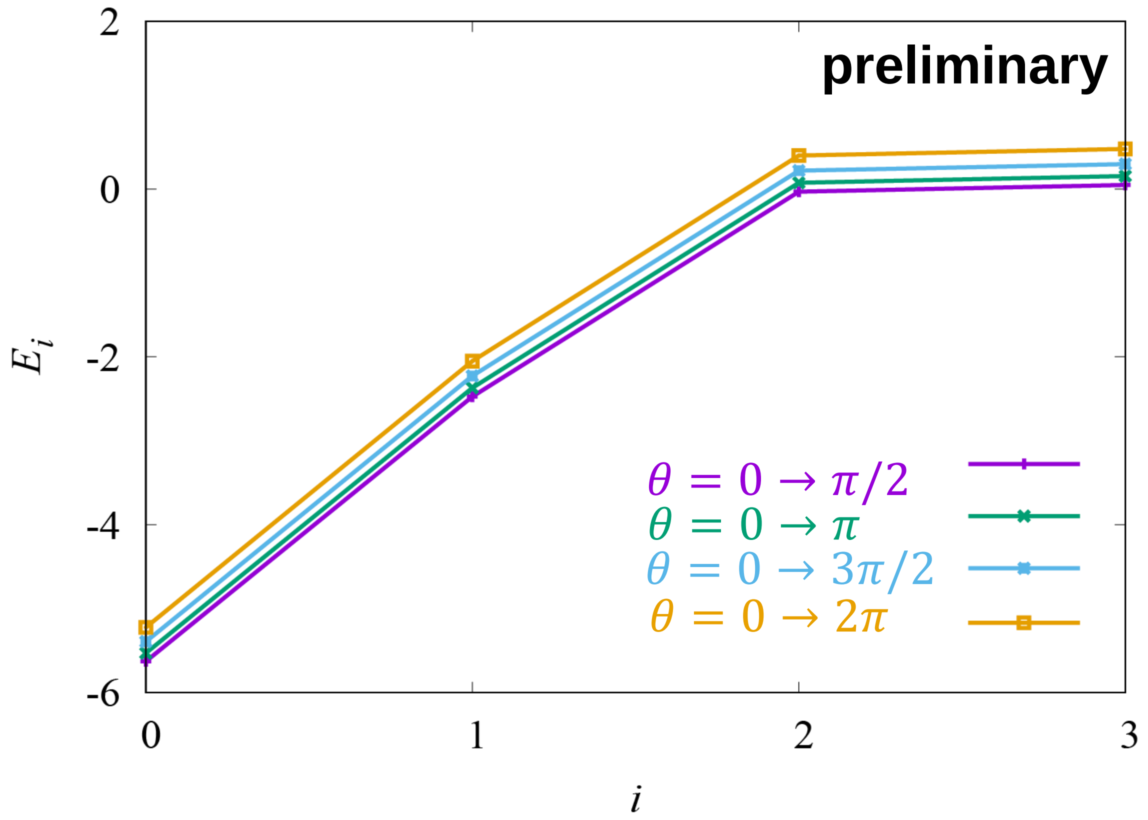
✓ Frequency of $\nu(t)$ does not strongly depend on θ.

"Chiral quench" ($\theta = 0 \rightarrow$ finite) $a = 0.2, M = 0.1, g = 1, N = 4$

$$|\psi(t=0)\rangle = \sum_i C_i |\phi_i\rangle$$

$$H|\phi_i\rangle = E_i|\phi_i\rangle$$





- ✓ Energy difference (= frequency of $\nu(t)$) is not strongly affected by changing θ
- ✓ (Because of light mass or finite size effects?)

Contents

Conclusion & Future works

- ✓ We investigate real time dynamics of particle number density $\nu(t)$ in (1+1)-D Schwinger model with topological θ term.
- ✓ From the time dependence of $\nu(t)$, we can extract information of excited states.
- ✓ It depends on the choice of initial state and target Hamiltonian which states dominantly contribute to the dynamics of $\nu(t)$.
- ✓ We calculate $\nu(t)$ with "chiral quench" ($\theta = 0 \to$ finite).
  So far, any signs of phase transition are not seen...

Future works

- ✓ What is the best choice of initial state for getting information of excitation spectrum?
- ✓ Can we see the phase transition from the real-time dynamics?
- ✓ Other quantities, large volume system, etc…