EFFICIENT HMC FOR PFAFFIAN QUANTUM MONTE CARLO

JULY 2026 | THOMAS HAUSCHILD | FORSCHUNGSZENTRUM JÜLICH

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BRIDGING QCD AND CONDENSED MATTER

What is our goal?

Treat strongly interacting condensed matter systems in an unbiased manner, e.g. the spinless tV-model:

$$-S/\beta = \underbrace{\sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \mathrm{H.c.}\right] - \mu\sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1} V c_j^\dagger c_j c_{j+1}^\dagger c_{j+1}}_{H_2}$$

Quartic interactions

No gauge field coupling

L : # fermionic sites

Hubbard-Stratonovich transformation:

$$\exp\left(Vc_j^\dagger c_j c_{j+1}^\dagger c_{j+1}\right) \sim \exp\left(\frac{V}{2}\left[c_j^\dagger c_j + c_{j+1}^\dagger c_{j+1}\right]^2 - \frac{V}{2}\left[c_j^\dagger c_j + c_{j+1}^\dagger c_{j+1}\right]\right) \sim \int \mathrm{d}\phi_j \exp\left(-\frac{\phi_j^2}{2V}\right)\exp\left(\phi_j\left[c_j^\dagger c_j + c_{j+1}^\dagger c_{j+1}\right]\right)$$

BRIDGING QCD AND CONDENSED MATTER

What is our goal?

Treat strongly interacting condensed matter systems in an unbiased manner, e.g. the spinless tV-model:

$$-S_{\text{eff}}/\beta = \underbrace{\sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \mathrm{H.c.}\right] - \left(\mu + \frac{V}{2}\right)\sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1}\frac{-\phi_j^2}{2V} + \phi_j\left[c_j^\dagger c_j + c_{j+1}^\dagger c_{j+1}\right]}_{H_2}$$

Now we also need to integrate over the auxiliary fields

L : # fermionic sites

N_t : # time slices

$$Z = \mathrm{Tr}\left\{e^{-\beta S}\right\}$$

$$\approx \int \mathscr{D}(\phi)\exp\left(-\frac{\phi^2}{2m}\right)\mathrm{Tr}\left\{\prod_{t=1}^{N_t}\exp\left(-\vec{c}^{\,\dagger}A\vec{c}\right)\exp\left(-\vec{c}^{\,\dagger}B\left[\phi^t\right]\vec{c}\right)\right\}$$

$$= \int \mathscr{D}(\phi)\exp\left(-\frac{\phi^2}{2m}\right)\det\left(\underbrace{I + e^{-A}e^{-B[\phi^1]}e^{-A}e^{-B[\phi^2]}\ldots e^{-A}e^{-\tilde{B}[\phi^{N_t}]}}_{:=M[\phi]}\right)$$

$M : L\times L$

$2N_t$ matrix multiplications

➡ $\mathcal{O}\left(N_t L^3\right)$

BRIDGING QCD AND CONDENSED MATTER: DQMC

What is our goal?

Treat strongly interacting condensed matter systems in an unbiased manner, e.g. the spinless tV-model:

$$-S_{\text{eff}} = -\frac{\boldsymbol{\phi}^2}{2V} + \log\left(\det\left[M\right]\right)$$

Now we also need to integrate over the auxiliary fields

$$\begin{aligned} Z &= \operatorname{Tr}\left\{e^{-\beta S}\right\} \\ &\approx \int \mathscr{D}\left(\phi\right) \exp\left(-\frac{\boldsymbol{\phi}^2}{2m}\right) \operatorname{Tr}\left\{\prod_{t=1}^{N_t} \exp\left(-\vec{c}^{\dagger} A \vec{c}\right) \exp\left(-\vec{c}^{\dagger} B\left[\phi^t\right] \vec{c}\right)\right\} \\ &= \int \mathscr{D}\left(\phi\right) \exp\left(-\frac{\boldsymbol{\phi}^2}{2m}\right) \det\left(\underbrace{I + e^{-A} e^{-B[\phi^1]} e^{-A} e^{-B[\phi^2]} \ldots e^{-A} e^{-\tilde{B}[\phi^{N_t}]}}_{:=M[\boldsymbol{\phi}]}\right) \end{aligned}$$

L : # fermionic sites

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$2N_t$ matrix multiplications

➔ $\mathcal{O}\left(N_t L^3\right)$

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INGREDIENTS FOR DETERMINANT QMC

Via HMC sample from:

$$Z = \int \mathscr{D}(\phi) \exp\left(-\frac{\boldsymbol{\phi}^2}{2m}\right) \det\left(M[\boldsymbol{\phi}]\right)$$

Force term:

$$\frac{\partial S_{\text{eff}}}{\partial \phi_x^t} \propto \left[R_{t+1\ldots N_t} M^{-1} R_{1\ldots t}\right]_{xx}$$

Correlator/Measurements

$$C_{ij}(t) = \left\langle c_i(t) c_j^\dagger \right\rangle \propto \left[M^{-1} R_{1\ldots t}\right]_{ij}$$

$$M[\boldsymbol{\phi}] = I + \underbrace{e^{-A}}_{:=\mathscr{K}} \underbrace{e^{-B[\phi^1]}}_{:=\Phi_1} e^{-A} e^{-B[\phi^2]} \ldots e^{-A} e^{-B[\phi^{N_t}]}$$

$$R_{a\ldots b} = \mathscr{K}\Phi_a \mathscr{K}\Phi_{a+t} \ldots \mathscr{K}\Phi_{b-1} \mathscr{K}\Phi_b$$

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$$R_{a\ldots b} = \mathscr{K}\Phi_a \mathscr{K}\Phi_{a+t} \ldots \mathscr{K}\Phi_{b-1} \mathscr{K}\Phi_b$$

When evaluating force terms correlators come for free

Luu, Ostmeyer, Sinilkov & Temmen, "Stable Determinant Monte Carlo Simulations", arXiv:2604.00815 (2026)

MOTIVATION FOR PFAFFIAN QMC

Pfaffian quantum Monte Carlo: solution to Majorana sign ambiguity and applications

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Institute for Advanced Study, Tsinghua University, Beijing 100084, China
(Dated: August 21, 2024)

Determinant quantum Monte Carlo (DQMC), formulated in complex-fermion representation, has played a key role in studying strongly-correlated fermion systems. However, its applicability is limited due to the requirement of particle-number conservation after Hubbard-Stratonovich transformation. In going beyond the conventional DQMC, one encouraging development occurred when Majorana fermions were introduced for QMC [1, 2]. But in previous Majorana-based QMC, Boltzmann weight is determined often with a sign ambiguity. Here we successfully resolved this ambiguity by deriving a *closed-form* Pfaffian formula for the weight, enabling efficient calculation of the weight with its sign in polynomial time. We call it “Pfaffian quantum Monte Carlo” (PfQMC), which can be applied to generic interacting fermion models. We have successfully employed PfQMC to explore how robust Majorana edge modes in Kitaev chain are against strong interactions. By offering greater flexibility, PfQMC can potentially enhance existing sign-mitigating and approximation methods and help address challenging issues such as the ground-state properties of the doped Hubbard model.

- From 2024
- By Han, Wan, Yao
- Generalization of DQMC
- No HMC implementation

Han, Wan & Yao, “Pfaffian quantum Monte Carlo,” arXiv:2408.10311 (2024)

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MOTIVATION FOR PFAFFIAN QMC

Non-particle-number-conserving terms?

$$-S/\beta = \underbrace{\sum_{j=1}^{L-1} \left[-t c_j^\dagger c_{j+1} \qquad\qquad + \mathrm{H.c.} \right] - \mu \sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1} V c_j^\dagger c_j c_{j+1}^\dagger c_{j+1}}_{H_2}$$

PfQMC advantages:

MOTIVATION FOR PFAFFIAN QMC

Interacting Kitaev Chain:

$$-S/\beta = \underbrace{\sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger + \mathrm{H.c.}\right] - \mu \sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1} V c_j^\dagger c_j c_{j+1}^\dagger c_{j+1}}_{H_2}$$

DQMC Kernels cannot support these:

$$Z = \approx \int \mathscr{D}(\phi) \exp\left(-\frac{\phi^2}{2m}\right) \mathrm{Tr}\left\{\prod_{t=1}^{N_t} \exp\left(-\vec{c}^\dagger A \vec{c}\right) \exp\left(-\vec{c}^\dagger B\left[\phi^t\right]\vec{c}\right)\right\}$$

PfQMC advantages:

1. Can handle non-particle-number-conserving systems

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MOTIVATION FOR PFAFFIAN QMC

Interacting Kitaev Chain:

$$-S/\beta = \underbrace{\sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger + \mathrm{H.c.}\right] - \mu \sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1} V c_j^\dagger c_j c_{j+1}^\dagger c_{j+1}}_{H_2}$$

PfQMC advantages:

1. Can handle non-particle-number-conserving systems
2. Allows additional decoupling channels

Hubbard-Stratonovich transfomation is not unique:

$$H_2 \sim V c_j^\dagger c_j c_{j+1}^\dagger c_{j+1} \sim \frac{V}{2}\left[c_j^\dagger c_j + c_{j+1}^\dagger c_{j+1}\right]^2 \sim -\frac{V}{2}\left[c_j^\dagger c_j - c_{j+1}^\dagger c_{j+1}\right]^2 \sim \frac{V}{2}\left[c_{j+1}^\dagger c_j^\dagger + c_j c_{j+1}\right]^2 \sim -\frac{V}{2}\left[c_{j+1}^\dagger c_j^\dagger - c_j c_{j+1}\right]^2$$

DQMC Kernels cannot support these either:

$$Z = \approx \int \mathscr{D}(\phi) \exp\left(-\frac{\phi^2}{2m}\right) \mathrm{Tr}\left\{\prod_{t=1}^{N_t} \exp\left(-\vec{c}^\dagger A \vec{c}\right) \exp\left(-\vec{c}^\dagger B\left[\phi^t\right]\vec{c}\right)\right\}$$

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MOTIVATION FOR PFAFFIAN QMC

Interacting Kitaev Chain:

$$-S/\beta = \underbrace{\sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger + \mathrm{H.c.}\right] - \mu\sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1} V c_j^\dagger c_j c_{j+1}^\dagger c_{j+1}}_{H_2}$$

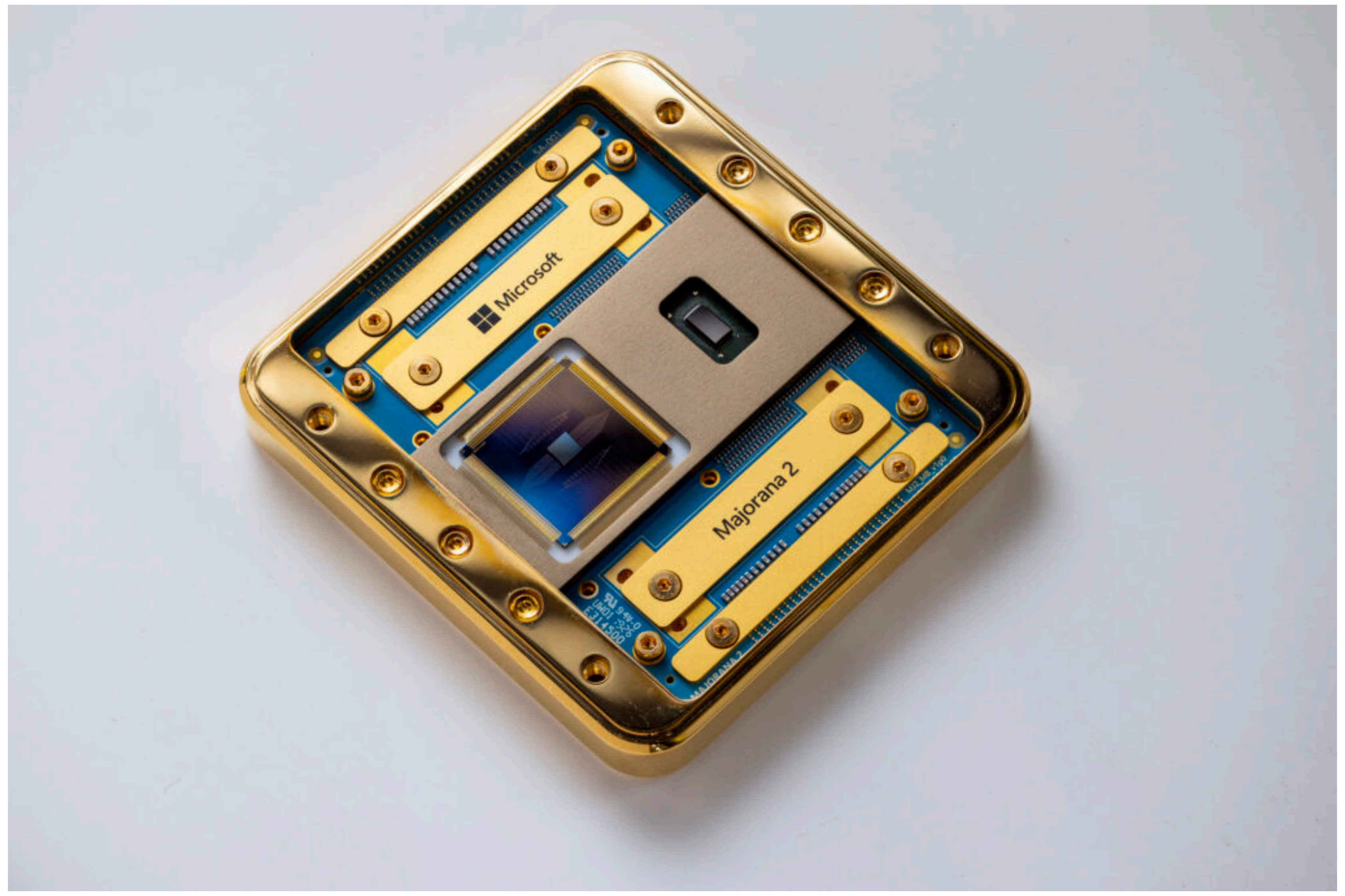
PfQMC advantages:

1. Can handle non-particle-number-conserving systems
2. Allows additional decoupling channels
3. Natural formalism to treat Majorana-physics

The non-interacting model supports Majorana edge states

In some regions the interacting model does too

PfQMC → Access to Majorana correlators



Microsoft press release July 2nd 2026

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MOTIVATION FOR PFAFFIAN QMC WITH HMC

HMC advantages:

1. Global updates
2. Control over acceptance rate
3. Combination with pseudo fermions gives very good scaling

PfQMC advantages:

1. Can handle non-particle-number-conserving systems
2. Allows additional decoupling channels
3. Natural formalism to treat Majorana-physics

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PFAFFIAN QMC LEAP

Double the Hilbert space:

Determinant QMC		Pfaffian QMC
Dirac basis		Bogoliubov - de Gennes basis
$\mathscr{K} = \exp\left(-\vec{c}^{\dagger} A \vec{c}\right)$	$\rightarrow$	$\mathscr{K} = \exp\left(-\frac{1}{2}\begin{bmatrix}\vec{c}^{\dagger}\\ \vec{c}\end{bmatrix}^{\mathrm{T}} A \begin{bmatrix}\vec{c}\\ \vec{c}^{\dagger}\end{bmatrix}\right)$
$\Phi^{t} = \exp\left(-\vec{c}^{\dagger} B[\phi^{t}]\vec{c}\right)$	$\rightarrow$	$(\Phi^{t}) = \exp\left(-\frac{1}{2}\begin{bmatrix}\vec{c}^{\dagger}\\ \vec{c}\end{bmatrix}^{\mathrm{T}} B[\phi^{t}]\begin{bmatrix}\vec{c}\\ \vec{c}^{\dagger}\end{bmatrix}\right)$
$-S_{\mathrm{eff}} = \frac{\boldsymbol{\phi}^{2}}{2V} - \log\left(\det(M)\right)$		$-S_{\mathrm{eff}} = ?$

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PFAFFIAN QMC LEAP

Majorana representation

Transformation:

$$c_j = \frac{1}{2}\left(\gamma_j^{(1)} + i\gamma_j^{(2)}\right)$$

$$c_j^\dagger = \frac{1}{2}\left(\gamma_j^{(1)} - i\gamma_j^{(2)}\right)$$

$$\Rightarrow \begin{bmatrix} \vec{c} \\ \vec{c}^\dagger \end{bmatrix} = \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix} I & +iI \\ I & -iI \end{bmatrix}}_{:=U} \begin{bmatrix} \vec{\gamma}^{(1)} \\ \vec{\gamma}^{(2)} \end{bmatrix}$$

Properties:

- Hermitian $\gamma_i^a = \left(\gamma_i^a\right)^\dagger$
- Clifford algebra $\left\{\gamma_i^a, \gamma_j^b\right\} = 2\delta_{ab}\delta_{ij}$

Similarity transform:

Pfaffian QMC

Bogoliubov - de Gennes basis

$$\mathscr{K} = \exp\left(-\frac{1}{2}\begin{bmatrix} \vec{c}^\dagger \\ \vec{c} \end{bmatrix}^{\mathrm{T}} A \begin{bmatrix} \vec{c} \\ \vec{c}^\dagger \end{bmatrix}\right)$$

$$(\Phi^t) = \exp\left(-\frac{1}{2}\begin{bmatrix} \vec{c}^\dagger \\ \vec{c} \end{bmatrix}^{\mathrm{T}} B[\phi^t] \begin{bmatrix} \vec{c} \\ \vec{c}^\dagger \end{bmatrix}\right)$$

$$-S_{\mathrm{eff}} = ?$$

$\rightarrow$

$\rightarrow$

Pfaffian QMC

Majorana basis

$$\mathscr{K} = \exp\left(-\frac{1}{2}\begin{bmatrix} \vec{\gamma}^{(1)} \\ \vec{\gamma}^{(2)} \end{bmatrix}^{\mathrm{T}} A \begin{bmatrix} \vec{\gamma}^{(1)} \\ \vec{\gamma}^{(2)} \end{bmatrix}\right)$$

$$(\Phi^t) = \exp\left(-\frac{1}{2}\begin{bmatrix} \vec{\gamma}^{(1)} \\ \vec{\gamma}^{(2)} \end{bmatrix}^{\mathrm{T}} B[\phi^t] \begin{bmatrix} \vec{\gamma}^{(1)} \\ \vec{\gamma}^{(2)} \end{bmatrix}\right)$$

$$-S_{\mathrm{eff}} = ?$$

PROMOTING DQMC TO PFQMC

Pfaffian Weight

After reducing the fermion matrix

$$S_{\text{eff}} \sim \log\left(\mathrm{Tr}\left\{\prod_{t=1}^{N_t} e^{-\frac{1}{4}\vec{\gamma}^{\mathrm{T}}A\vec{\gamma}}e^{-\frac{1}{4}\vec{\gamma}^{\mathrm{T}}B[\phi^t]\vec{\gamma}}\right\}\right) + \text{gaussian part}$$

$$\propto \log\left(\left[\prod_{t=1}^{N_t}\eta(B[\phi^t])\right]\left[\prod_{t=1}^{N_t-1}\mathrm{Pf}\left(\begin{bmatrix} G\left(AB[\phi^1]\cdots AB[\phi^t]\right) & -I \\ I & G\left(AB[\phi^{t+1}]\right)\end{bmatrix}\right)\right]\right) + \text{gaussian part}$$

$\sim \mathcal{O}\left(N_t L^3\right)$

$$\eta(X) = \mathrm{Pf}\left(\begin{bmatrix}\sqrt{2}\sinh\left(\frac{X}{4}\right) & -I \\ I & \sqrt{2}\sinh\left(\frac{X}{4}\right)\end{bmatrix}\right), \quad G(X) = \tanh\left(\frac{X}{2}\right)$$

Han, Wan & Yao, “Pfaffian quantum Monte Carlo,” arXiv:2408.10311 (2024)

PROMOTING DQMC TO PFQMC

Pfaffian Gradient

$$S_{\mathrm{eff}} \sim \log\left(\mathrm{Tr}\left\{\prod_{t=1}^{N_t} e^{-\frac{1}{4}\vec{\gamma}^{\mathrm{T}} A\vec{\gamma}} e^{-\frac{1}{4}\vec{\gamma}^{\mathrm{T}} B[\phi^t]\vec{\gamma}}\right\}\right) + \text{gaussian part}$$

After reducing the fermion matrix

$$\propto \log\left(\left[\prod_{t=1}^{N_t} \eta(B[\phi^t])\right]\left[\prod_{t=1}^{N_t-1} \mathrm{Pf}\left(\begin{bmatrix} G\left(AB[\phi^1]\cdots AB[\phi^t]\right) & -I \\ I & G\left(AB[\phi^{t+1}]\right)\end{bmatrix}\right)\right]\right) + \text{gaussian part}$$

$$\sim \mathcal{O}\left(N_t L^3\right)$$

Force terms:

$$\mathrm{Re}\left(\frac{\partial}{\partial \phi_x^t} S_{\mathrm{eff}}(\phi)\right) \propto -\frac{\partial}{\partial \phi_x^t} \log\left(\underbrace{\left|\mathrm{Tr}\left\{\prod_{t=1}^{N_t} e^{-\frac{1}{4}\vec{\gamma}^{\mathrm{T}} A\vec{\gamma}} e^{-\frac{1}{4}\vec{\gamma}^{\mathrm{T}} B[\phi^t]\vec{\gamma}}\right\}\right|}_{\sqrt{\det(M)}}\right)$$

$$|S_{\mathrm{eff}}| \sim \log\left(\sqrt{\det(M)}\right)$$

PROMOTING DQMC TO PFQMC

Pfaffian Gradient

Action:

$$S_{\text{eff}} \propto \log\left(\left[\prod_{t=1}^{N_t}\eta(B[\phi^t])\right]\left[\prod_{t=1}^{N_t-1}\mathrm{Pf}\left(\begin{bmatrix} G\left(AB[\phi^1]\cdots AB[\phi^t]\right) & -I \\ I & G\left(AB[\phi^{t+1}]\right)\end{bmatrix}\right)\right]\right] \right) + \text{gaussian part} \qquad \sim \mathcal{O}\left(N_t L^3\right)$$

Force terms:

$$\mathrm{Re}\left(\frac{\partial}{\partial \phi_x^t} S_{\text{eff}}(\phi)\right) \propto \frac{1}{2}\,\mathrm{Re}\left(\left[R_{t+1\ldots N_t} M^{-1} R_{1\ldots t}\right]_{xx}\right) \quad \sim \mathcal{O}\left(N_t L^3\right)$$

Correlators:

$$C_{ij}(t) = \langle \gamma_i(t)\gamma_j\rangle \propto \left[M^{-1}R_{1\ldots t}\right]_{ij}$$

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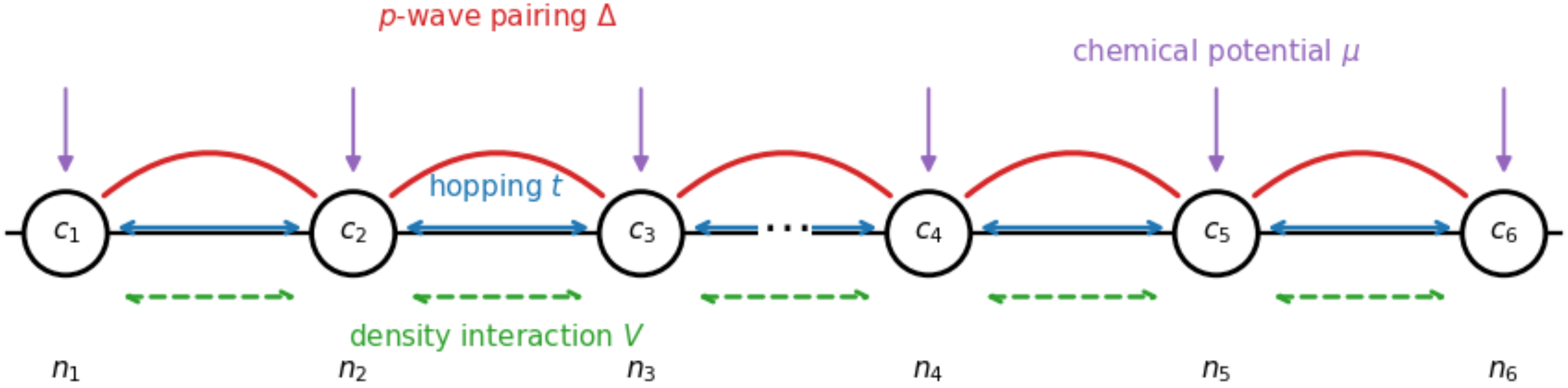
THE INTERACTING SPINLESS KITAEV CHAIN

$$H = \sum_{j=1}^{L-1} \left[-tc_j^\dagger c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger + \mathrm{H.c.} \right] - \mu \sum_{j=1}^{L} n_j + \sum_{j=1}^{L-1} V \left(n_j - \frac{1}{2} \right) \left(n_{j+1} - \frac{1}{2} \right)$$



Non-interacting System:

- System is gapped i.g.
- Low energy sector can support Majorana zero modes
- Localization at edges
- Robust with respect to local perturbations

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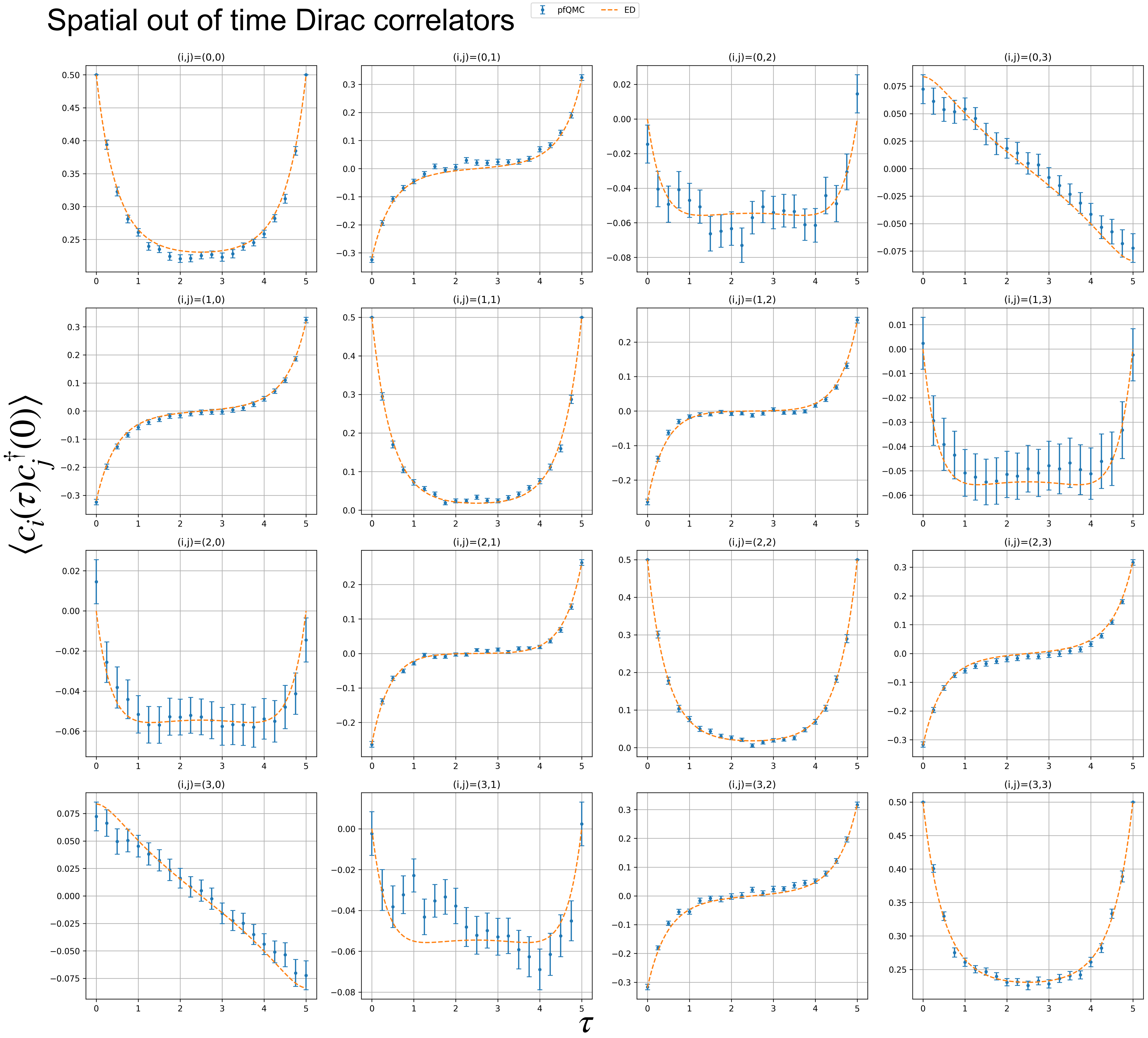
PROOF OF CONCEPT

Spinless Kitaev Chain with density-density interactions:

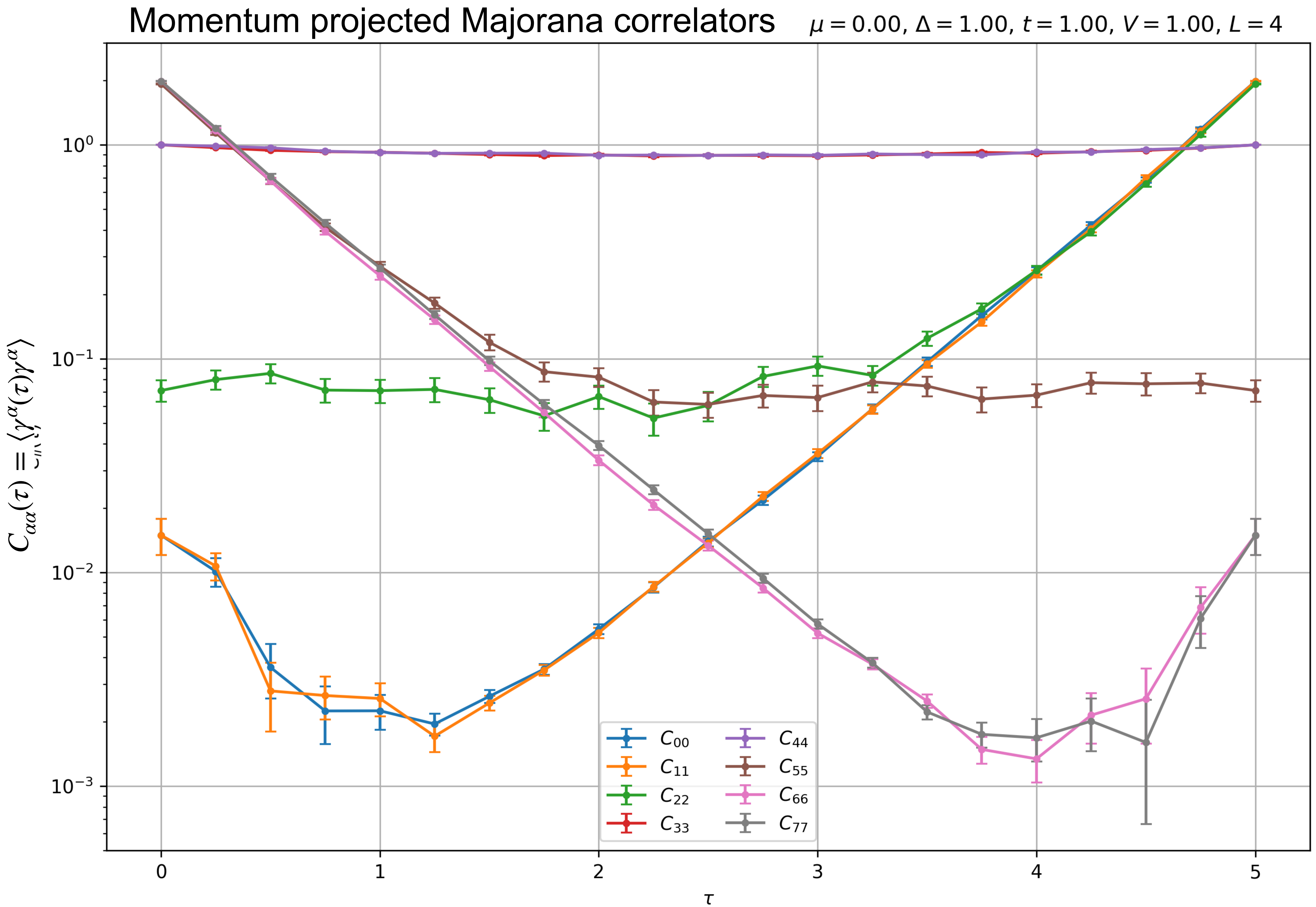
$$H = \sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \Delta c_{j+1}^\dagger c_j^\dagger + \mathrm{H.c.}\right] - \mu\sum_{j=1}^{L} n_j + \sum_{j=1}^{L-1} V\left(n_j - \frac{1}{2}\right)\left(n_{j+1} - \frac{1}{2}\right)$$

$$t = 1.0$$
$$\Delta = 1.0$$
$$V = 1.0$$
$$\mu = 0.0$$

Spatial out of time Dirac correlators

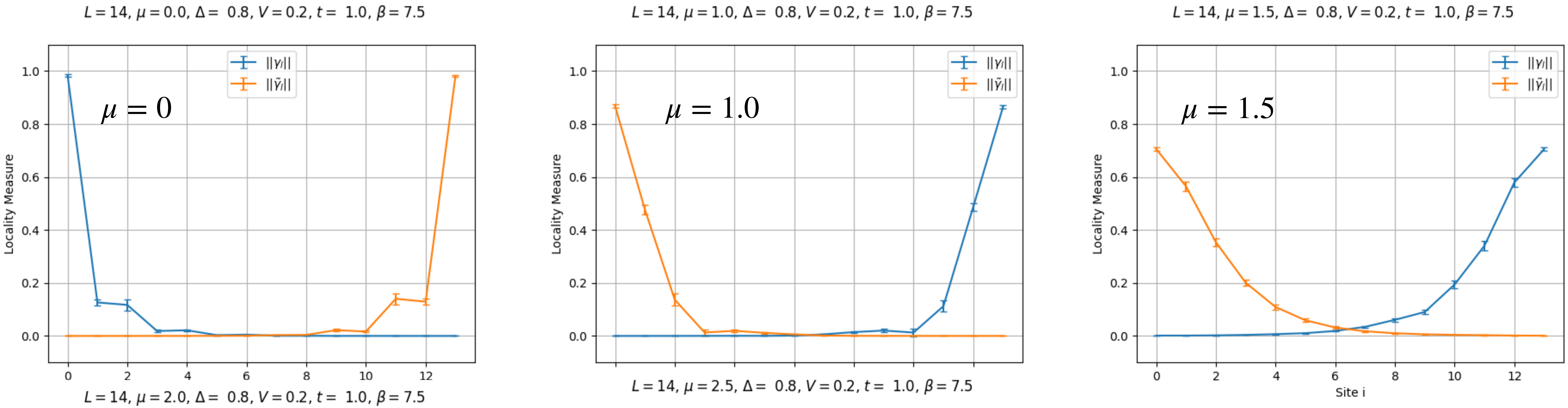


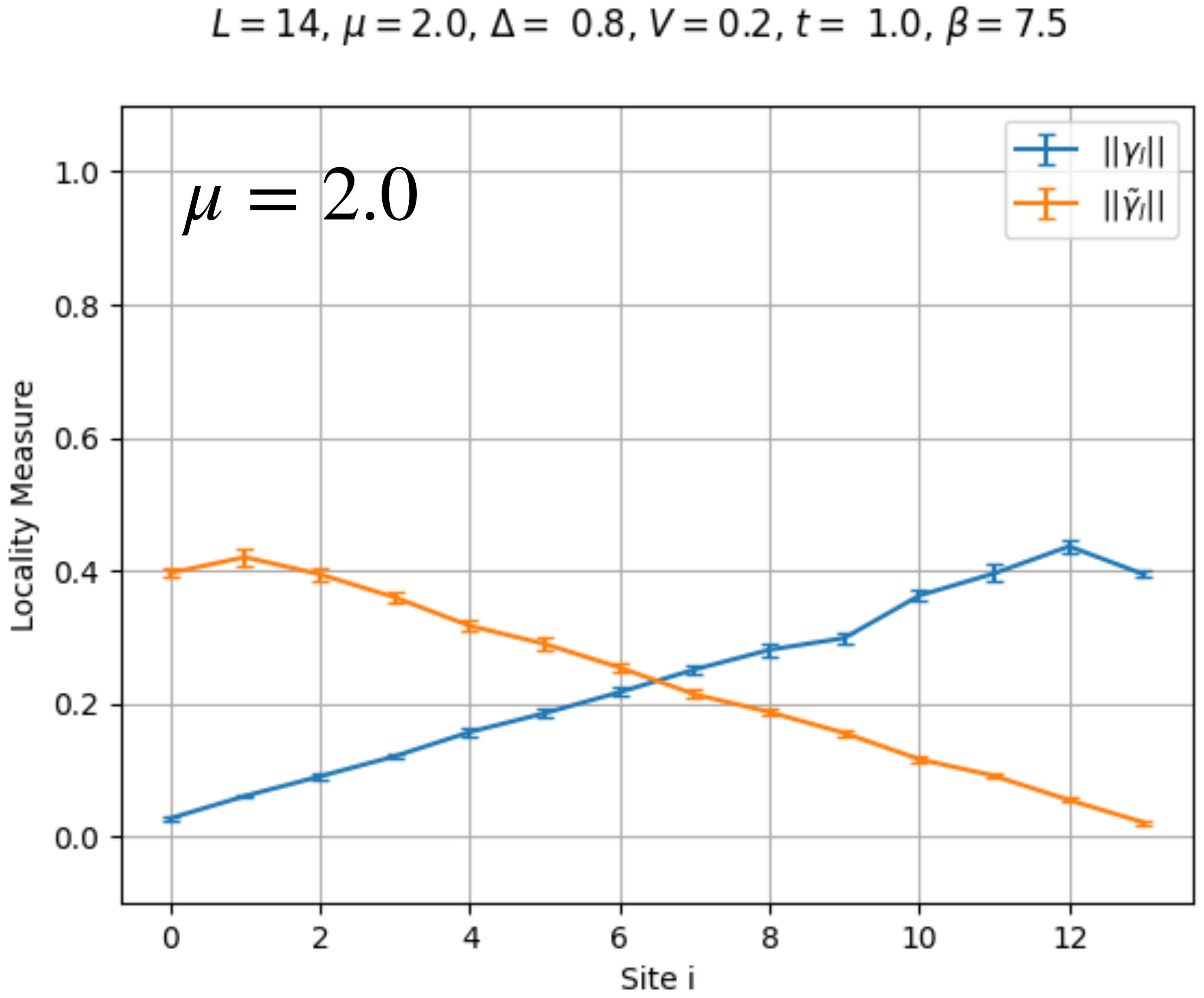
EXTRACTING MAJORANA EXCITATION ENERGIES

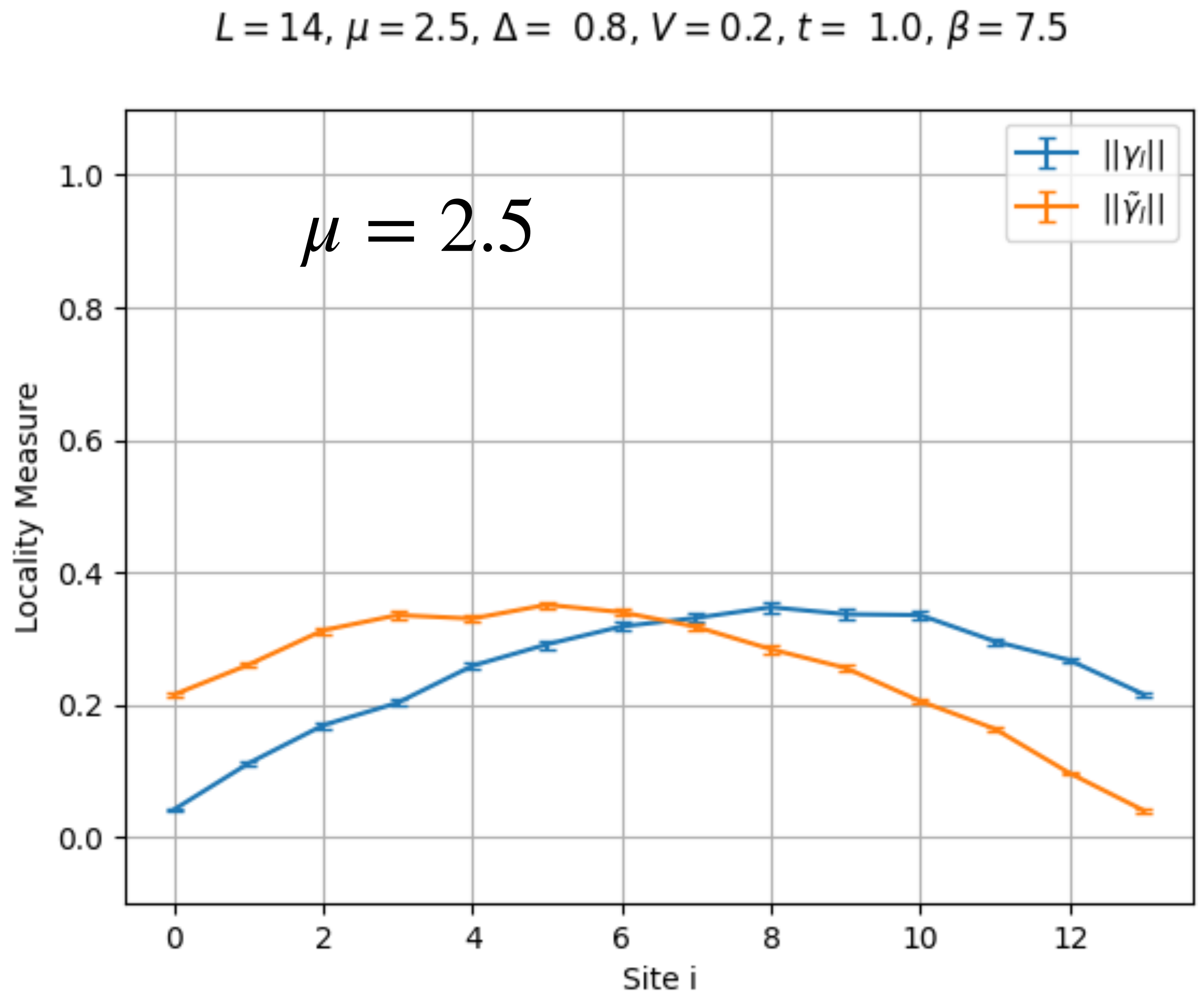


- Momentum projected Majorana correlators
- Exponential decay gives information on excitation energies
- Flat correlators hint at low energy excitations

LOCALITY PROFILES







- Under open boundary conditions:
  - Edgemodes at $\mu < 2t$
  - Trivial for $\mu > 2t$
  - Seems to still hold for small V

SUMMARY AND OUTLOOK

Summary:

DQMC → PfQMC — handle pairing terms, more decoupling channels, Majorana physics

Retained advantages — same time complexity, correlators are calculated from force terms

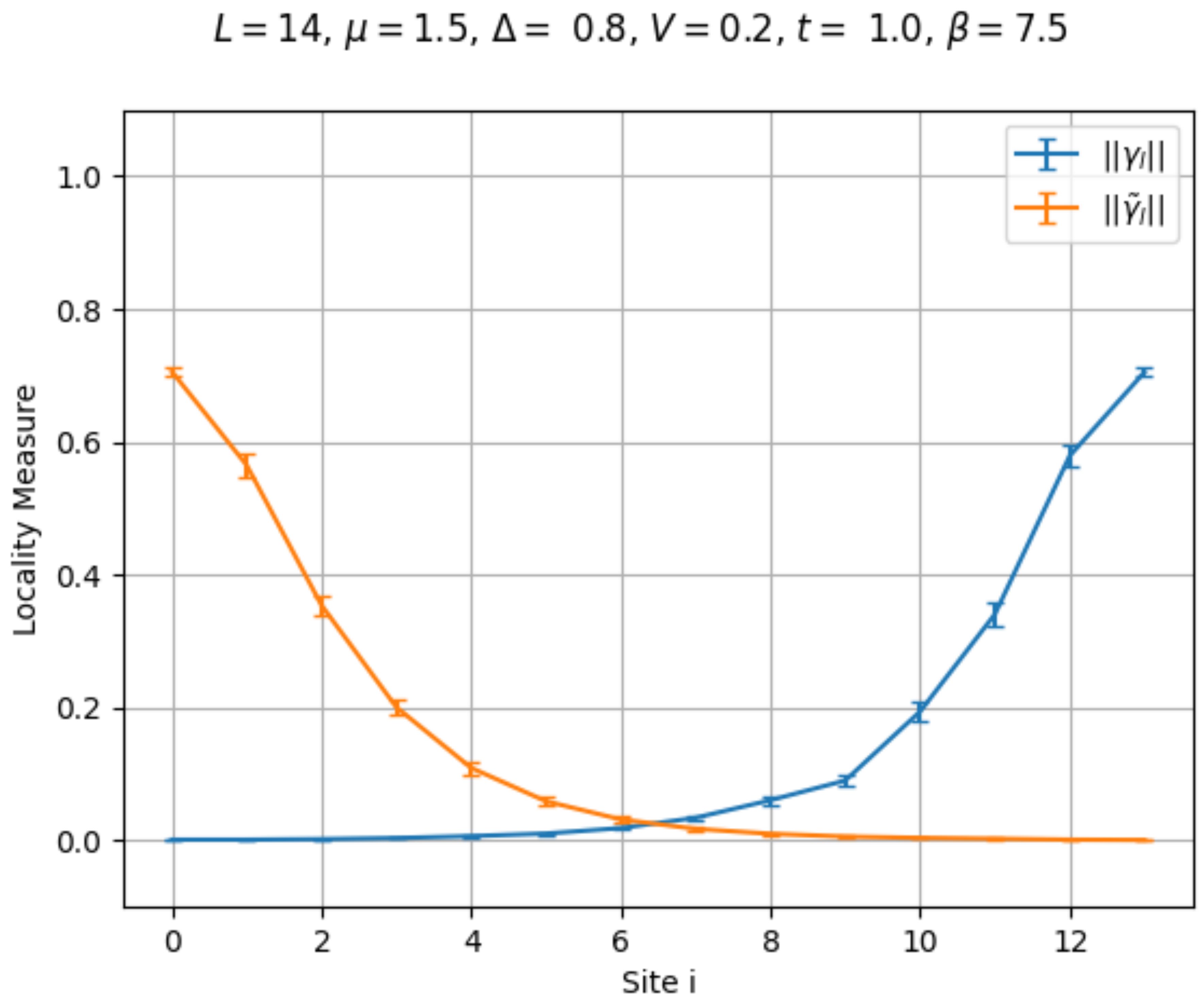
Preliminary results — matching ED for small systems, found low energy modes, localization

Remaining problems:

- Ergodicity
- Stability
- Non-diagonal interactions

Future Work:

- Improve scaling with pseudo fermions
- Identify systems with no or mild sign problem



BACKUP SLIDES

THE MAJORANA HOPPING CHANNEL

$$H = \sum_{j=1}^{L-1} \left(\frac{i}{2}\left[(-1)^j t - \Delta\right]\eta_j\eta_{j+1} + \frac{i}{2}\left[(-1)^j t + \Delta\right]\gamma_j\gamma_{j+1} + \frac{V}{4}\eta_j\eta_{j+1}\gamma_j\gamma_{j+1} \right) - \frac{i}{2}\mu \sum_{j=1}^{L} \eta_j\gamma_j$$

$$c_j = \frac{1}{2}\left(\eta_j - i\gamma_j\right), \quad c_j = \frac{1}{2}\left(\eta_j + i\gamma_j\right), \quad n_j \sim i\eta_j\gamma_j$$

$$\eta_j\eta_{j+1}\gamma_j\gamma_{j+1} = -\frac{1}{2}\left(\eta_j\gamma_j + \eta_{j+1}\gamma_{j+1}\right)^2 + \mathrm{const}$$

Charge Channel

$$= +\frac{1}{2}\left(\eta_j\gamma_j - \eta_{j+1}\gamma_{j+1}\right)^2 + \mathrm{const}$$

Spin Channel

$$= +\frac{1}{2}\left(\eta_j\eta_{j+1} + \gamma_j\gamma_{j+1}\right)^2 + \mathrm{const}$$

Majorana Hopping Channel

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THE MAJORANA HOPPING CHANNEL

$$
B[\phi^t] = \left[\begin{array}{ccccc|ccccc}
0 & -\phi_1^t & & & & & & & & \\
+\phi_1^t & 0 & -\phi_2^t & & & & & & & \\
 & +\phi_2^t & 0 & \ddots & & & & & & \\
 & & \ddots & \ddots & -\phi_{L-1}^t & & & & & \\
 & & & +\phi_{L-1}^t & 0 & & & & & \\
\hline
 & & & & & 0 & \phi_1^t & & & \\
 & & & & & -\phi_1^t & 0 & \phi_2^t & & \\
 & & & & & & -\phi_2^t & 0 & \ddots & \\
 & & & & & & & \ddots & \ddots & \phi_{L-1}^t \\
 & & & & & & & & -\phi_{L-1}^t & 0
\end{array}\right]
$$

TREATING NON-DIAGONAL INTERACTIONS

$$\frac{\partial}{\partial \phi_i^t}\Phi[\phi] = \frac{\partial}{\partial \phi_i^t}\exp\left(-\boldsymbol{B}_t\right) \approx \sum_{n=1}^{n_{\text{cut}}} \frac{(-1)^n}{n\,!} \sum_{k=0}^{n-1} \boldsymbol{B}_t^k \frac{\partial \boldsymbol{B}_t}{\partial \phi_i^t} \boldsymbol{B}_t^{n-1-k}$$

Gradient:

$$\mathrm{Re}\left(\frac{\partial}{\partial \phi_x^t} U(\phi)\right) \sim \mathrm{Re}\left(\left[\sum_{n=1}^{n_{\text{cut}}} \frac{(-1)^n}{n\,!} \sum_{k=0}^{n-1} \boldsymbol{B}_t^{n-1-k} \left[R_{t+1\ldots N_t} \underbrace{M^{-1}\mathscr{K} R_{1\ldots t-1}}_{=C(t-1)} \mathscr{K}\right] \boldsymbol{B}_t^k\right]_{i,i+1}\right)$$

Computational Complexity: $\mathscr{O}\left(n_{\text{cut}} N_t L^3\right)$

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TREATING NON-DIAGONAL INTERACTIONS

Gradient:

$$\mathrm{Re}\left(\frac{\partial}{\partial \phi_x^t} U(\phi)\right) \sim \mathrm{Re}\left(\left[\sum_{n=1}^{n_{\mathrm{cut}}} \frac{(-1)^n}{n!} \sum_{k=0}^{n-1} \boldsymbol{B}_t^{n-1-k} \left[R_{t+1\dots N_t} \underbrace{M^{-1} \mathscr{K} R_{1\dots t-1}}_{=C(t-1)} \mathscr{K}\right] \boldsymbol{B}_t^k\right]_{i,i+1}\right)$$

Consequences of truncation	
Computational complexity	$\mathcal{O}\left(n_{\mathrm{cut}} N_t L^3\right)$
Sampling	Remains exact
Correlators	Remain exact
Acceptance rate	Might suffer

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BRIDGING QCD AND CONDENSED MATTER

What is our goal?

Treat strongly interacting condensed matter systems in an unbiased manner, e.g. the spinless tV-model:

$$-S/\beta = \underbrace{\sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \mathrm{H.c.}\right] - \mu\sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1} V\left(c_j^\dagger c_j - \frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2}\right)}_{H_2}$$

Quartic interactions
no gauge field coupling

L : # fermionic sites

Hubbard-Stratonovich Transformation:

$$\exp\left(V\left(c_j^\dagger c_j - \frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2}\right)\right) \propto \exp\left(-\frac{V}{2}\left[c_j^\dagger c_j - c_{j+1}^\dagger c_{j+1}\right]^2\right) \propto \int \mathrm{d}\phi_j \exp\left(-\frac{\phi_j^2}{2V}\right)\exp\left(i\phi_j\left[c_j^\dagger c_j - c_{j+1}^\dagger c_{j+1}\right]\right)$$

BRIDGING QCD AND CONDENSED MATTER

What is our goal?

Treat strongly interacting condensed matter systems in an unbiased manner, e.g. the spinless tV-model:

$$-S_{\text{eff}}/\beta = \underbrace{\sum_{j=1}^{L-1}\left[-tc_j^\dagger c_{j+1} + \mathrm{H.c.}\right] - \mu\sum_{j=1}^{L} n_j}_{H_1} + \underbrace{\sum_{j=1}^{L-1}\frac{-\phi_j^2}{2V} + i\phi_j\left[c_j^\dagger c_j + c_{j+1}^\dagger c_{j+1}\right]}_{H_2}$$

Now we also need to integrate over the auxiliary fields

$$Z = \int \mathscr{D}(\phi)\, \mathrm{Tr}\left\{e^{-\beta S_{\text{eff}}}\right\}$$

$$\approx \int \mathscr{D}(\phi)\exp\left(-\frac{\boldsymbol{\phi}^2}{2m}\right)\mathrm{Tr}\left\{\prod_{t=1}^{N_t}\exp\left(-\vec{c}^\dagger A\vec{c}\right)\exp\left(-\vec{c}^\dagger B\left[\phi^t\right]\vec{c}\right)\right\}$$

$$= \int \mathscr{D}(\phi)\exp\left(-\frac{\boldsymbol{\phi}^2}{2m}\right)\det\left(\underbrace{I + e^{-A}e^{-B[\phi^1]}e^{-A}e^{-B[\phi^2]}\ldots e^{-A}e^{-\tilde{B}[\phi^{N_t}]}}_{:=M[\boldsymbol{\phi}]}\right)$$

L : # fermionic sites

N_t : # time slices

$M : L\times L$

$2N_t$ matrix multiplications

➡ $\mathcal{O}\left(N_t L^3\right)$

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BRIDGING QCD AND CONDENSED MATTER

$$\mathrm{pf}(A) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \mathrm{sgn}(\sigma) \prod_{i=1}^{n} a_{\sigma(2i-1),\sigma(2i)}$$

$$\det(A) = \sum_{\sigma \in S_n} \left(\mathrm{sgn}(\sigma) \prod_{i=1}^{n} a_{i,\sigma(i)} \right)$$