Quantum-classical hybrid method for microcanonical ensembles

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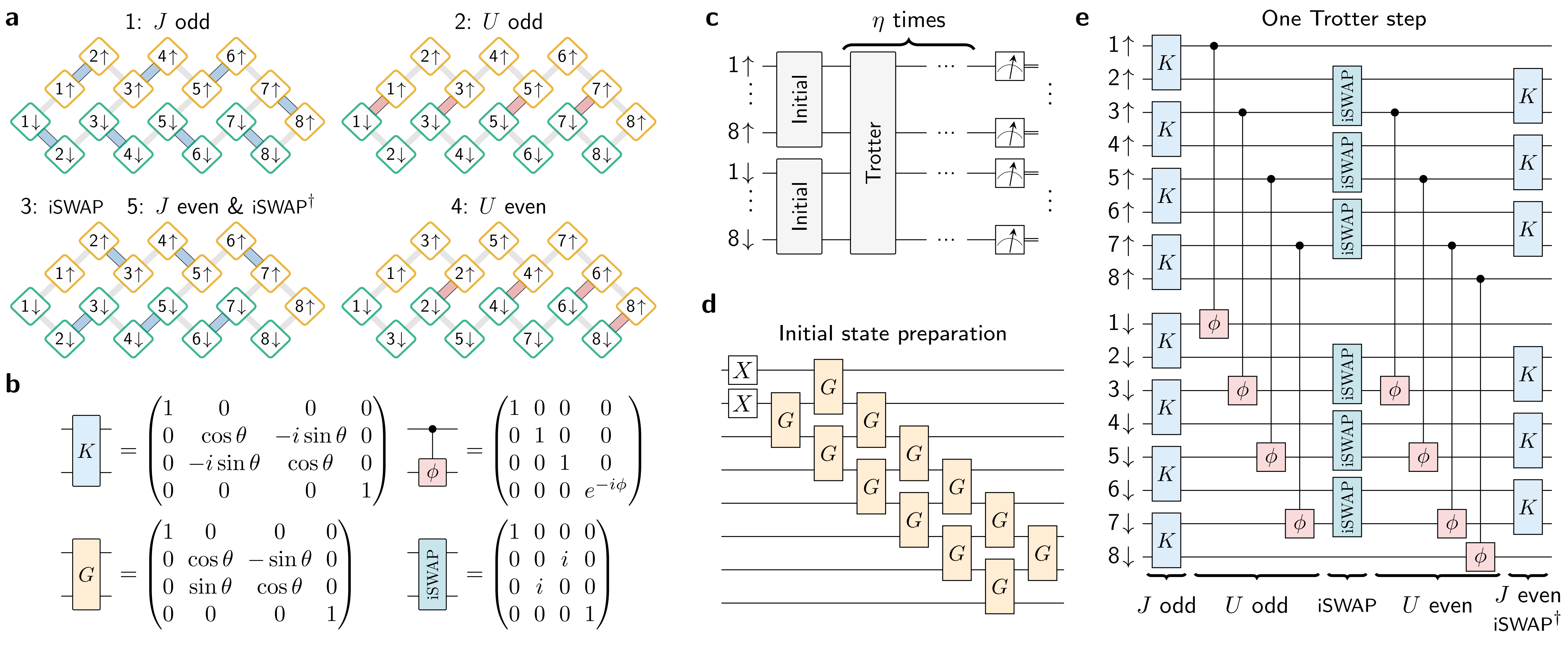
K. Seki and S. Yunoki, Phys. Rev. B **106**, 155111 (2022)

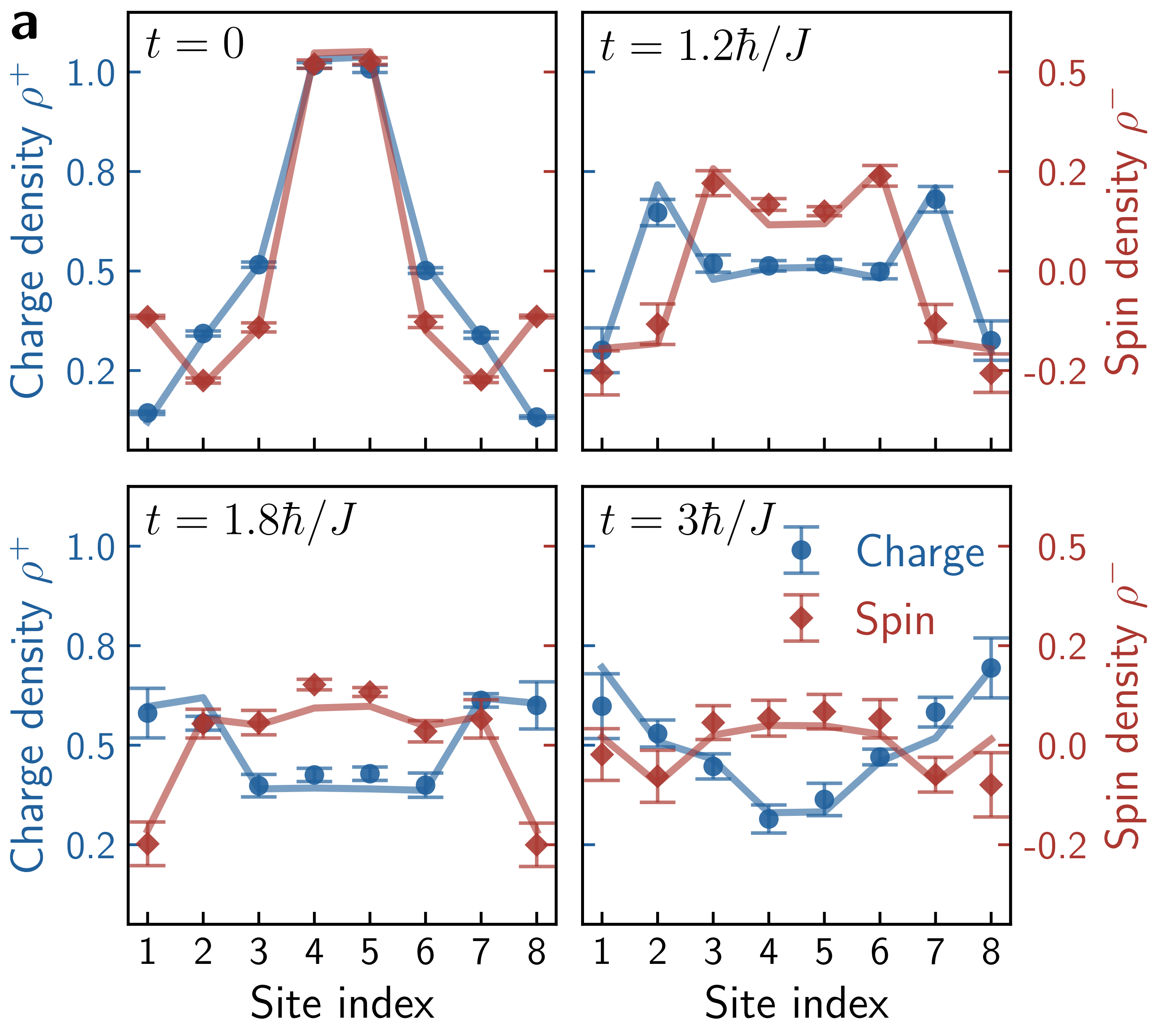
Outline

- Background and motivation
- Quantum-classical hybrid method for microcanonical ensembles
- Numerical results
    - Classical simulation
    - Quantum simulation (preliminary)
- Summary

Dynamics of quantum many-body systems on quantum computers

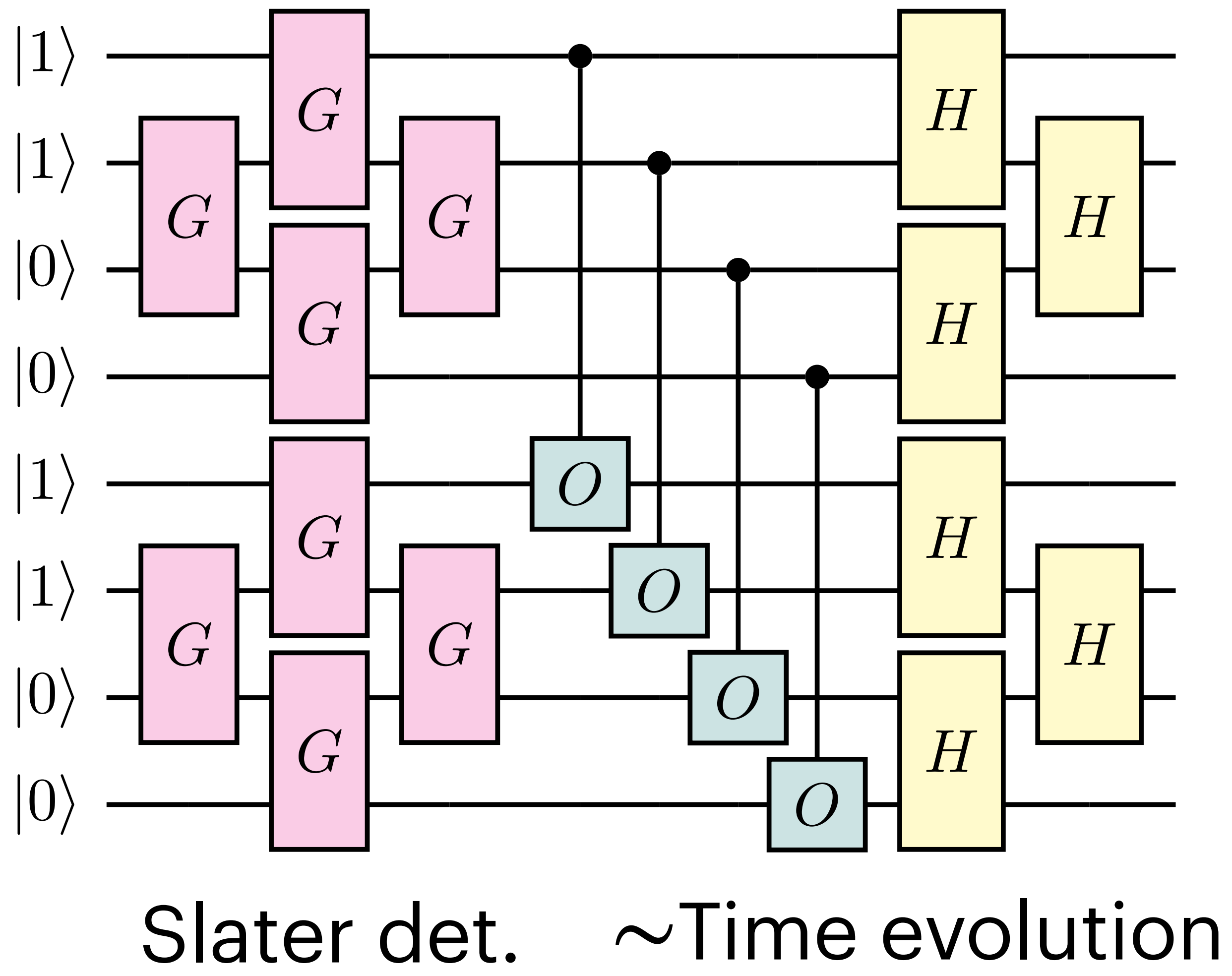
Time evolution of a state by the 1D Hubbard Hamiltonian Arute *et al.*, arXiv:2010.07965

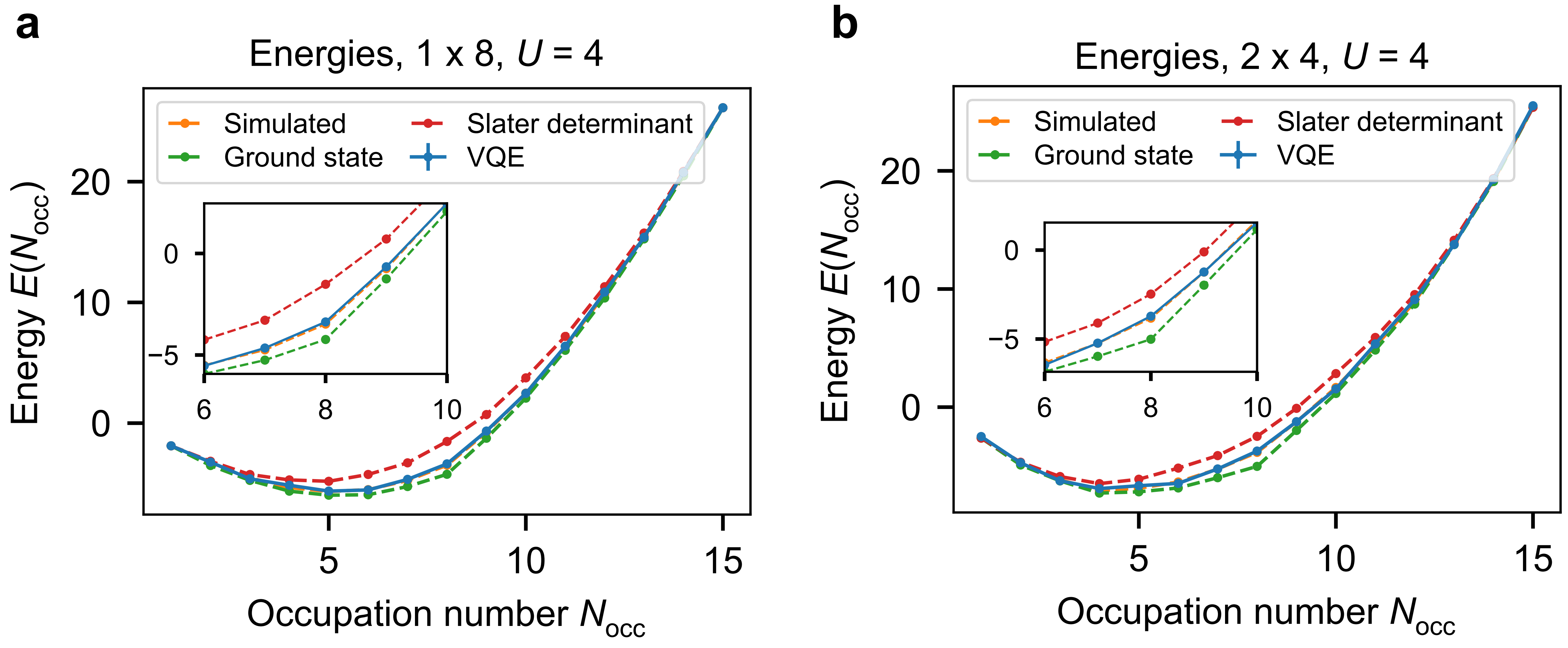




Variational (VQE) calculation for the Hubbard model Stanisic *et al.*, Nature communications **13**, 5743 (2022)

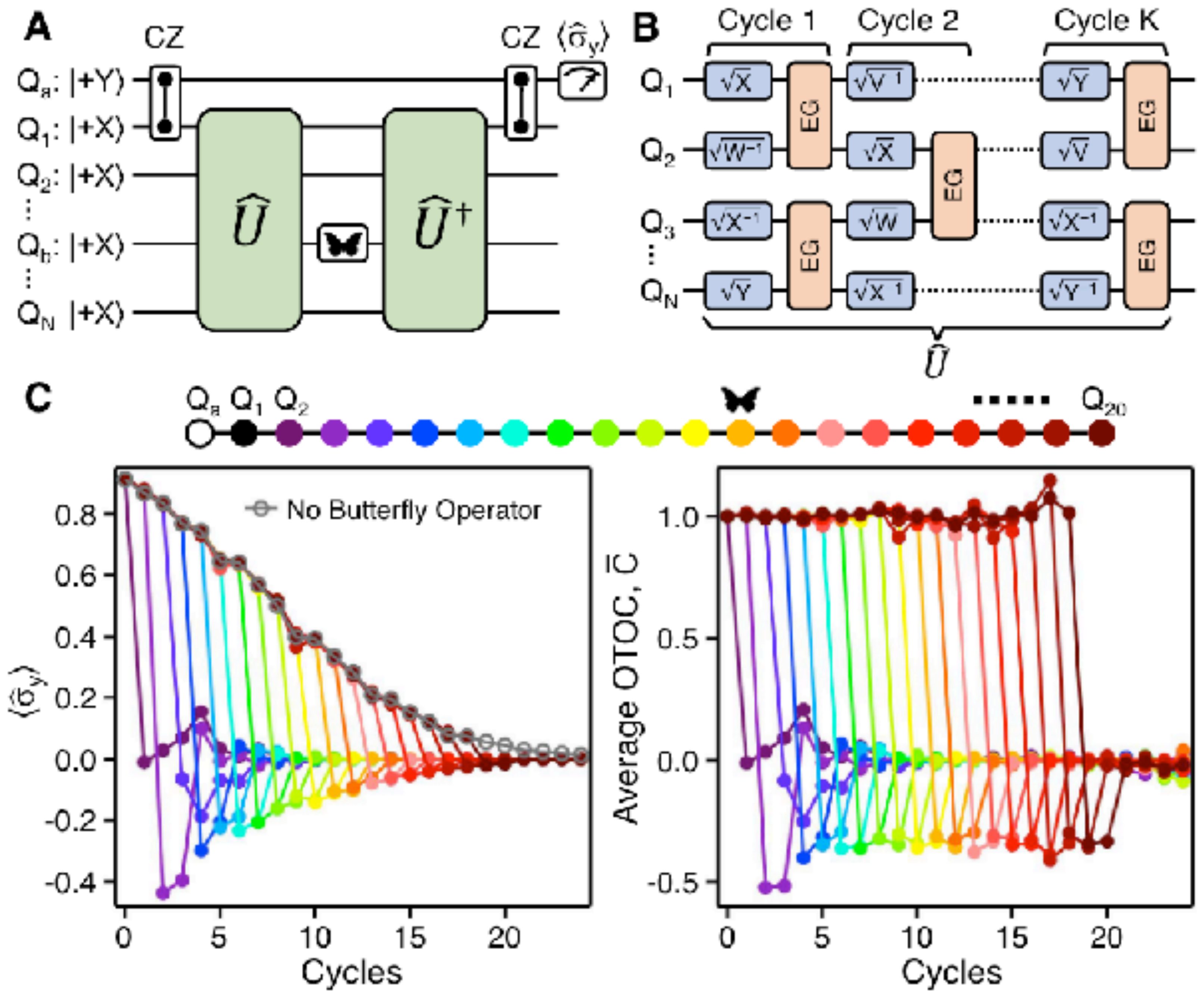
Hamiltonian-variational ansatz





Dynamics of quantum many-body systems on quantum computers

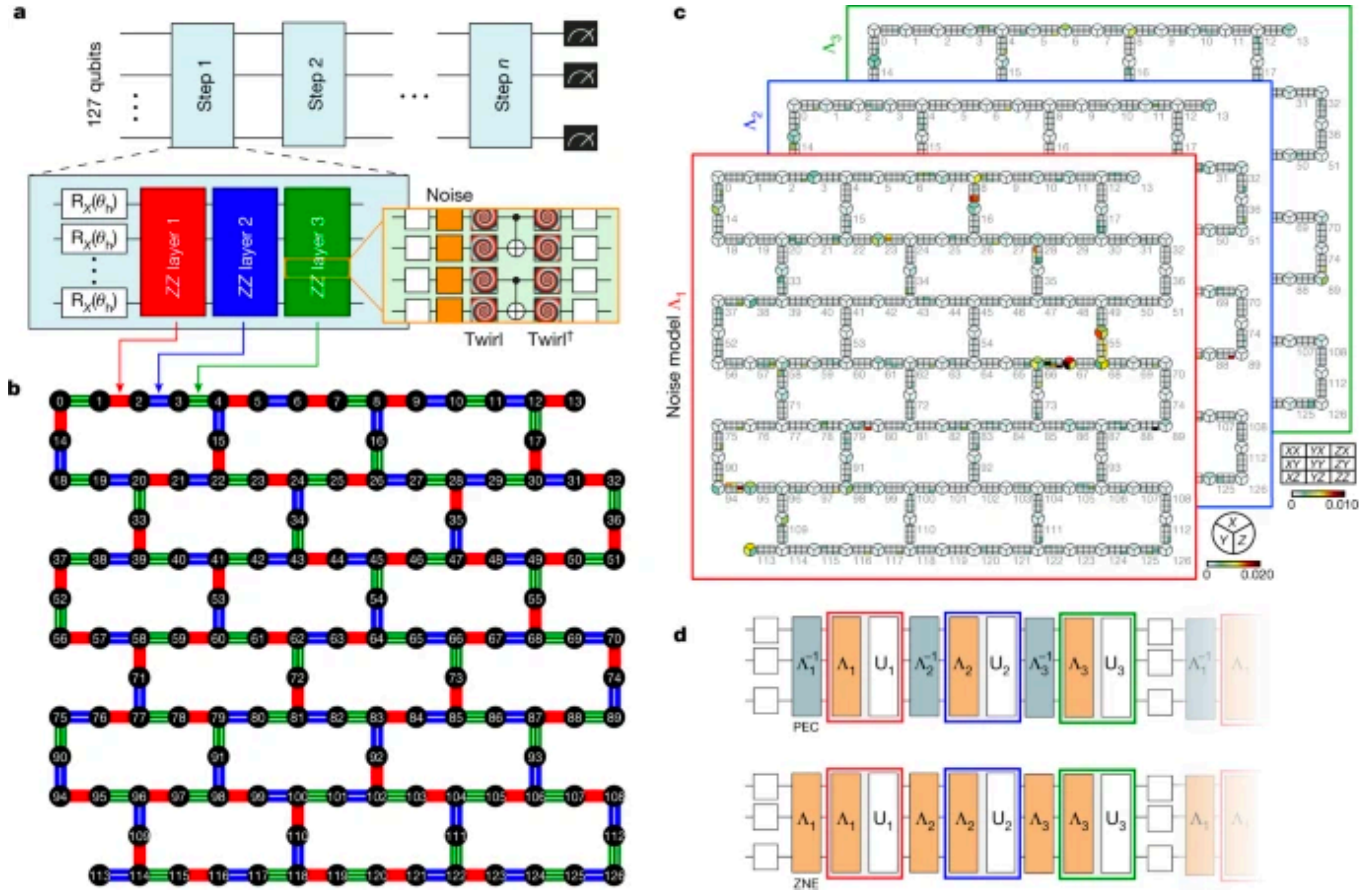
Mi *et al.*, Science **374**, 1479 (2021)



Out-of-time-order correlators with random unitaries $\hat{U}$
(not a Hamiltonian dynamics)

$$\left\langle \hat{X}_b(t)\hat{Z}_1\hat{X}_b(t)\hat{Z}_1 \right\rangle, \ \hat{X}_b(t) = \hat{U}^\dagger \hat{X}_b \hat{U}$$

Kim *et al.*, Nature **618**, 500 (2023)



Dynamics of transverse-field Ising model

A finite signal of $\langle \hat{Z}_{62} \rangle$ with
20 Trotter steps (144 x 20 = 2880 CNOTs)

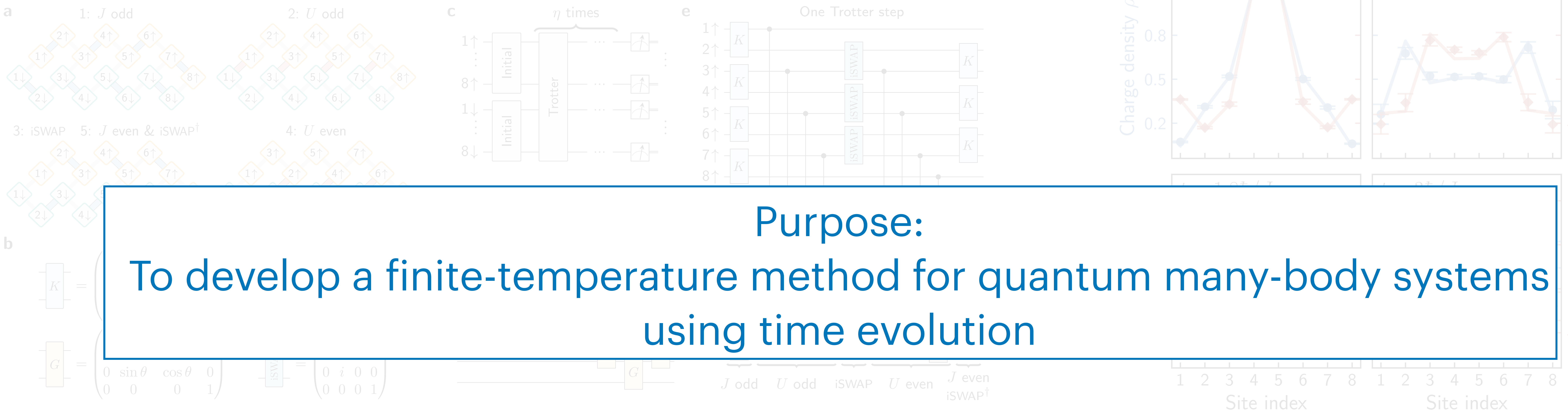
A naive estimation of circuit fidelity

$$(0.99)^{2880} \sim 3 \times 10^{-13}$$

0.99: median 2Q gate fidelity
Several followup papers appeared

Dynamics of quantum many-body systems on quantum computers

Time evolution of a state by the 1D Hubbard Hamiltonian Arute *et al.*, arXiv:2010.07965



Purpose:
To develop a finite-temperature method for quantum many-body systems using time evolution

Variational (VQE) calculation fo

Variational wave function (Ham

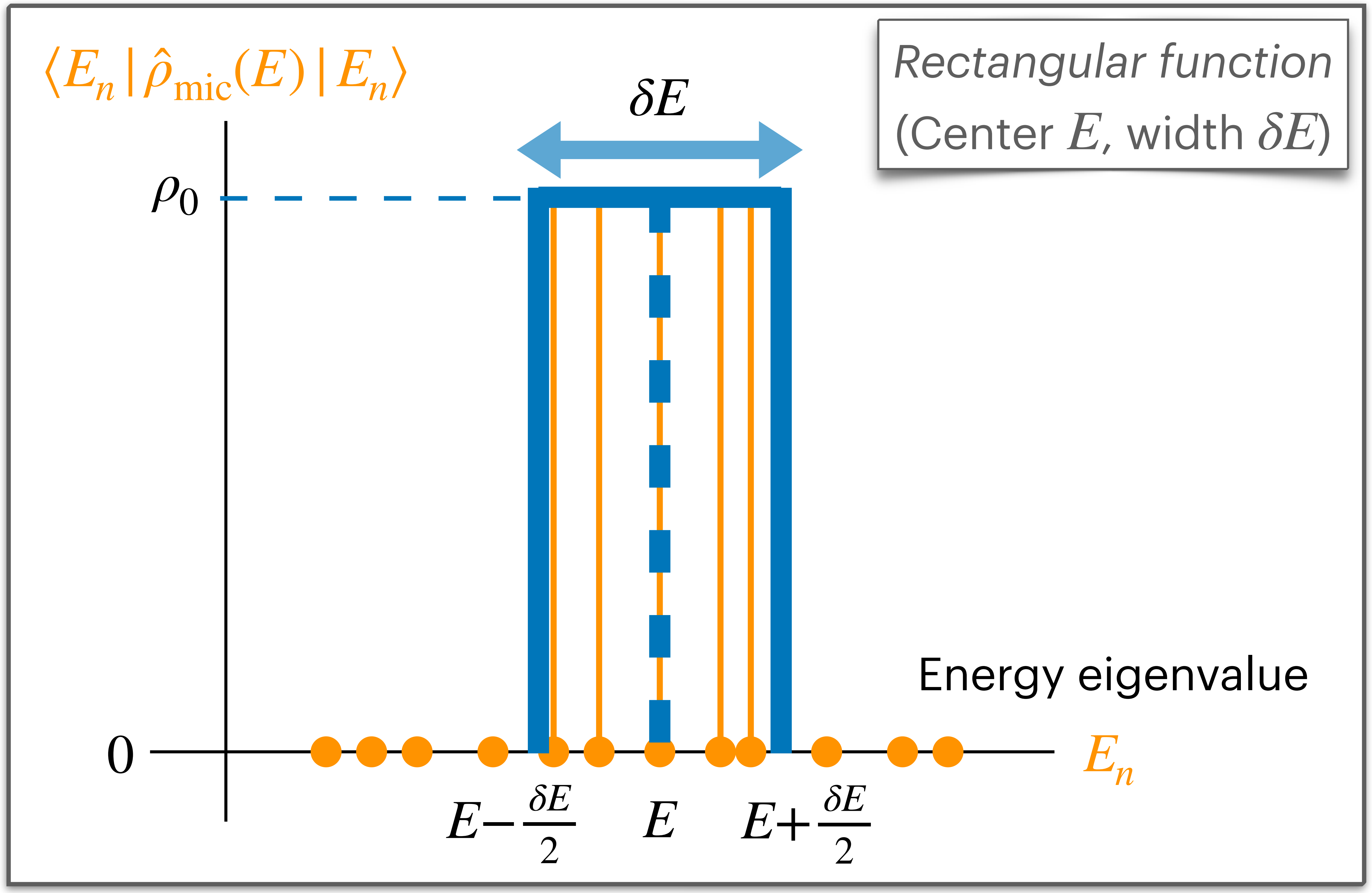
Time evolution by quantum many-body Hamiltonians is getting feasible

3 (2022)

Quantum-classical hybrid method for microcanonical ensembles

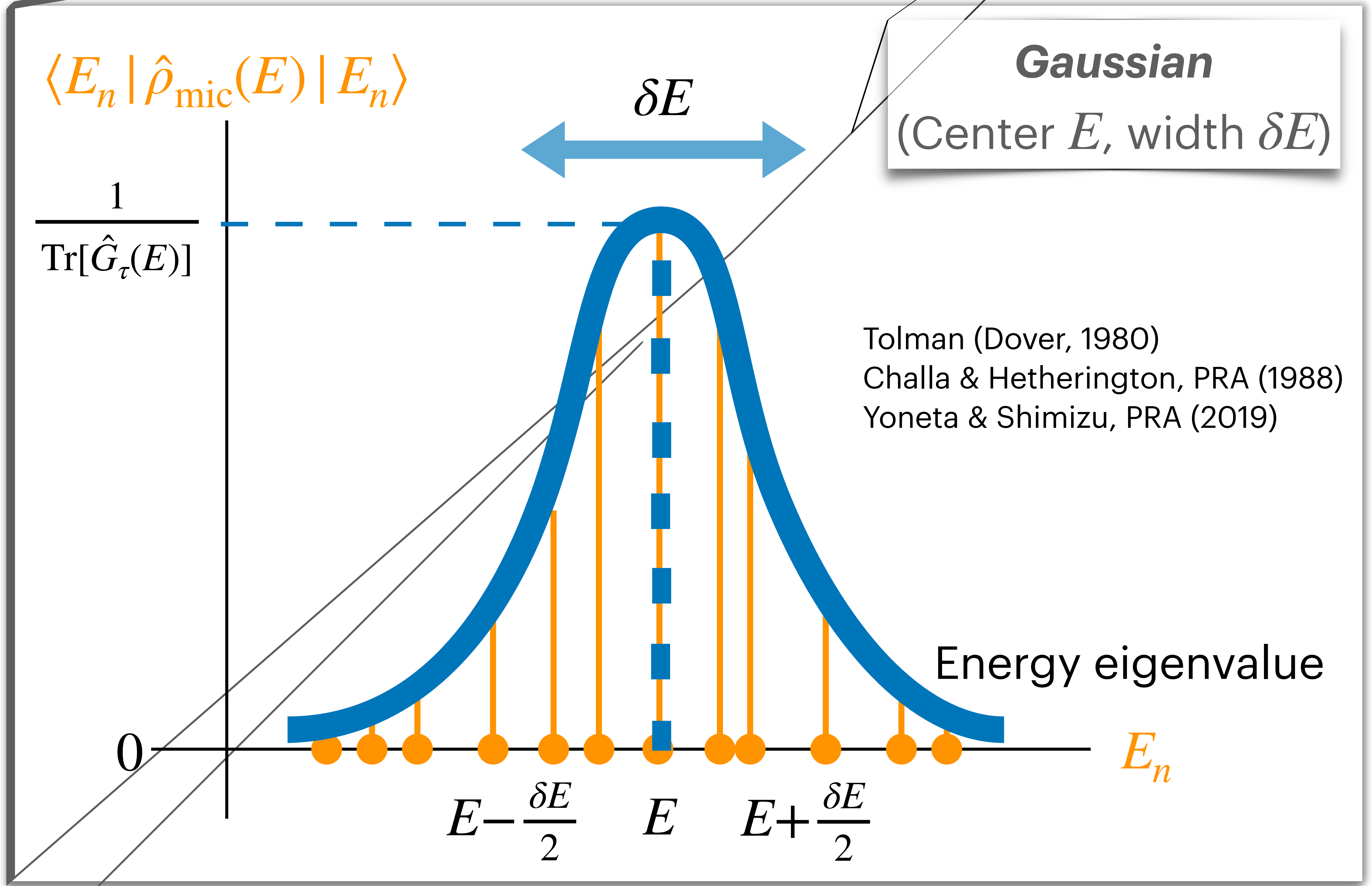
Definition of microcanonical density matrix

Conventional definition



$$\langle E_m | \hat{\rho}_{\mathrm{mic}}(E) | E_n \rangle = \begin{cases} \rho_0 \delta_{mn} & (E - \frac{\delta E}{2} \leqslant E_n < E + \frac{\delta E}{2}) \\ 0 & (\text{otherwise}) \end{cases}$$

Our definition



$$\langle E_m | \hat{\rho}_{\mathrm{mic},\tau}(E) | E_n \rangle = \frac{\mathrm{e}^{-(E_n - E)^2 \tau^2}}{\sum_{n=0}^{D-1} \mathrm{e}^{-(E_n - E)^2 \tau^2}} \delta_{mn} \qquad \delta E = \frac{\sqrt{\pi}}{\tau}$$

Density matrix operator :

$$\hat{\rho}_{\mathrm{mic},\tau}(E) \equiv \frac{\hat{G}_\tau(E)}{\mathrm{Tr}\left[\hat{G}_\tau(E)\right]}, \qquad \hat{G}_\tau(E) = \mathrm{e}^{-(\hat{\mathscr{H}} - E)^2 \tau^2}$$

Pure state $|\psi_{\tau,r}(E)\rangle$ corresponding to the density matrix $\hat{\rho}_{\mathrm{mic},\tau}(E)$

"Random state"(r : label for random seeds)

$$|\psi_{\tau,r}(E)\rangle = [\hat{G}_\tau(E)]^{\frac{1}{2}}|\phi_r\rangle$$

Gaussian (center E, width $\sim 1/\tau$)

$$\hat{G}_\tau(E) = \mathrm{e}^{-(\hat{\mathscr{H}}-E)^2\tau^2}$$

Density matrix

$$\hat{\rho}_{\mathrm{mic},\tau}(E) \equiv \frac{\hat{G}_\tau(E)}{\mathrm{Tr}\left[\hat{G}_\tau(E)\right]}$$

- N: Number of qubits
- $D = 2^N$
- $\hat{\mathscr{H}}$: Hamiltonian
- E: Target energy
- τ: ~1/(energy width δE)

❖ Thermodynamic quantities

- $\left\langle\left\langle\langle\psi_{\tau,r}(E)|\psi_{\tau,r}(E)\rangle\right\rangle\right\rangle = \frac{1}{D}\mathrm{Tr}\left[\hat{G}_\tau(E)\right]$ # states $/D$

- $S_\tau(E) = \ln \mathrm{Tr}[\hat{G}_\tau(E)]$ Entropy
- $\beta_\tau(E) = \partial_E S_\tau(E) = 2\tau^2\left(\mathscr{E}_\tau(E) - E\right)$ Inverse temperature
- $\mathscr{E}_\tau(E) = \mathrm{Tr}\left[\hat{\rho}_{\mathrm{mic},\tau}(E)\hat{\mathscr{H}}\right] = \frac{\mathrm{Tr}[\hat{\mathscr{H}}\hat{G}_\tau(E)]}{\mathrm{Tr}[\hat{G}_\tau(E)]}$ Energy expectation

- $|\psi_{\tau,r}(E)\rangle$: a microcanonical version of the canonical TPQ state $\mathrm{e}^{-\frac{1}{2}\beta\hat{H}}|\phi_r\rangle$ Sugiura and Shimizu, PRL **111**, 010401 (2013)

(norm of canonical TPQ state ~ partition function Z)

- $|\psi_{\tau,r}(E)\rangle$: a linear combination of energy eigenstates $|E_n\rangle$ s.t.

$$E-\frac{\sqrt{2\pi}}{\tau} \lesssim E_n \lesssim E+\frac{\sqrt{2\pi}}{\tau}$$

$$|\psi_{\tau,r}(E)\rangle = \sum_{n=0}^{D-1} \mathrm{e}^{-\frac{1}{2}(E_n-E)^2\tau^2} c_{n,r}|E_n\rangle \text{ where } c_{n,r} = \langle E_n|\phi_r\rangle$$

- $|\psi_{\tau,r}(E)\rangle$ was introduced in the filter-diagonalization method Wall and Neuhauser, J. Chem. Phys. **102**, 8011 (1995)

Random state $|\phi_r\rangle$ on quantum circuit

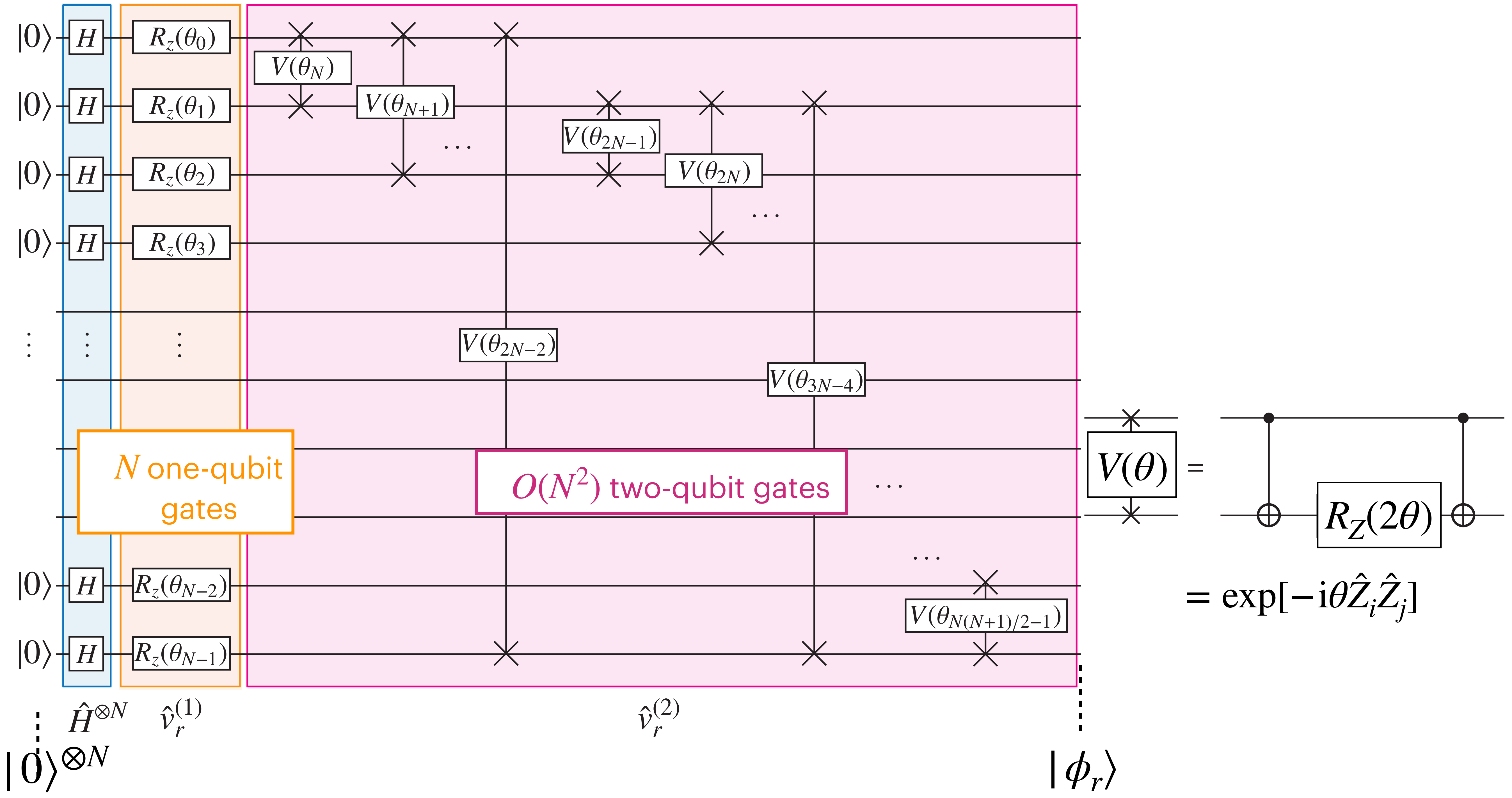
$|\phi_r\rangle$ should satisfy...

- ***Statistical average*** of $x_r \equiv \langle\phi_r|\hat{X}|\phi_r\rangle$ coincides with $\mathrm{Tr}[\hat{X}]/D$
- ***Covariance*** $\mathrm{Cov}(x,y)$ decreases exponentially in N

Random phase states $|\Phi_r\rangle$ satisfy the above properties, but require exponentially large number of gates. However, it suffices to prepare states $|\phi_r\rangle$ which reproduce the properties of $|\Phi_r\rangle$ up to ***2nd statistical moment***.

Diagonal-unitary 2-designs

Nakata and Murao, Int. J. Quantum Inf. **11**, 07 1350062 (2013)
Nakata *et al.*, J. Math. Phys. 58, 052203 (2017)



Variance of ratio (from error propagation) is :

$$\mathrm{Var}\left[\frac{\frac{1}{R}\sum_r x_r}{\frac{1}{R}\sum_r y_r}\right] \approx \frac{1}{R}\mathrm{Var}\left[\frac{x}{y}\right]$$

For a review, see
Jin *et al.*, JPSJ **90**, 012001 (2021)

$$\mathrm{Var}\left[\frac{x}{y}\right] \approx \left(\frac{\mathbb{E}[x]}{\mathbb{E}[y]}\right)^2 \left[\frac{\mathrm{Var}[x]}{\mathbb{E}[x]^2} + \frac{\mathrm{Var}[y]}{\mathbb{E}[y]^2} - 2\frac{\mathrm{Cov}(x,y)}{\mathbb{E}[x]\mathbb{E}[y]}\right]$$

$|\Phi_r\rangle \equiv \frac{1}{\sqrt{D}}\sum_{b=0}^{D-1} e^{i\theta_{b,r}}|b\rangle$, $D = 2^N$ with $\mathbb{E}[\cdots] = \int_0^{2\pi}\prod_{b=0}^{D-1}\frac{d\theta_b}{2\pi}\cdots$ satisfies

$$\mathrm{Cov}(x,y) = \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y] = \frac{1}{D^2}\left[\mathrm{Tr}[\hat{X}\hat{Y}] - \sum_{i=0}^{D-1}[\hat{X}]_{ii}[\hat{Y}]_{ii}\right],$$

where

$$\mathbb{E}[x] = \frac{1}{D}\mathrm{Tr}[\hat{X}],\ \mathbb{E}[y] = \frac{1}{D}\mathrm{Tr}[\hat{Y}],\ x_r = \langle\Phi_r|\hat{X}|\Phi_r\rangle,\ y_r = \langle\Phi_r|\hat{Y}|\Phi_r\rangle$$

($\hat{X}, \hat{Y}$: Hermitian)

Let $\hat{X}, \hat{Y}$ be $\hat{X} = \hat{G}_\tau(E)^{\frac{1}{2}}\mathscr{H}\hat{G}_\tau(E)^{\frac{1}{2}}$, $\hat{Y} = \hat{G}_\tau(E)$, where $\frac{\mathbb{E}[x]}{\mathbb{E}[y]} = \mathscr{E}_\tau(E)$.

Since eigenvalues of $\hat{X}, \hat{Y}$ are $O(N)$, $O(1)$, $\mathrm{Cov}(x,y)$ is $O(ND^{-1})$.
Assuming that the energy window considered contains sufficiently large number of states, $\mathrm{Tr}[\hat{G}_\tau(E)] = fD$, $1/D \ll f \leqslant 1$, then
$\mathbb{E}[x] = f\mathscr{E}_\tau(E)$, $\mathbb{E}[y] = f$, and $\mathrm{Var}(x/y) \sim e^{-N}$.

Cf. Lu et al., PRX Quantum **2**, 020321 (2021), Schuckert et al., PRB **107**, L140410 (2023): Micorocanonical, random product states
Cf. Coopmans et al., PRX Quantum **4**, 010305 (2023): Canonical TPQ with Random Clifford circuits

Fourier representation of the Gaussian operator

How to compute $\mathrm{Tr}\left[\hat{G}_\tau(E)\right]$ and $\mathrm{Tr}\left[\hat{\mathscr{H}}\hat{G}_\tau(E)\right]$

- $S_\tau(E) = \ln \mathrm{Tr}[\hat{G}_\tau(E)]$ Entropy
- $\beta_\tau(E) = \partial_E S_\tau(E) = 2\tau^2\left(\mathscr{E}_\tau(E) - E\right)$ Inverse temperature
- $\mathscr{E}_\tau(E) = \mathrm{Tr}\left[\hat{\rho}_{\mathrm{mic},\tau}(E)\hat{\mathscr{H}}\right] = \frac{\mathrm{Tr}[\hat{\mathscr{H}}\hat{G}_\tau(E)]}{\mathrm{Tr}[\hat{G}_\tau(E)]}$ Energy expectation

Represent $\hat{G}_\tau(E)$ as a sum of time-evolution operators

$$\hat{G}_\tau(E) = e^{-(\hat{\mathscr{H}}-E)^2\tau^2} = \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty} dt\, e^{-\frac{t^2}{4\tau^2}} e^{iEt}\hat{U}(t), \quad \hat{U}(t) = e^{-i\hat{\mathscr{H}}t}$$

- Gaussian of energy E = Fourier transform of gaussian of time t
- Unitary time-evolution operator $\hat{U}(t)$ appears naturally

Evaluate $\langle\phi_r|\hat{U}(t)|\phi_r\rangle$ and $\langle\phi_r|\hat{\mathscr{H}}\hat{U}(t)|\phi_r\rangle$ on a quantum computer, integrate them over t on a classical computer.

$$\mathrm{Tr}[\hat{G}_\tau(E)] \approx D\langle\langle \mathscr{N}_{\tau,r}(E)\rangle\rangle_R, \quad \mathscr{N}_{\tau,r}(E) \equiv \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty} dt\, e^{-\frac{t^2}{4\tau^2}} e^{iEt}\langle\phi_r|\hat{U}(t)|\phi_r\rangle$$

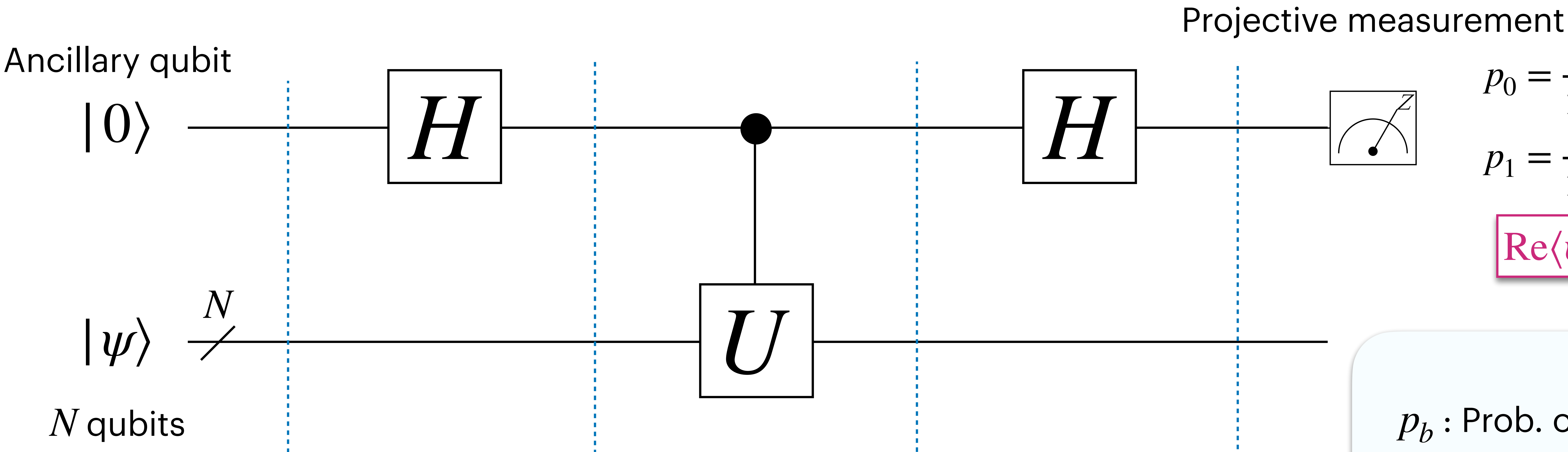
$$\mathrm{Tr}[\hat{\mathscr{H}}\hat{G}_\tau(E)] \approx D\langle\langle \mathscr{E}_{\tau,r}(E)\rangle\rangle_R, \quad \mathscr{E}_{\tau,r}(E) \equiv \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty} dt\, e^{-\frac{t^2}{4\tau^2}} e^{iEt}\langle\phi_r|\hat{\mathscr{H}}\hat{U}(t)|\phi_r\rangle$$

$$\langle\langle\cdots\rangle\rangle_R \equiv \frac{1}{R}\sum_{r=1}^{R}\cdots$$

- $e^{-\frac{t^2}{4\tau^2}}$ in the integrand: Range of the integral is effectively $O(\tau)$

Evaluation of $\mathrm{Re}\langle\psi|\hat{U}|\psi\rangle$: Hadamard test

Basis states
$\hat{Z}|0\rangle = |0\rangle$
$\hat{Z}|1\rangle = -|1\rangle$



$|0\rangle \otimes |\psi\rangle$

$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |\psi\rangle$

$\frac{1}{\sqrt{2}}(|0\rangle \otimes |\psi\rangle + |1\rangle \otimes \hat{U}|\psi\rangle)$

$$p_0 = \frac{1}{2}\left(1 + \mathrm{Re}\langle\psi|\hat{U}|\psi\rangle\right)$$
$$p_1 = \frac{1}{2}\left(1 - \mathrm{Re}\langle\psi|\hat{U}|\psi\rangle\right)$$

$$\mathrm{Re}\langle\psi|\hat{U}|\psi\rangle = p_0 - p_1$$

Born's rule

p_b : Prob. of observing $|b\rangle$ $(b = 0,1)$

$$p_b = ||\hat{P}_b|\Psi\rangle||^2 = \langle\Psi|\hat{P}_b|\Psi\rangle$$

where $\hat{P}_b = |b\rangle\langle b| \otimes \hat{1}$ is the projection onto eigenspace of $\hat{Z} \otimes \hat{1}$ associated with eigenvalue $(-1)^b$

$$|\Psi\rangle \equiv |0\rangle \otimes \frac{1+\hat{U}}{2}|\psi\rangle + |1\rangle \otimes \frac{1-\hat{U}}{2}|\psi\rangle$$

$\hat{P}_0|\Psi\rangle$ $\hat{P}_1|\Psi\rangle$

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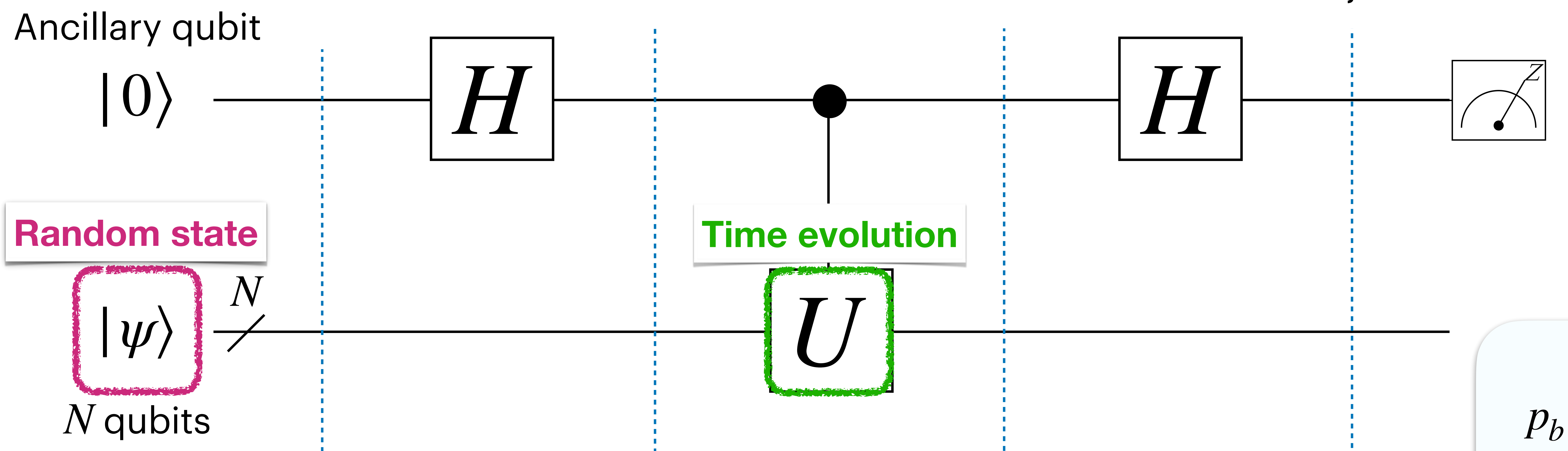

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Evaluation of $\mathrm{Im}\langle\psi|\hat{U}|\psi\rangle$: Hadamard test

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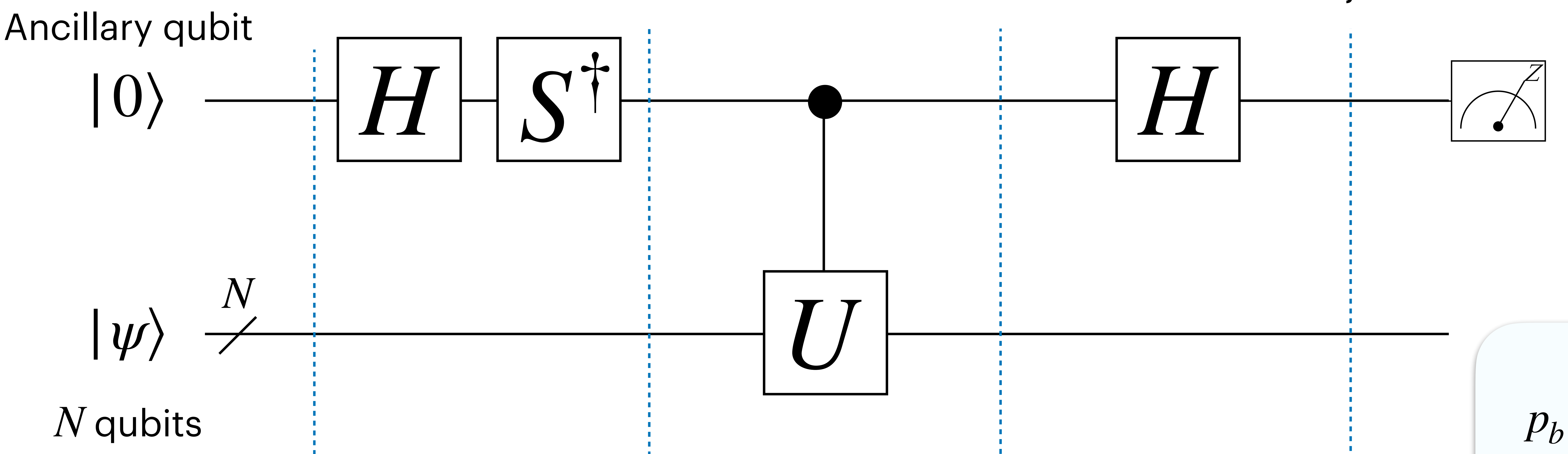
Projective measurement



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$|0\rangle \otimes |\psi\rangle$

$\frac{1}{\sqrt{2}}(|0\rangle - \mathrm{i}|1\rangle) \otimes |\psi\rangle$

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Phase gate

$$S \doteq \begin{bmatrix} 1 & 0 \\ 0 & \mathrm{i} \end{bmatrix}$$

$$|\Psi\rangle \equiv |0\rangle \otimes \underbrace{\frac{1 - \mathrm{i}\hat{U}}{2}|\psi\rangle}_{\hat{P}_0|\Psi\rangle} + \underbrace{|1\rangle \otimes \frac{1 + \mathrm{i}\hat{U}}{2}|\psi\rangle}_{\hat{P}_1|\Psi\rangle}$$

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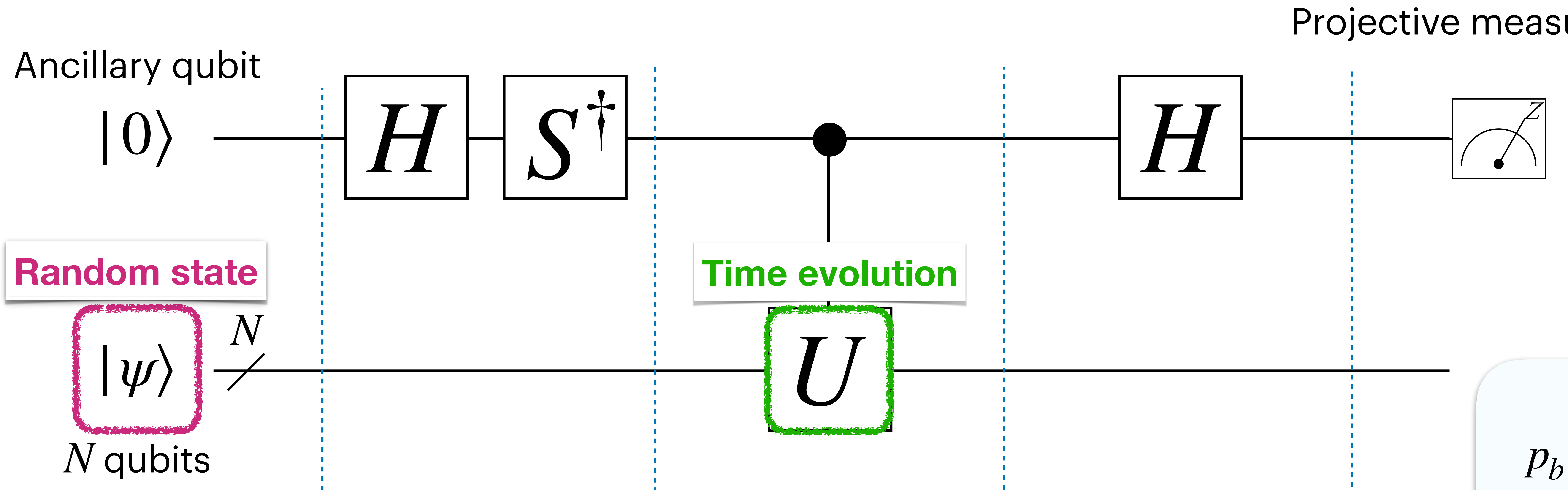

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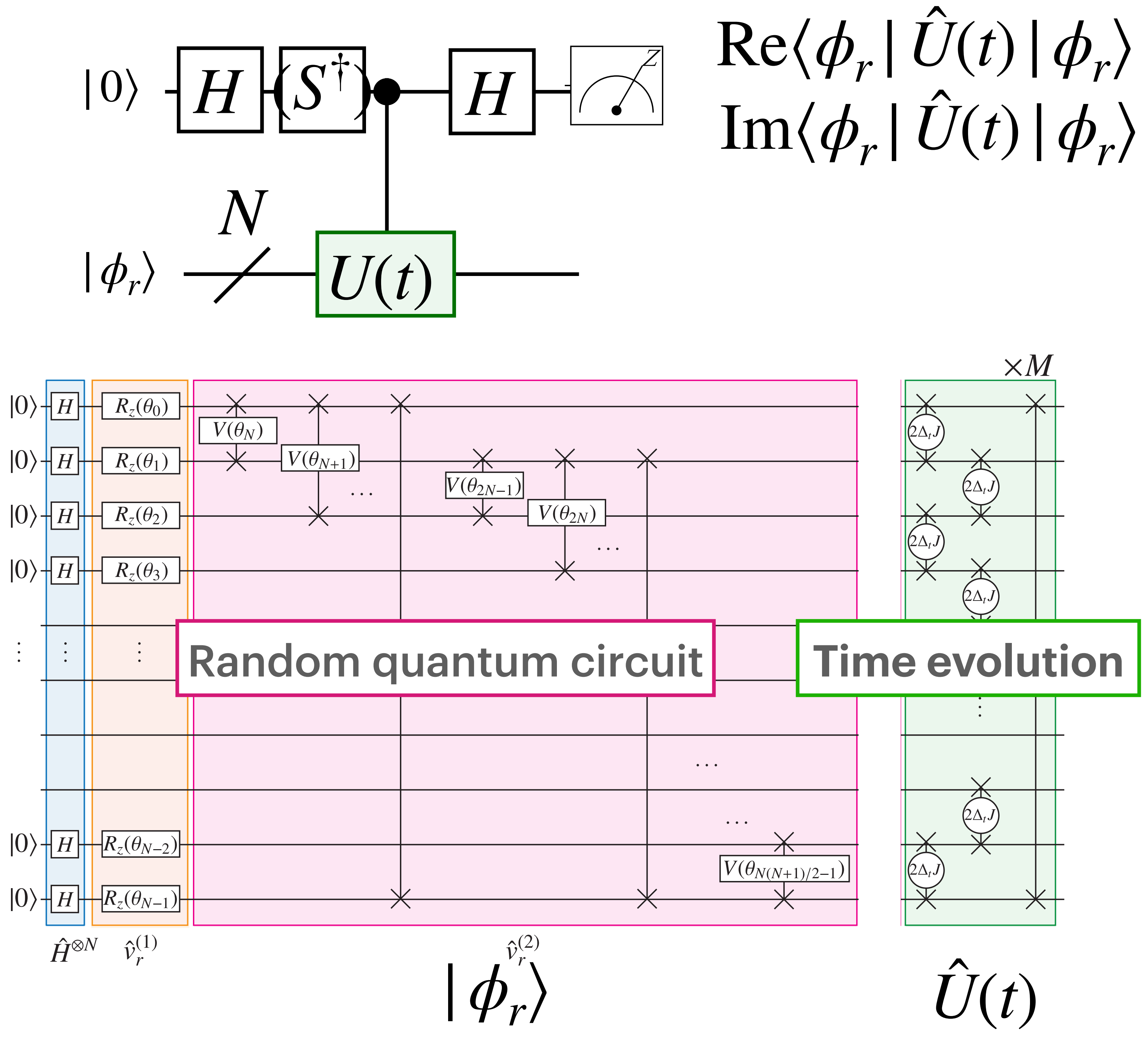
Phase gate

$$S \doteq \begin{bmatrix} 1 & 0 \\ 0 & \mathrm{i} \end{bmatrix}$$

Roles of quantum and classical computers

Quantum computer

Hadamard test

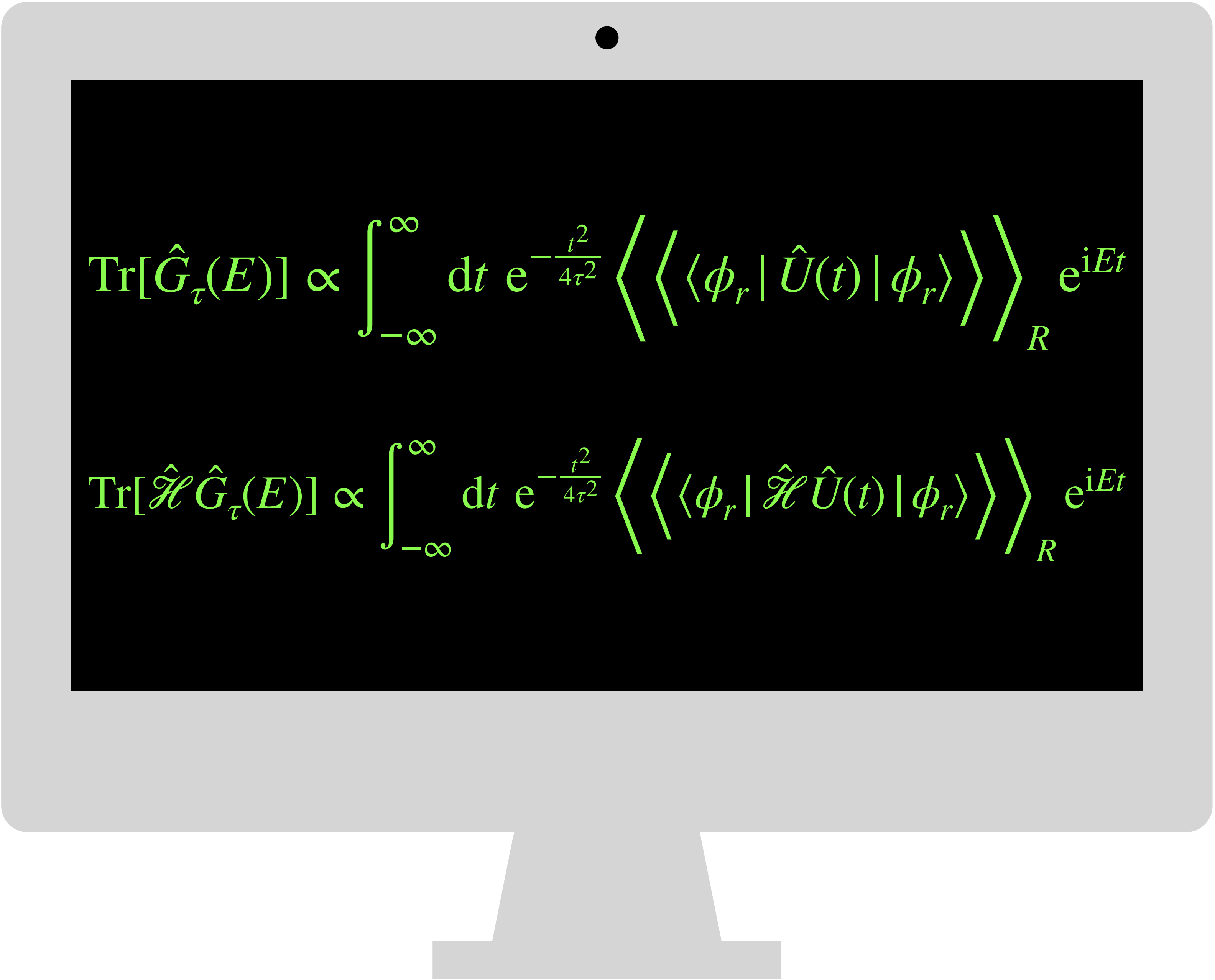


- Prepare random state $|\phi_r\rangle$ and time evolve it.
- Evaluate $\langle\phi_r|\hat{U}(t)|\phi_r\rangle$ and $\langle\phi_r|\hat{\mathscr{H}}\hat{U}(t)|\phi_r\rangle$ for $r = 1,\cdots,R$ and $0 \leqslant t \leqslant c\tau,\ c \sim O(1)$.

Classical computer

Fourier transformation

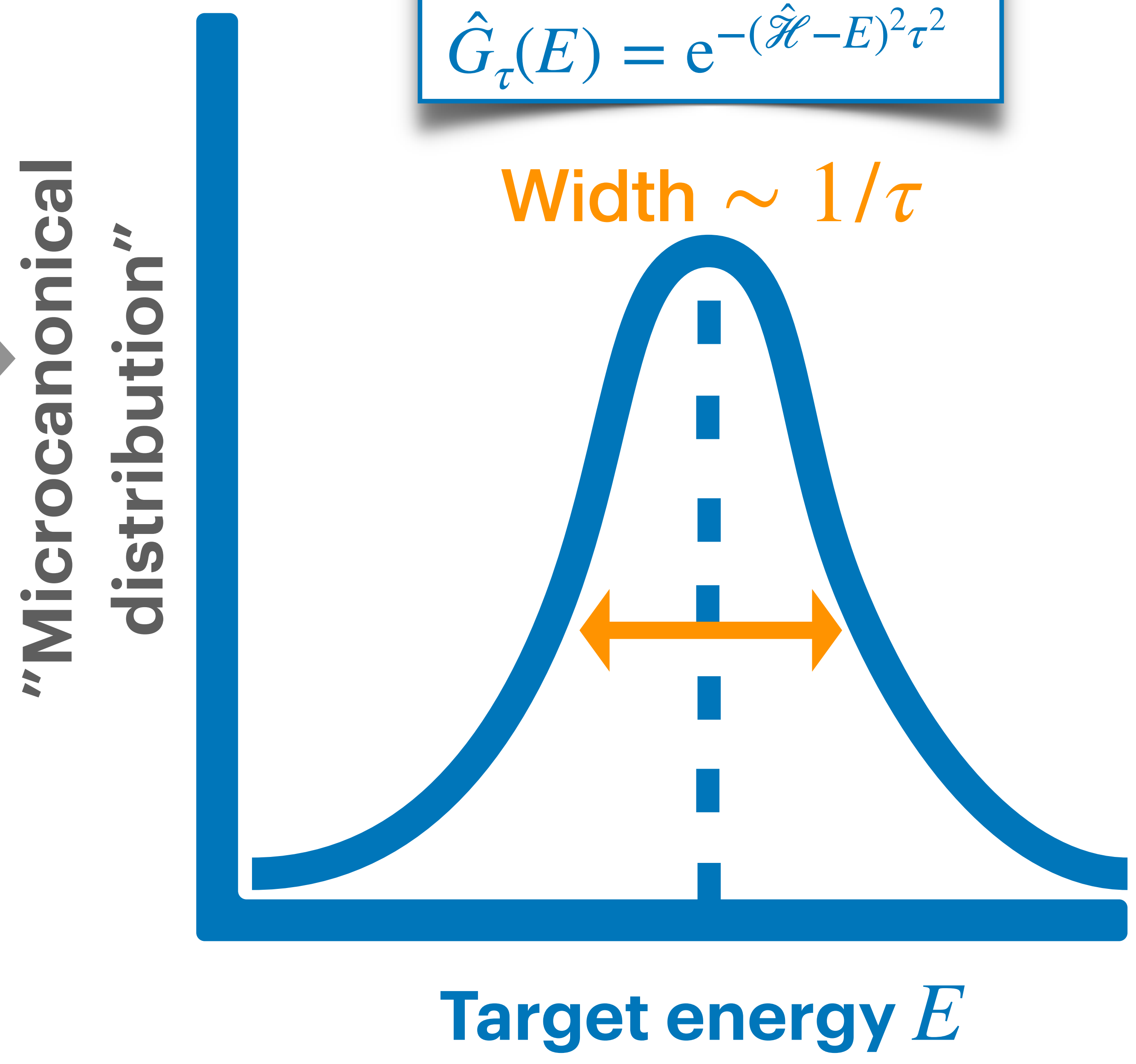
"From time-evolved states to energy-resolved states"



- Sum and Integrate $\langle\phi_r|\hat{U}(t)|\phi_r\rangle$ and $\langle\phi_r|\hat{\mathscr{H}}\hat{U}(t)|\phi_r\rangle$ over r and t.
- Target energy E can be varied solely with classical post processing.

Thermodynamic quantities

$$\hat{\rho}_{\mathrm{mic},\tau}(E) = \frac{\hat{G}_\tau(E)}{\mathrm{Tr}\left[\hat{G}_\tau(E)\right]},$$
$$\hat{G}_\tau(E) = e^{-(\hat{\mathscr{H}}-E)^2\tau^2}$$



- $S_\tau(E) = \ln \mathrm{Tr}[\hat{G}_\tau(E)]$
- $\beta_\tau(E) = \partial_E S_\tau(E) = 2\tau^2\left(\mathscr{E}_\tau(E) - E\right)$
- $\mathscr{E}_\tau(E) = \mathrm{Tr}\left[\hat{\rho}_{\mathrm{mic},\tau}(E)\hat{\mathscr{H}}\right] = \frac{\mathrm{Tr}[\hat{\mathscr{H}}\hat{G}_\tau(E)]}{\mathrm{Tr}[\hat{G}_\tau(E)]}$

Numerical results

Numerical Results

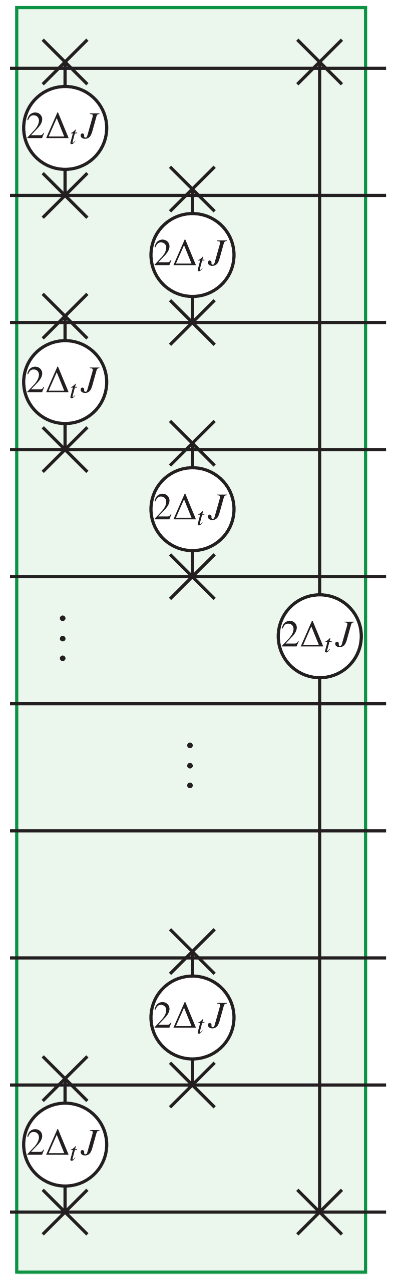
• Classical simulation

1D Heisenberg model, 20, 22, 24 and 28sites

- Time discretization : $\Delta_t J = 0.01$, number of samples $R = 64$ fixed
- First-order Suzuki-Trotter decomposition of $\hat{U}(t)$
- $\int_{-\infty}^{\infty} \mathrm{d}t \cdots \to \int_{-10\tau}^{10\tau} \mathrm{d}t \cdots$, trapezoidal rule

$$\mathrm{Tr}[\hat{G}_\tau(E)] \approx D \langle \langle \mathcal{N}_{\tau,r}(E) \rangle \rangle_R, \quad \mathcal{N}_{\tau,r}(E) \equiv \frac{1}{2\sqrt{\pi}\tau} \int_{-\infty}^{\infty} \mathrm{d}t \mathrm{e}^{-\frac{t^2}{4\tau^2}} \mathrm{e}^{\mathrm{i}Et} \langle \phi_r | \hat{U}(t) | \phi_r \rangle$$

1 time step



Suzuki-Trotter decomposition

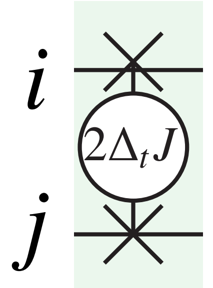
$$\hat{U}(\Delta_t) = \mathrm{e}^{-\mathrm{i}\hat{\mathscr{H}}_{\mathrm{even}}\Delta_t} \mathrm{e}^{-\mathrm{i}\hat{\mathscr{H}}_{\mathrm{odd}}\Delta_t} + O(\Delta_t^2)$$

1D Heisenberg model

$$\hat{\mathscr{H}} = J \sum_{\langle i,j \rangle} \widehat{\mathrm{SWAP}}_{ij} = 2J \sum_{\langle i,j \rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + \frac{JN_{\mathrm{bond}}}{2}$$

$$\widehat{\mathrm{SWAP}}_{ij} = \frac{1}{2} \left(\hat{X}_i \hat{X}_j + \hat{Y}_i \hat{Y}_j + \hat{Z}_i \hat{Z}_j + \hat{I}_i \hat{I}_j \right)$$

Exponential SWAP (e-SWAP) gate



$$= \exp(-\mathrm{i}\Delta_t J \widehat{\mathrm{SWAP}}_{ij})$$

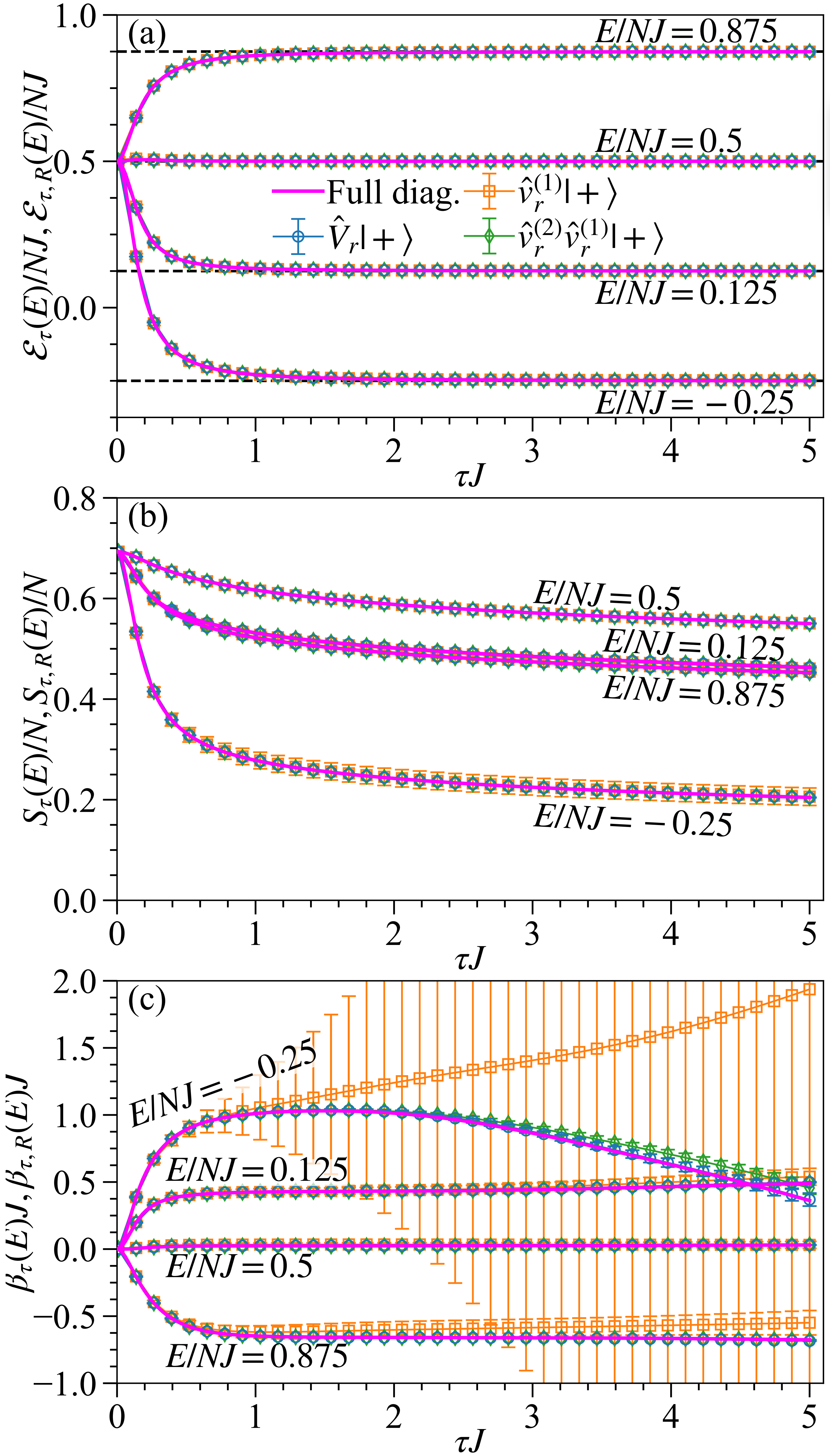
• Quantum simulation (preliminary results)

2-site Heisenberg model (No Trotter errors)

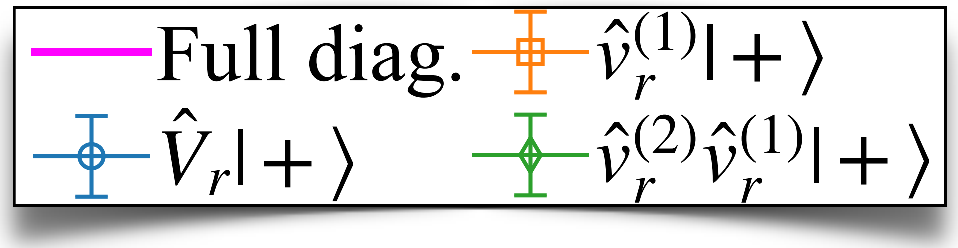
- ibm_manila (Superconducting qubits)
- ibm_kawasaki (Superconducting qubits)
- IonQ Harmony (Trapped ion qubits)

Classical simulation results

1D PBC $S = 1/2$ Heisenberg model, $N = 24$



Energy expectation/ site



$\mathscr{E}_\tau(E)$ approach E

Entropy / site

$S_\tau(E)$ decreases monotonically in τ

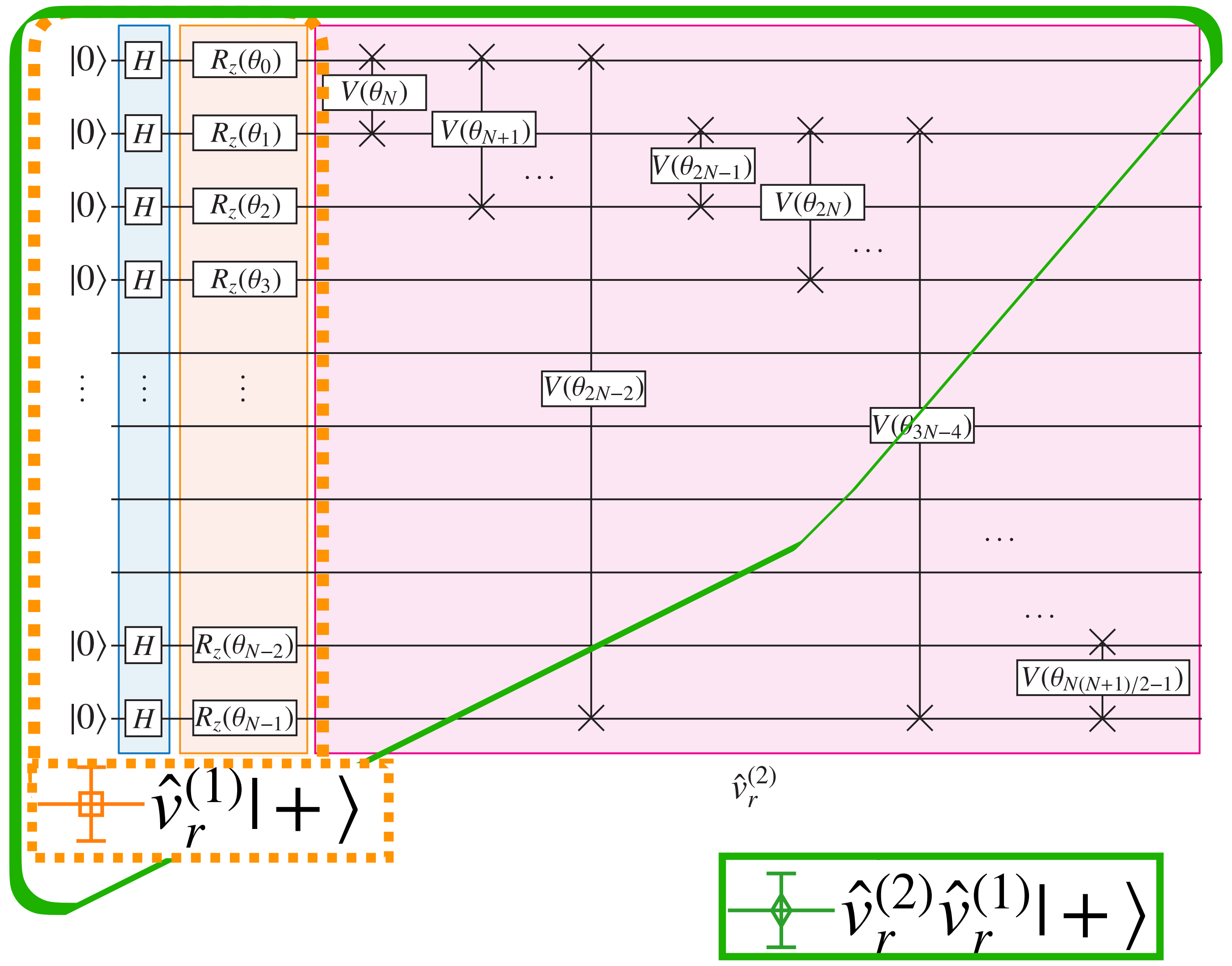
$$\frac{\partial S_\tau(E)}{\partial \tau} = \frac{\partial_\tau \mathrm{Tr}\left[\hat{G}_\tau(E)\right]}{\mathrm{Tr}\left[\hat{G}_\tau(E)\right]} \leqslant 0$$

Inverse temperature

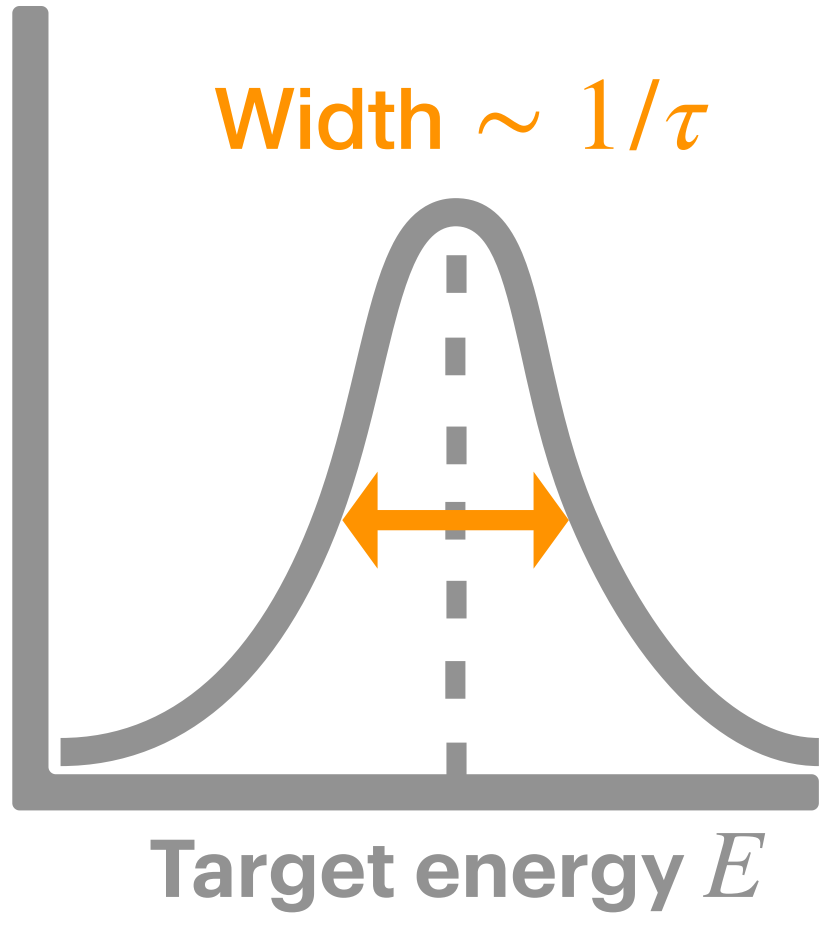
Sign of $\mathscr{E}_\tau(E) - E$ determines sign of $\beta_\tau(E)$

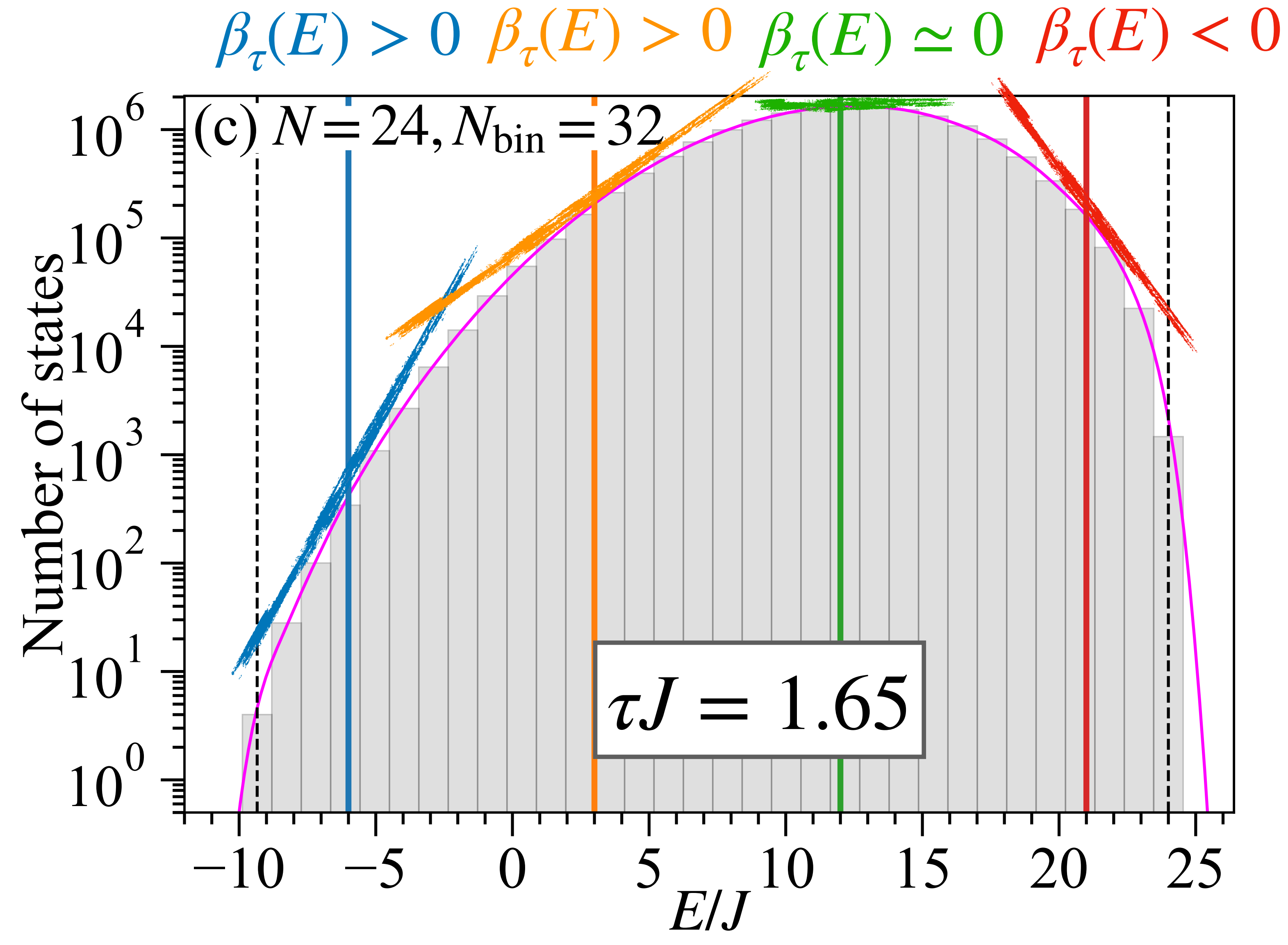
$$\beta_\tau(E) = \partial_E S_\tau(E) = 2\tau^2\left(\mathscr{E}_\tau(E) - E\right)$$

Random states



Energy window



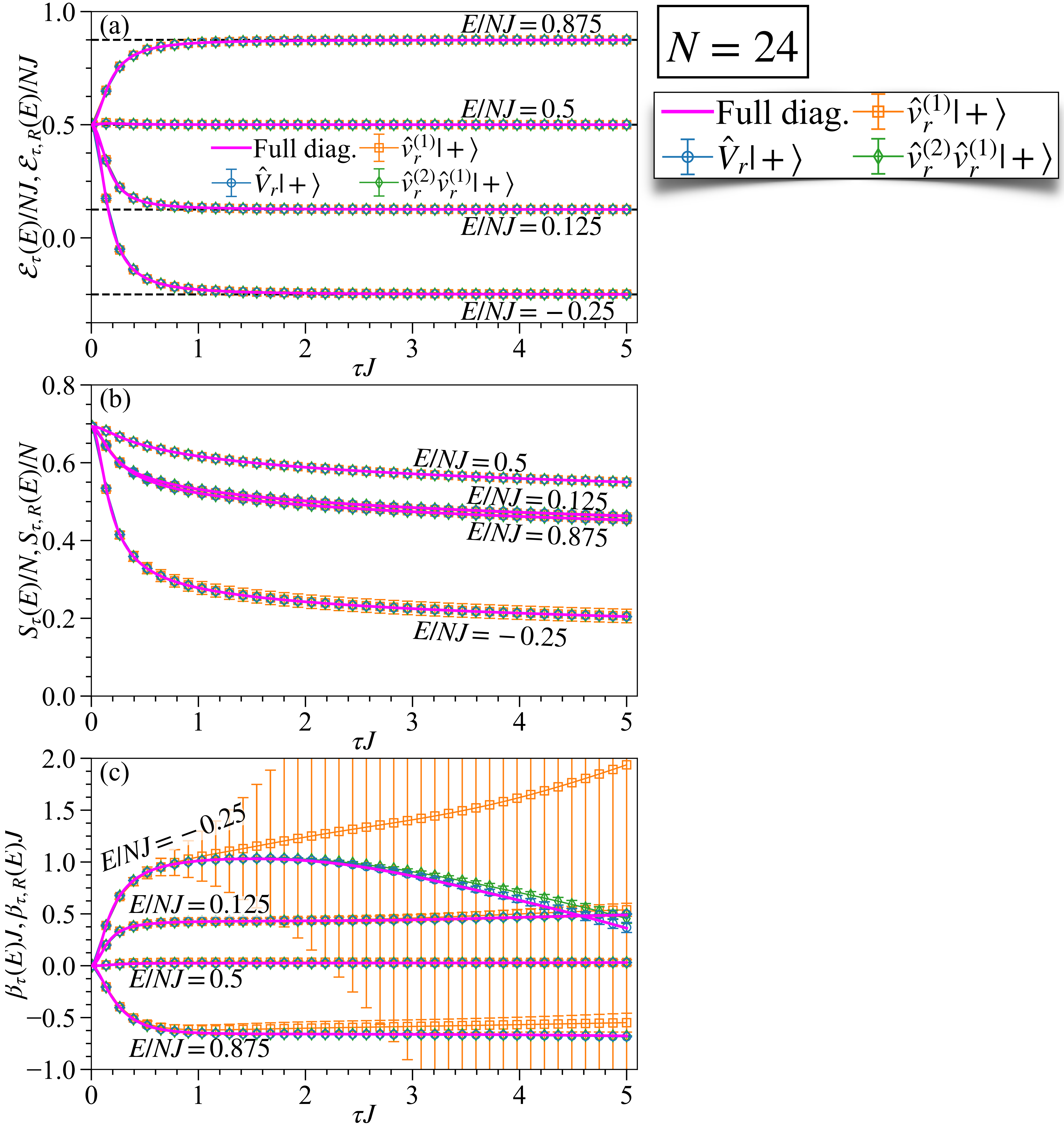


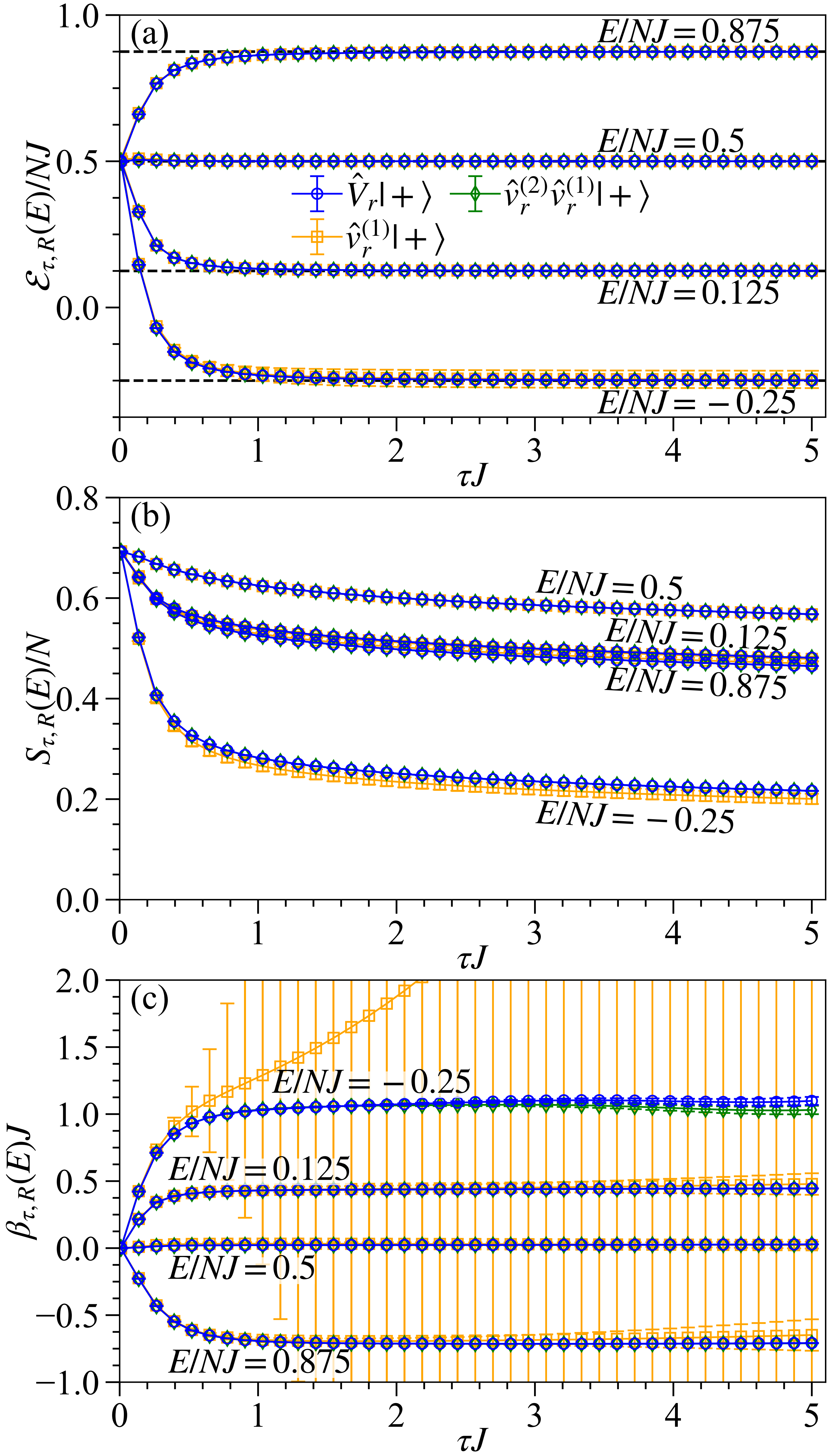
Target energies $E/NJ = -0.25, 0.125, 0.5, 0.875$

Importance of the number of states for thermodynamic quantities

e.g., $\beta_\tau(E)$ frequently changes its sign with increasing E

1D PBC $S = 1/2$ Heisenberg model, $N = 24$ and 28





$N = 28$

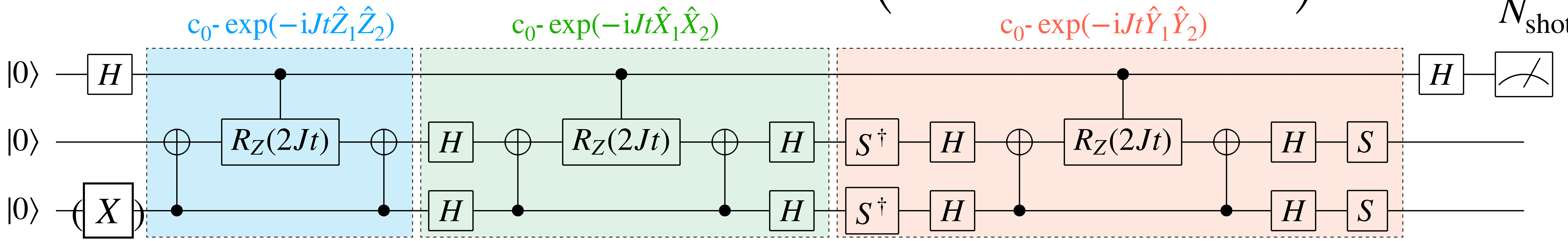
(No full-diagonalization results)

Quantum simulation results

Test on ibm_manila (work in progress)

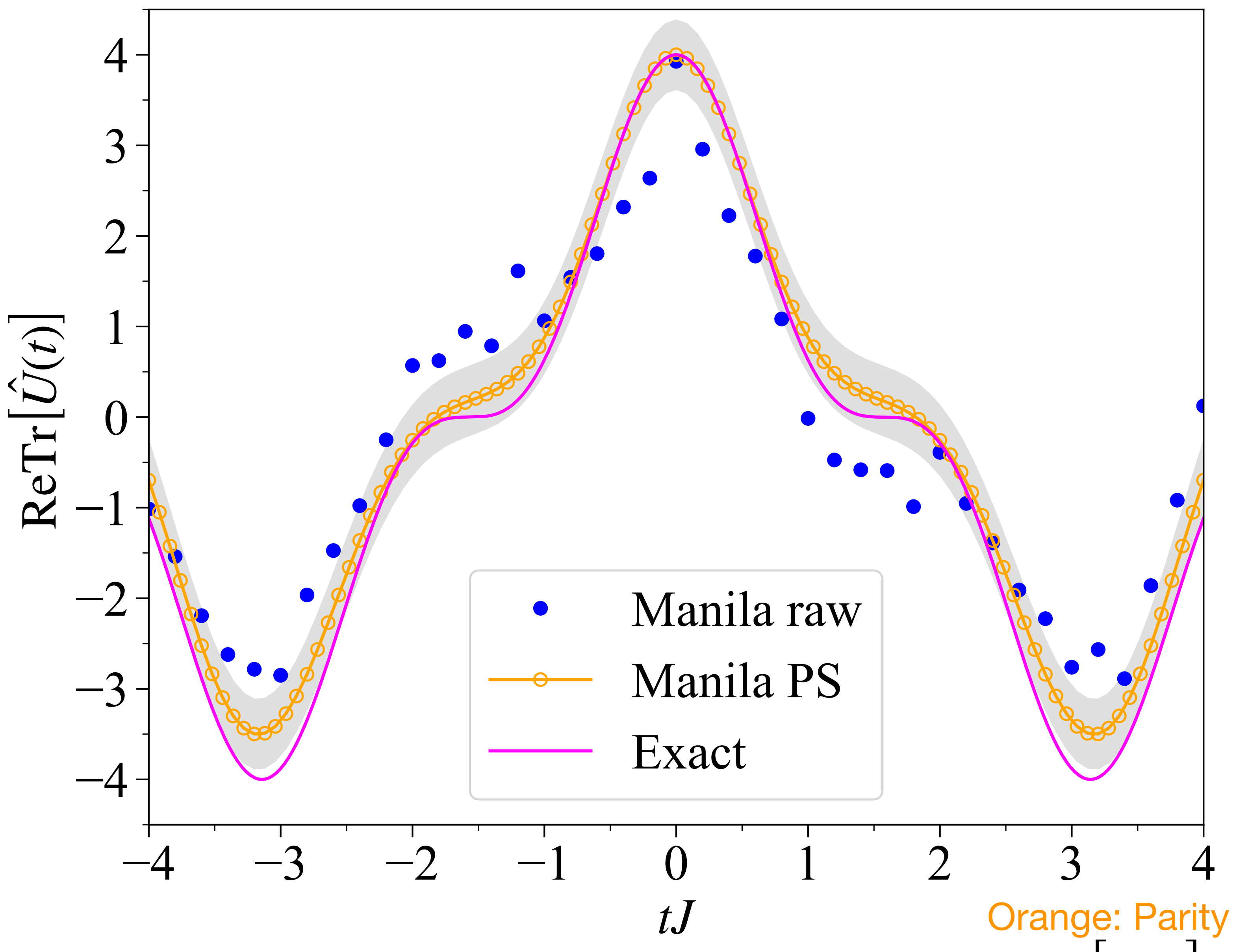
Two-site Heisenberg model: $\mathscr{H} = J\left(\hat{X}_1\hat{X}_2 + \hat{Y}_1\hat{Y}_2 + \hat{Z}_1\hat{Z}_2\right)$

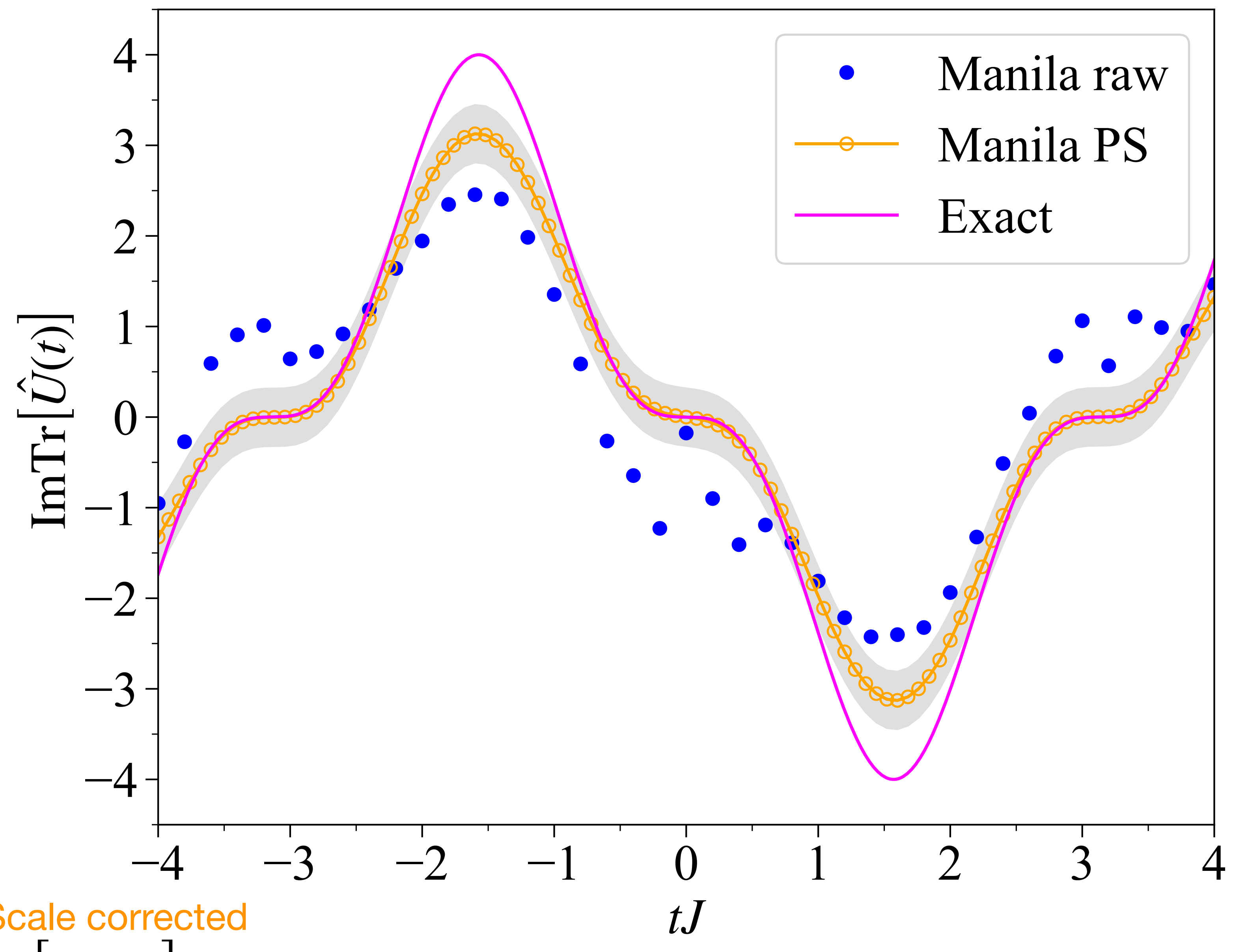
$N_{\rm shot} = 4096$

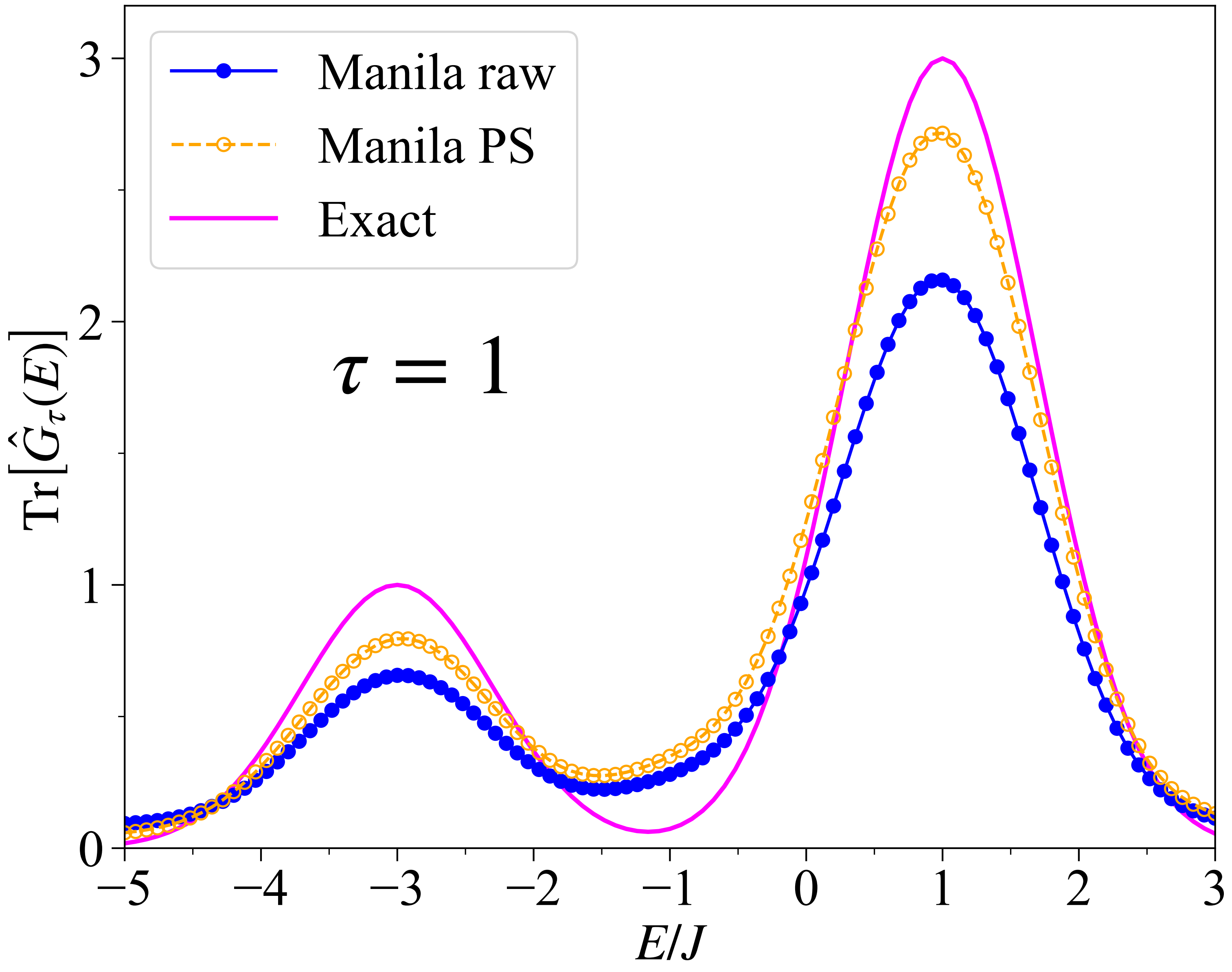


Evaluate $\langle 00|\hat{U}(t)|00\rangle$ **and** $\langle 01|\hat{U}(t)|01\rangle$

$${\rm Tr}\left[\hat{G}_\tau(E)\right] = e^{-(E+3J)^2\tau^2} + 3e^{-(E-J)^2\tau^2}$$







Orange: Parity and Scale corrected

$${\rm ReTr}\left[\hat{U}(t)\right] = {\rm ReTr}\left[\hat{U}(-t)\right]$$

$${\rm ImTr}\left[\hat{U}(t)\right] = -{\rm ImTr}\left[\hat{U}(-t)\right]$$

$${\rm ReTr}\left[\hat{U}(0)\right]/D = 1$$

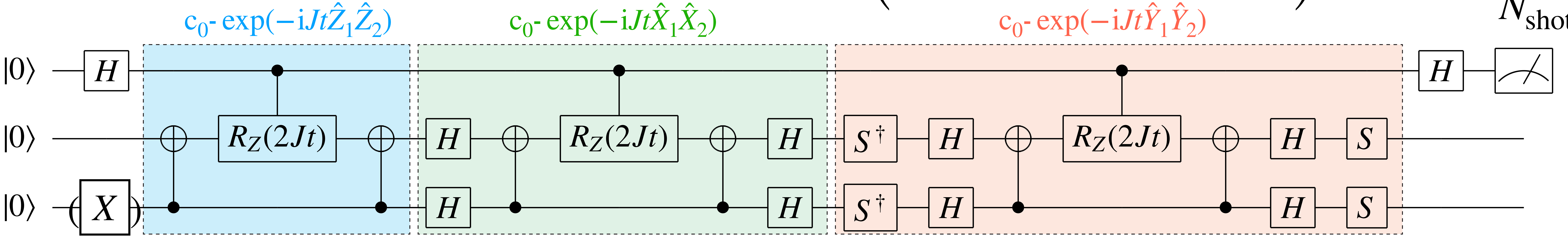
$$D = 2^2 = 4$$

$${\rm Tr}\left[\hat{G}_\tau(E)\right] = \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty} dt e^{-\frac{t^2}{4\tau^2}} e^{iEt}{\rm Tr}\left[\hat{U}(t)\right]$$

Test on ibm_kawasaki (work in progress)

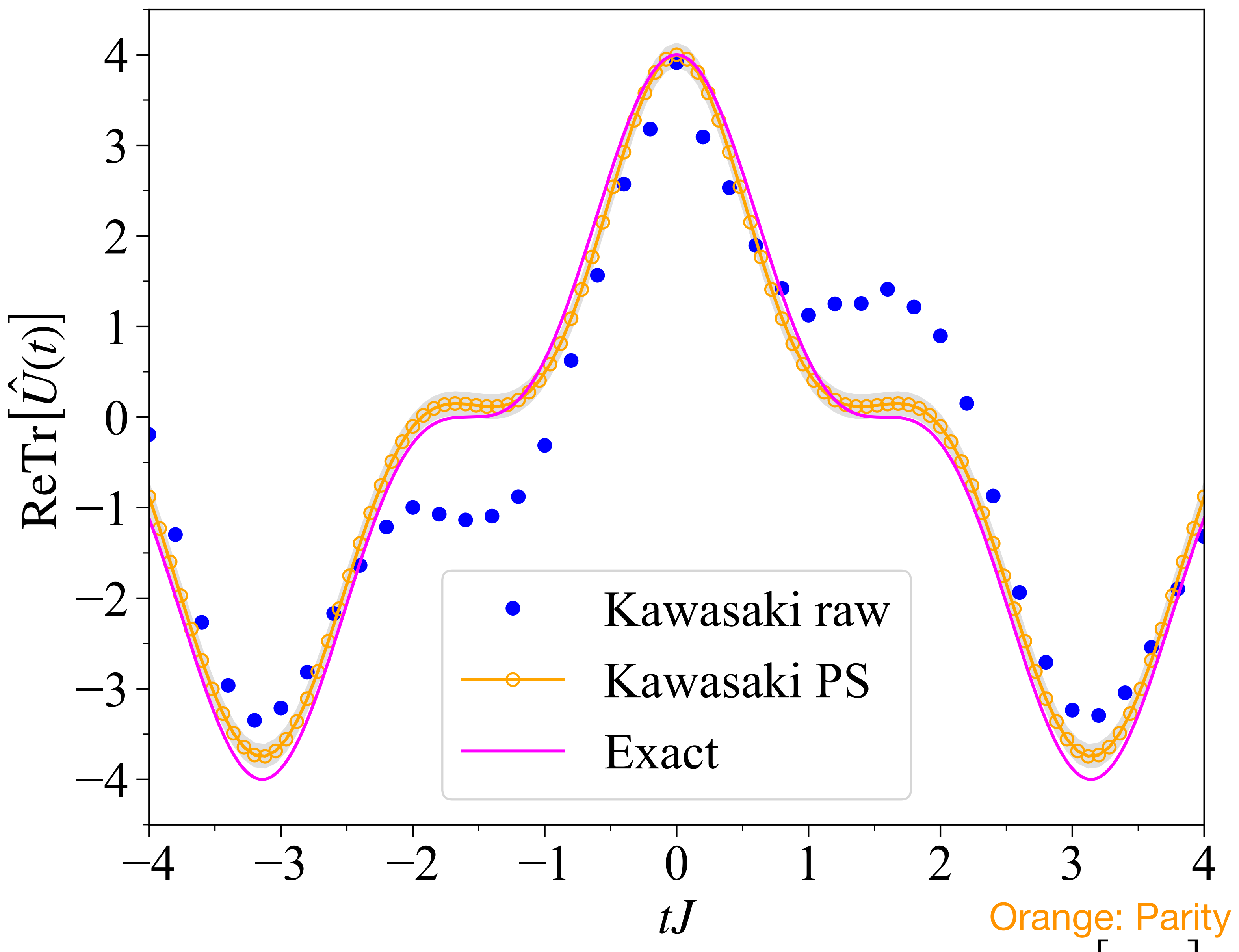
Two-site Heisenberg model: $\mathscr{H} = J\left(\hat{X}_1\hat{X}_2 + \hat{Y}_1\hat{Y}_2 + \hat{Z}_1\hat{Z}_2\right)$

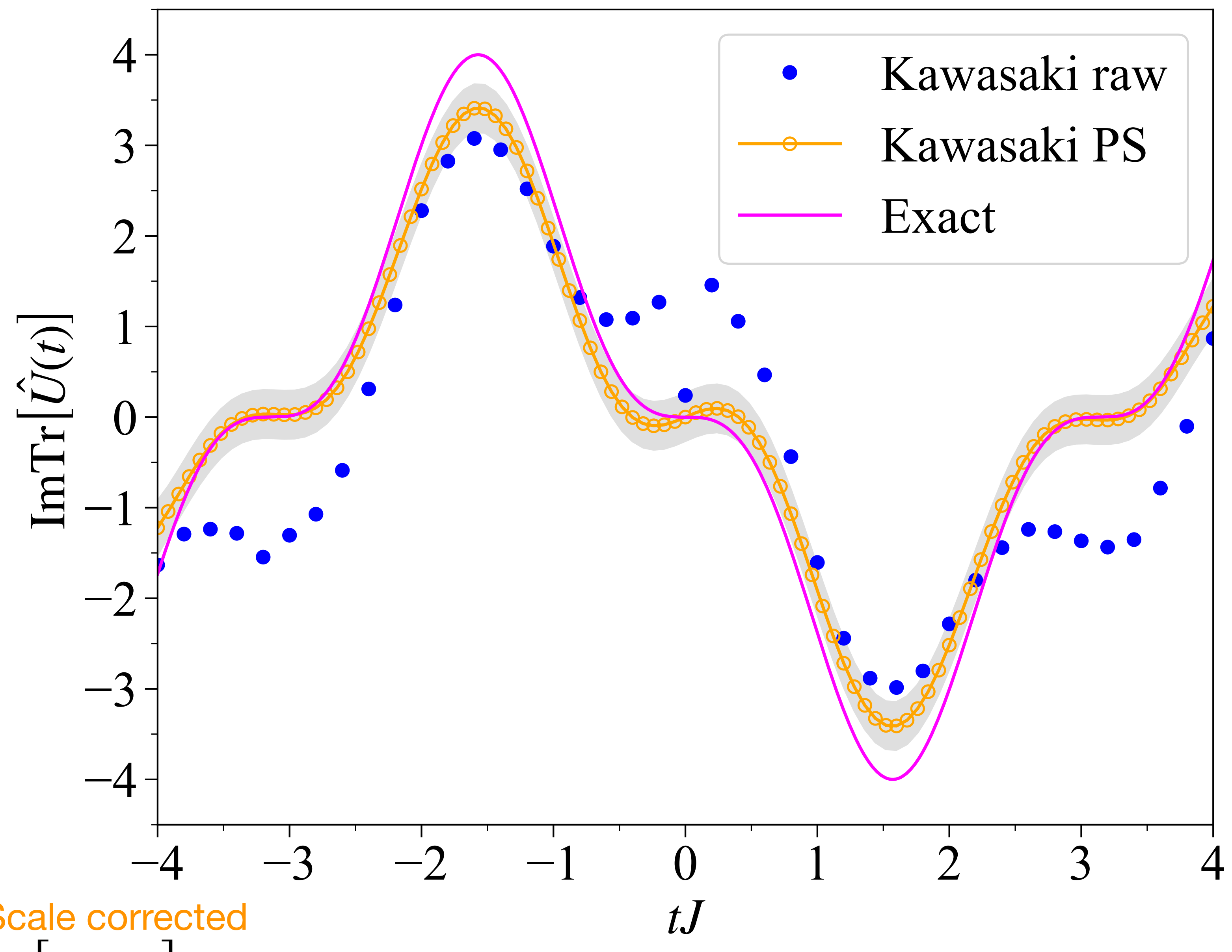
$N_{\mathrm{shot}} = 4096$

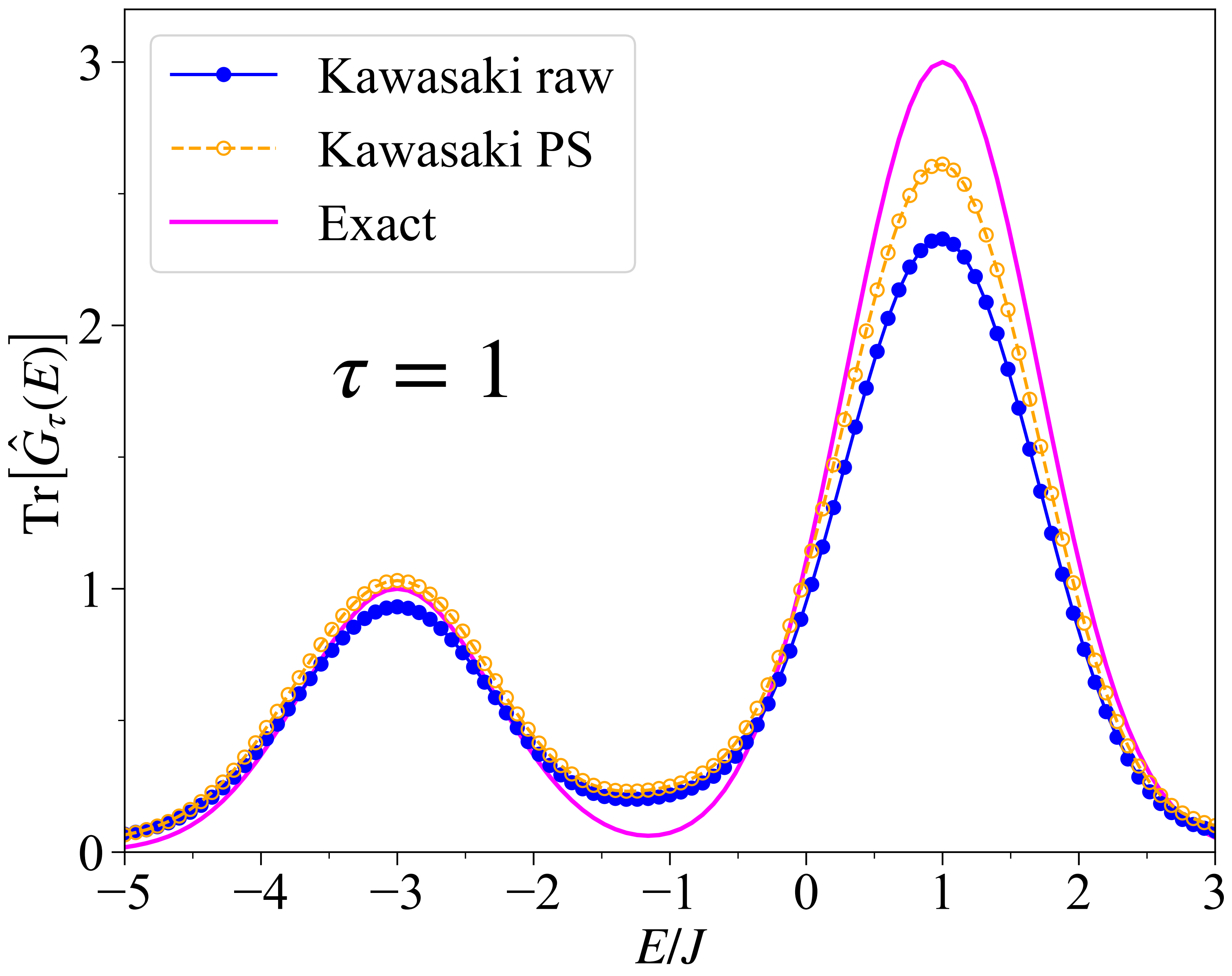


Evaluate $\langle 00|\hat{U}(t)|00\rangle$ **and** $\langle 01|\hat{U}(t)|01\rangle$

$$\mathrm{Tr}\left[\hat{G}_\tau(E)\right] = \mathrm{e}^{-(E+3J)^2\tau^2} + 3\mathrm{e}^{-(E-J)^2\tau^2}$$







Orange: Parity and Scale corrected

$$\mathrm{ReTr}\left[\hat{U}(t)\right] = \mathrm{ReTr}\left[\hat{U}(-t)\right]$$

$$\mathrm{ImTr}\left[\hat{U}(t)\right] = -\,\mathrm{ImTr}\left[\hat{U}(-t)\right]$$

$$\mathrm{ReTr}\left[\hat{U}(0)\right]/D = 1$$

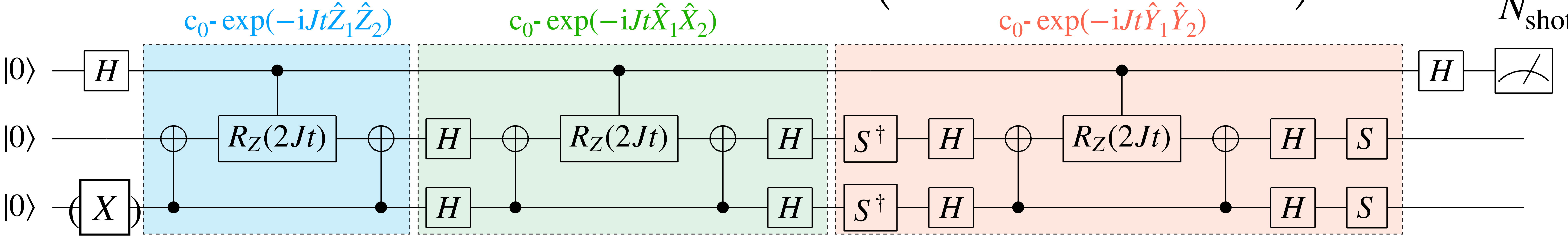
$$D = 2^2 = 4$$

$$\mathrm{Tr}\left[\hat{G}_\tau(E)\right] = \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty} \mathrm{d}t\,\mathrm{e}^{-\frac{t^2}{4\tau^2}}\mathrm{e}^{\mathrm{i}Et}\mathrm{Tr}\left[\hat{U}(t)\right]$$

Test on IonQ (work in progress)

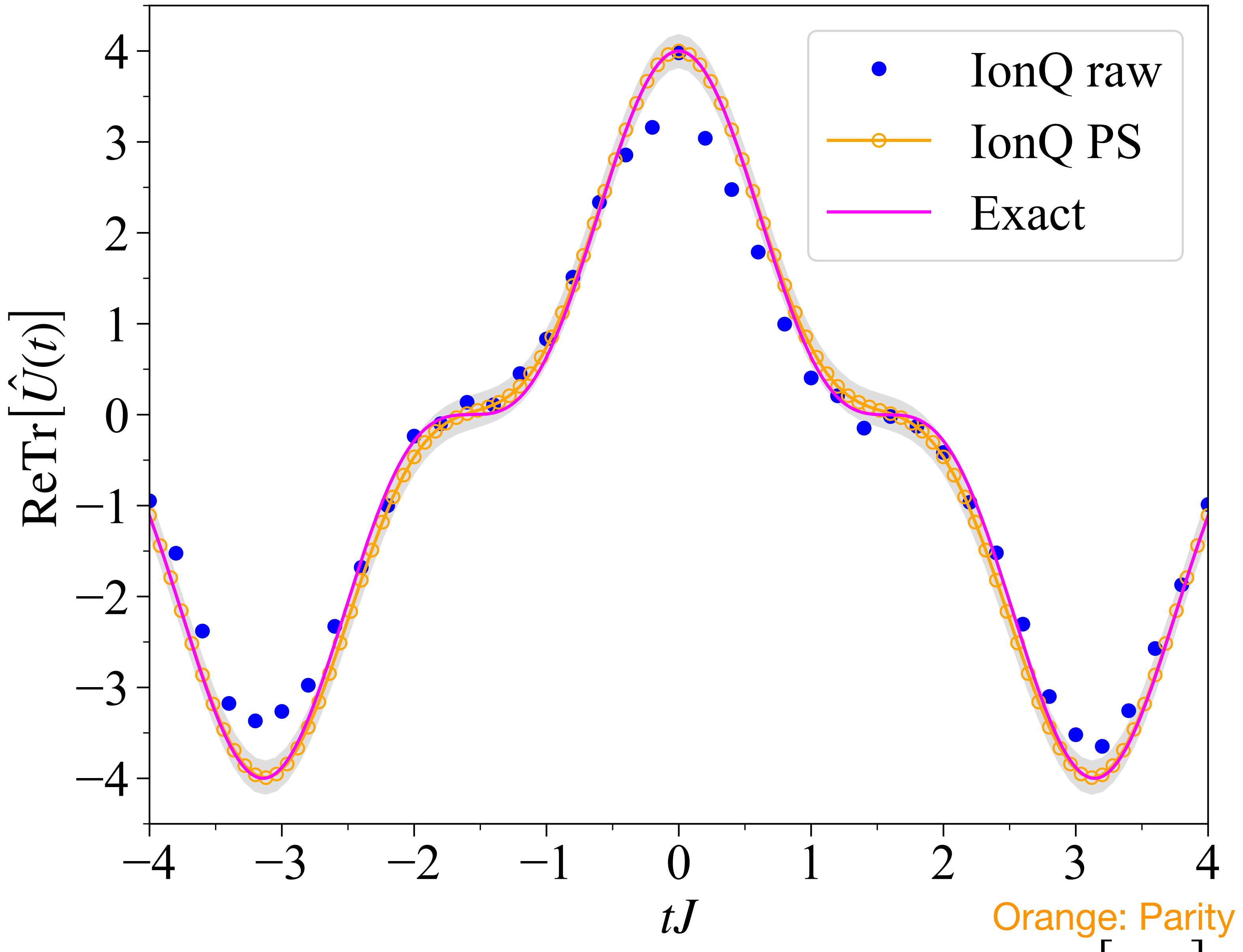
Two-site Heisenberg model: $\mathscr{H} = J\left(\hat{X}_1\hat{X}_2 + \hat{Y}_1\hat{Y}_2 + \hat{Z}_1\hat{Z}_2\right)$

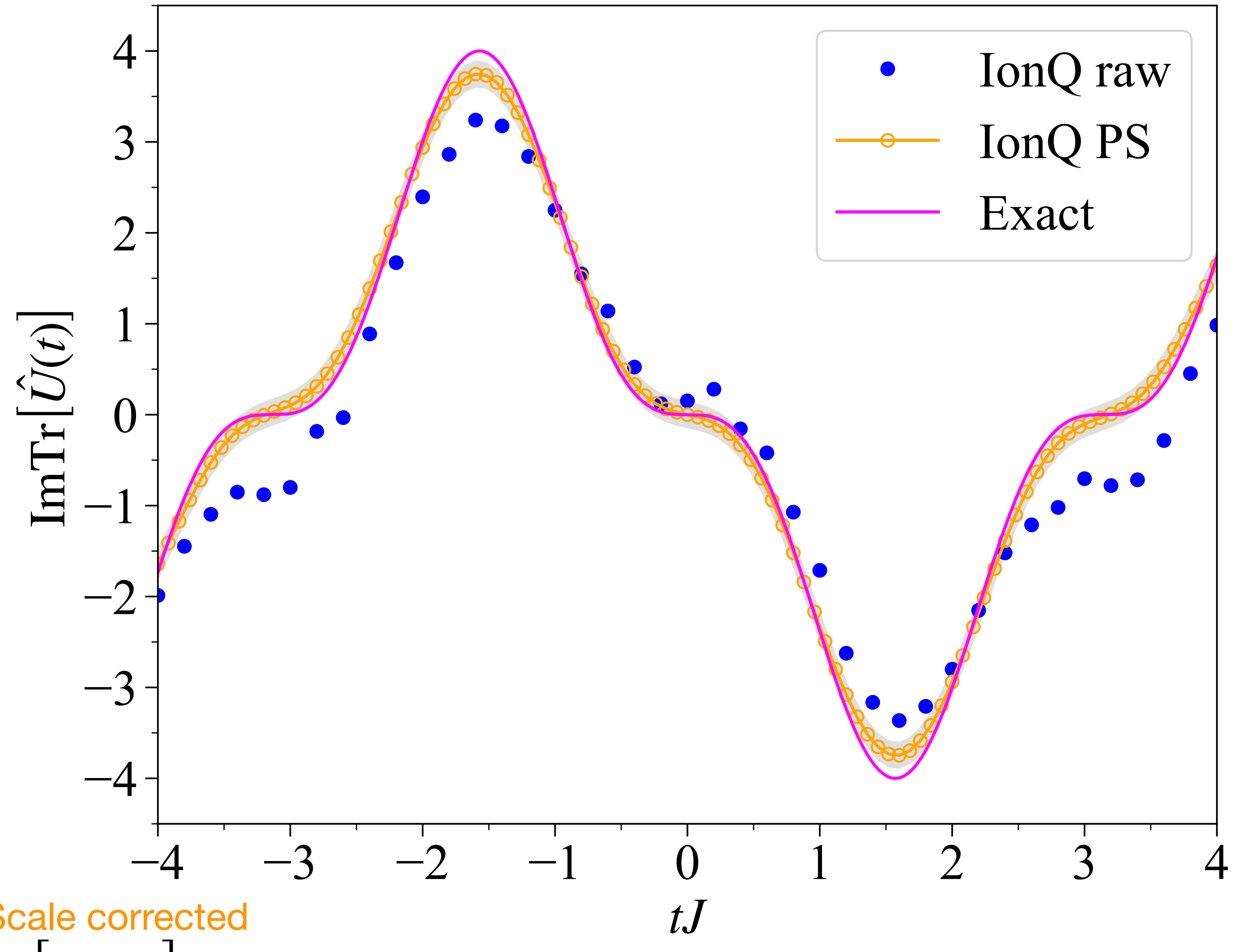
$N_{\text{shot}} = 4096$

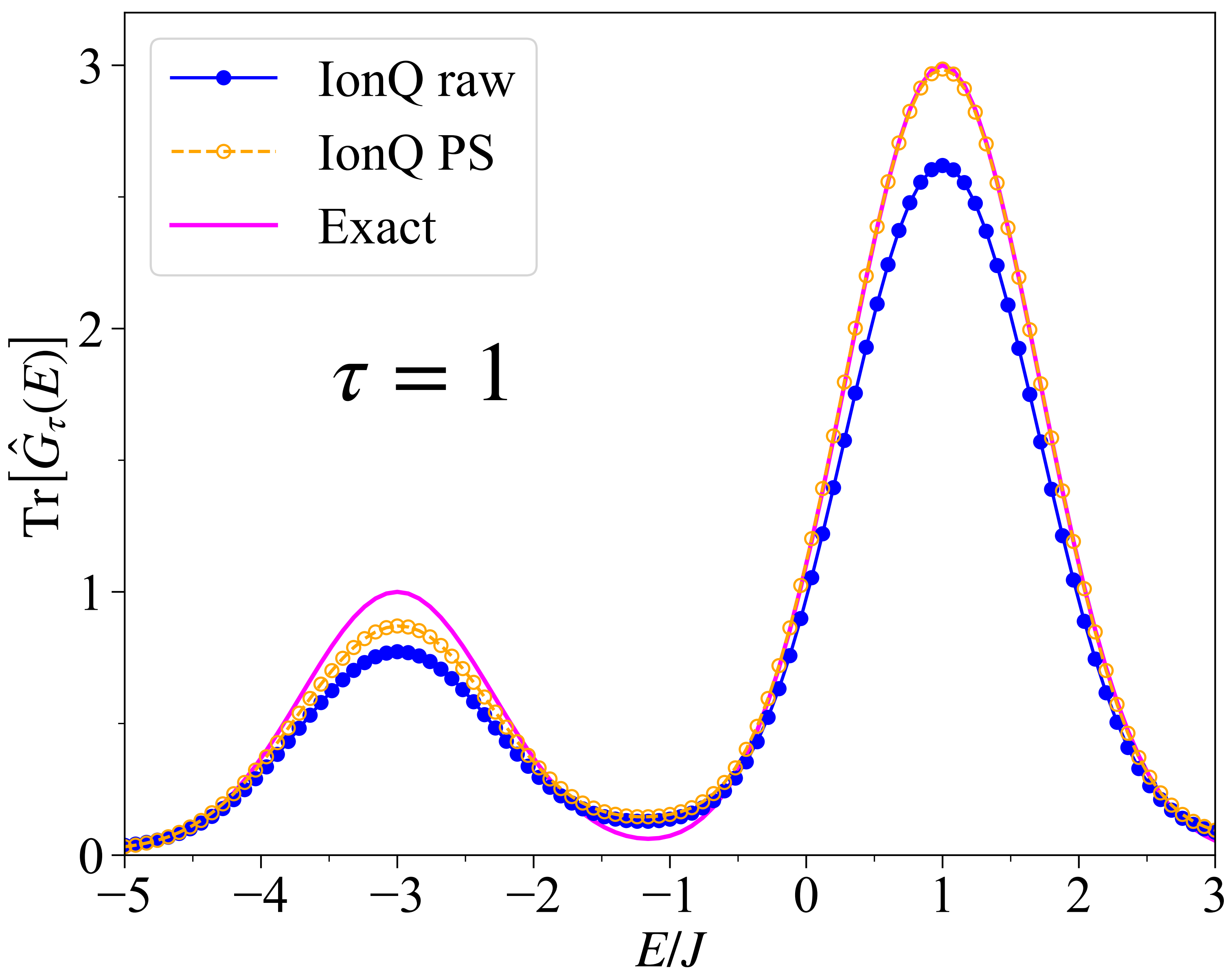


Evaluate $\langle 00 | \hat{U}(t) | 00 \rangle$ **and** $\langle 01 | \hat{U}(t) | 01 \rangle$

$\mathrm{Tr}\left[\hat{G}_\tau(E)\right] = e^{-(E+3J)^2\tau^2} + 3e^{-(E-J)^2\tau^2}$







Orange: Parity and Scale corrected

$\mathrm{ReTr}\left[\hat{U}(t)\right] = \mathrm{ReTr}\left[\hat{U}(-t)\right]$

$\mathrm{ImTr}\left[\hat{U}(t)\right] = -\,\mathrm{ImTr}\left[\hat{U}(-t)\right]$

$\mathrm{ReTr}\left[\hat{U}(0)\right]/D = 1$

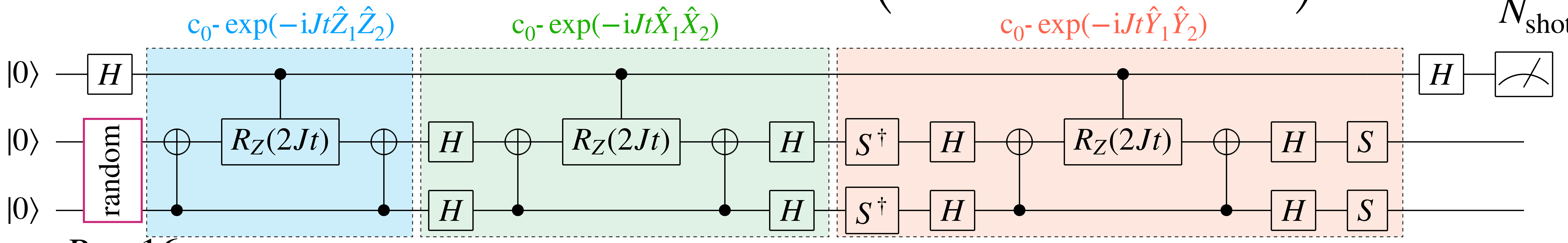
$D = 2^2 = 4$

$$\mathrm{Tr}\left[\hat{G}_\tau(E)\right] = \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty} dt\, e^{-\frac{t^2}{4\tau^2}} e^{iEt}\,\mathrm{Tr}\left[\hat{U}(t)\right]$$

Test on ibm_kawasaki with random states (work in progress)

Two-site Heisenberg model: $\mathscr{H} = J\left(\hat{X}_1\hat{X}_2 + \hat{Y}_1\hat{Y}_2 + \hat{Z}_1\hat{Z}_2\right)$

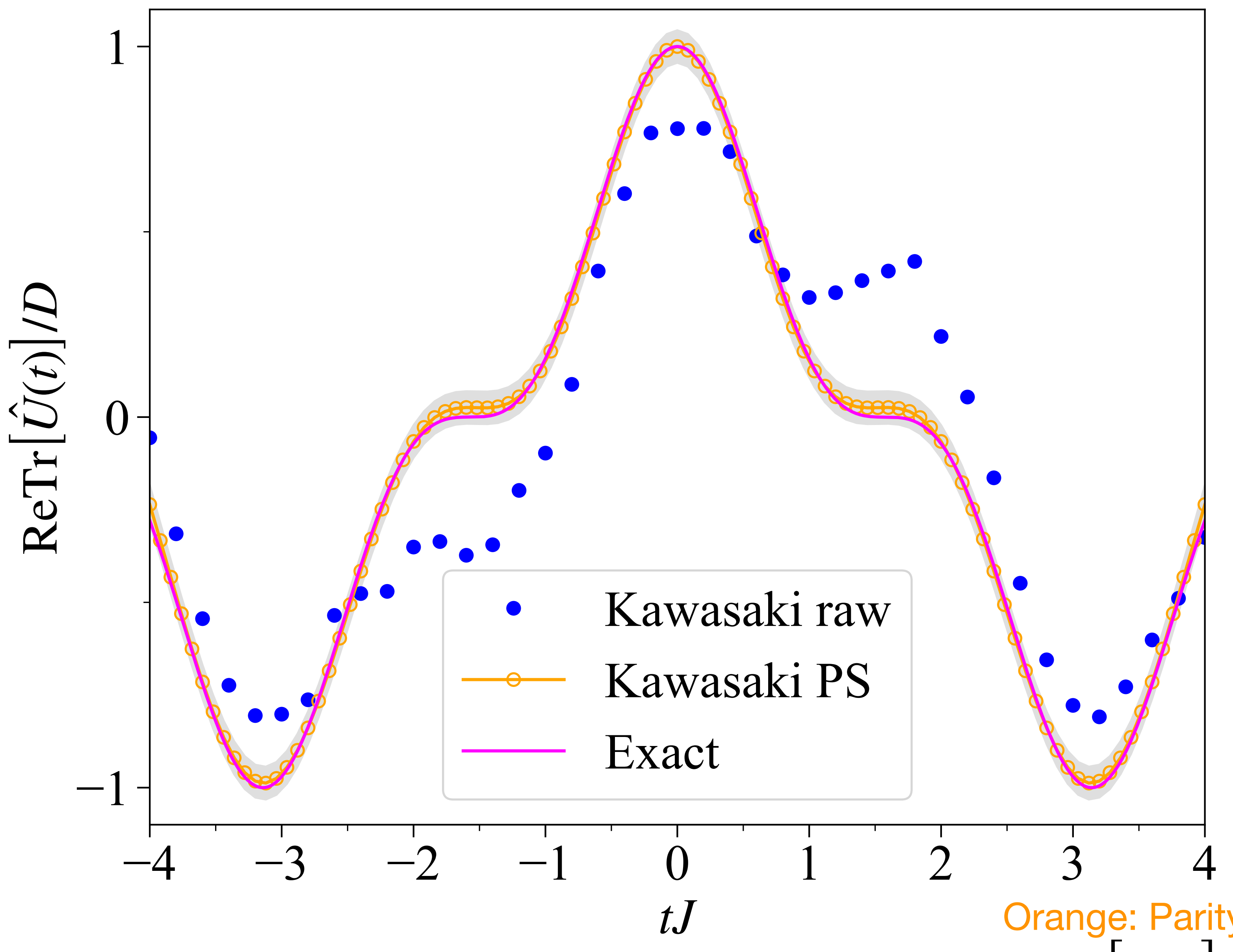
$N_{\mathrm{shot}} = 4096$

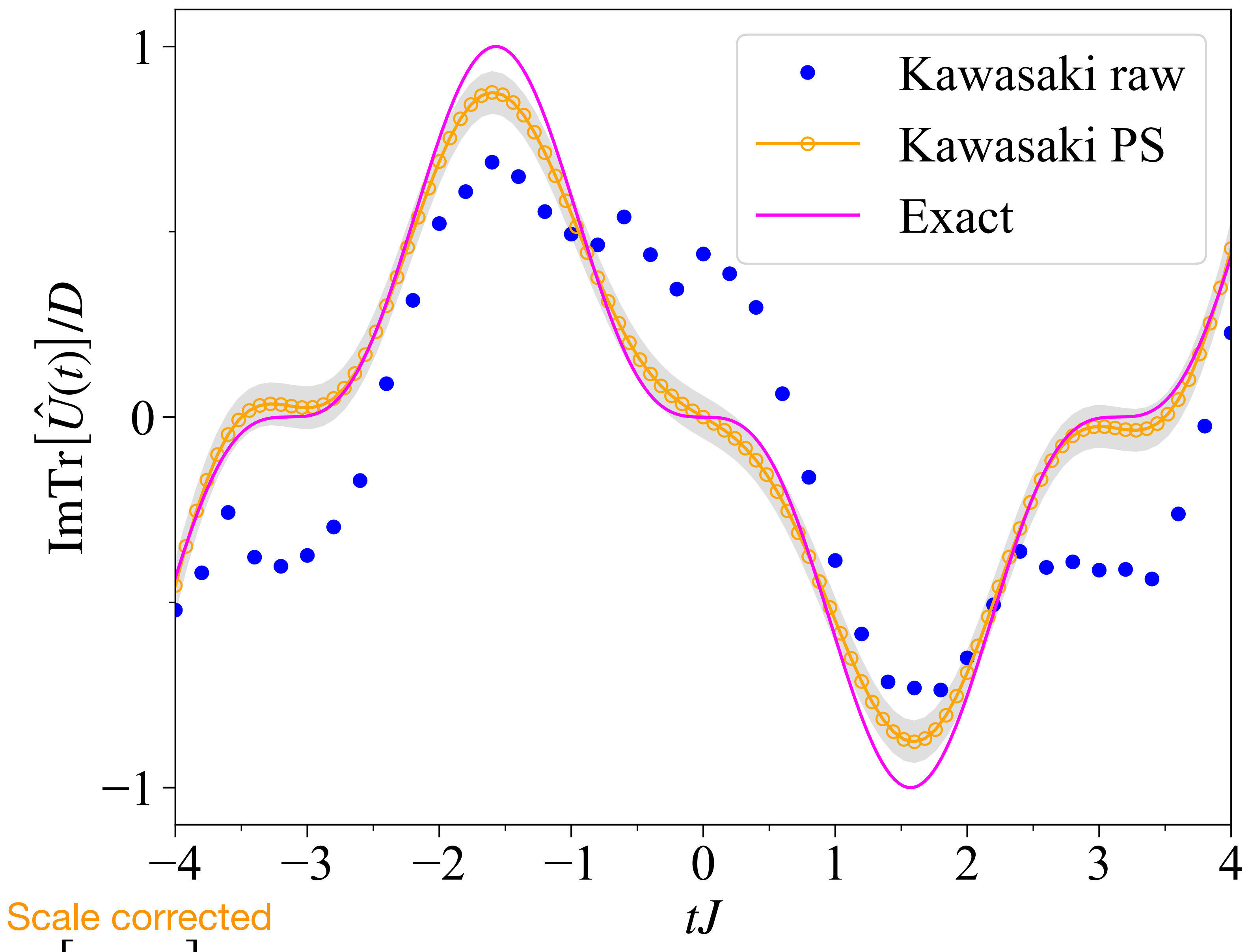


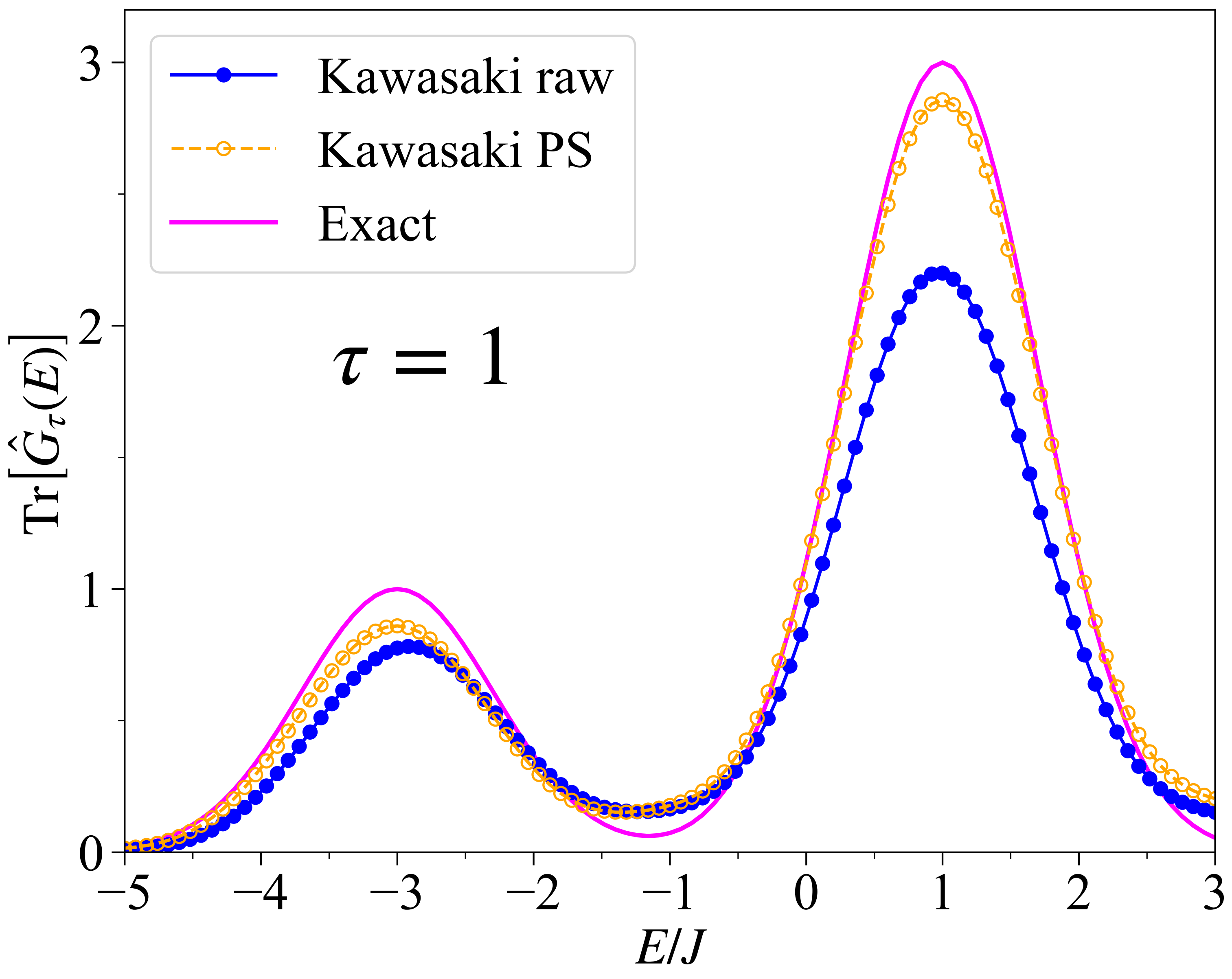
$R = 16$

Evaluate $\mathrm{Tr}[\hat{U}(t)]/D$ **directly**

$$\mathrm{Tr}\left[\hat{G}_\tau(E)\right] = \mathrm{e}^{-(E+3J)^2\tau^2} + 3\mathrm{e}^{-(E-J)^2\tau^2}$$







Orange: Parity and Scale corrected

$$\mathrm{ReTr}\left[\hat{U}(t)\right] = \mathrm{ReTr}\left[\hat{U}(-t)\right]$$

$$\mathrm{ImTr}\left[\hat{U}(t)\right] = -\,\mathrm{ImTr}\left[\hat{U}(-t)\right]$$

$$\mathrm{ReTr}\left[\hat{U}(0)\right]/D = 1$$

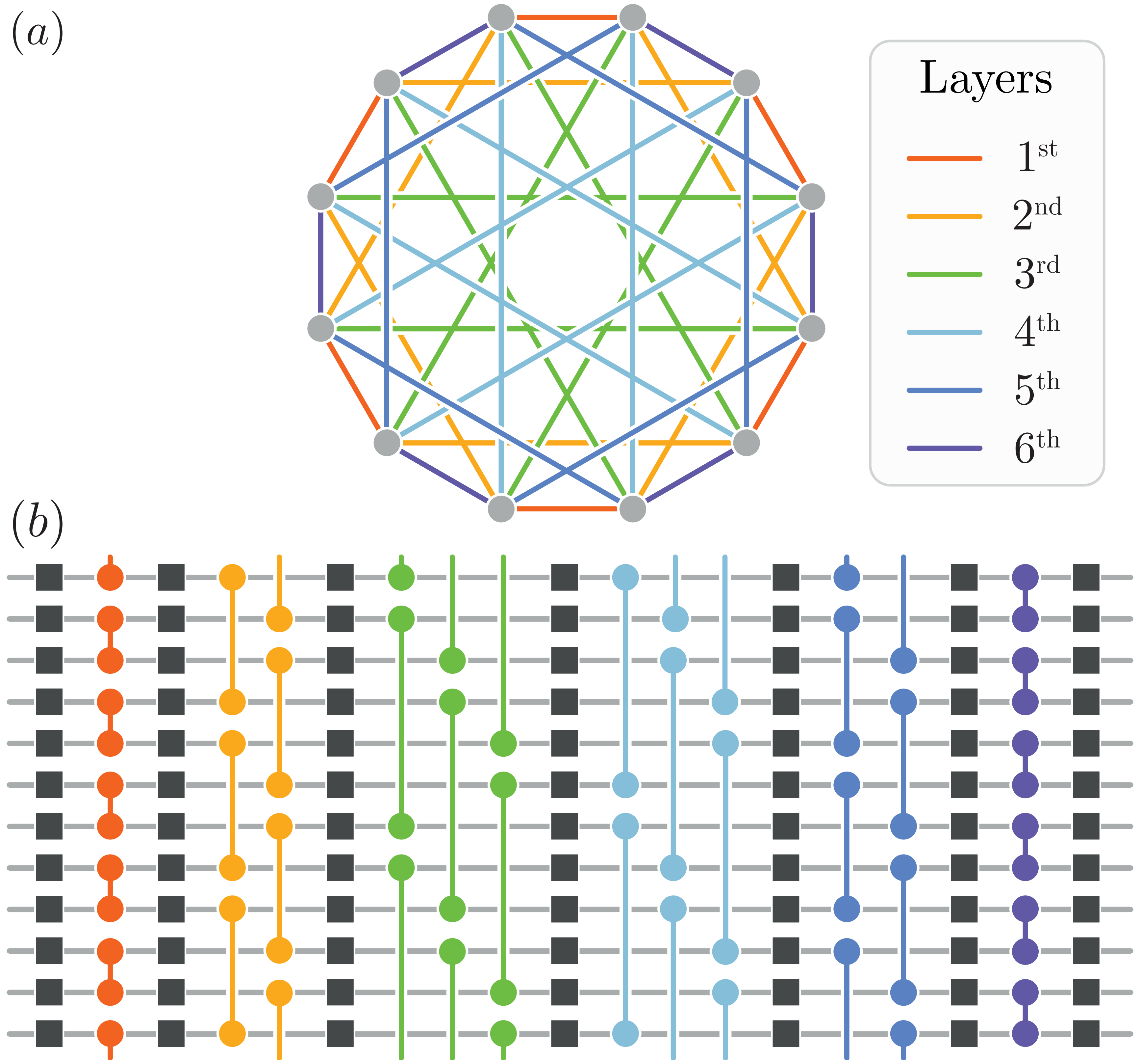
$D = 2^2 = 4$

$$\mathrm{Tr}\left[\hat{G}_\tau(E)\right] = \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty} \mathrm{d}t\,\mathrm{e}^{-\frac{t^2}{4\tau^2}}\mathrm{e}^{\mathrm{i}Et}\mathrm{Tr}\left[\hat{U}(t)\right]$$

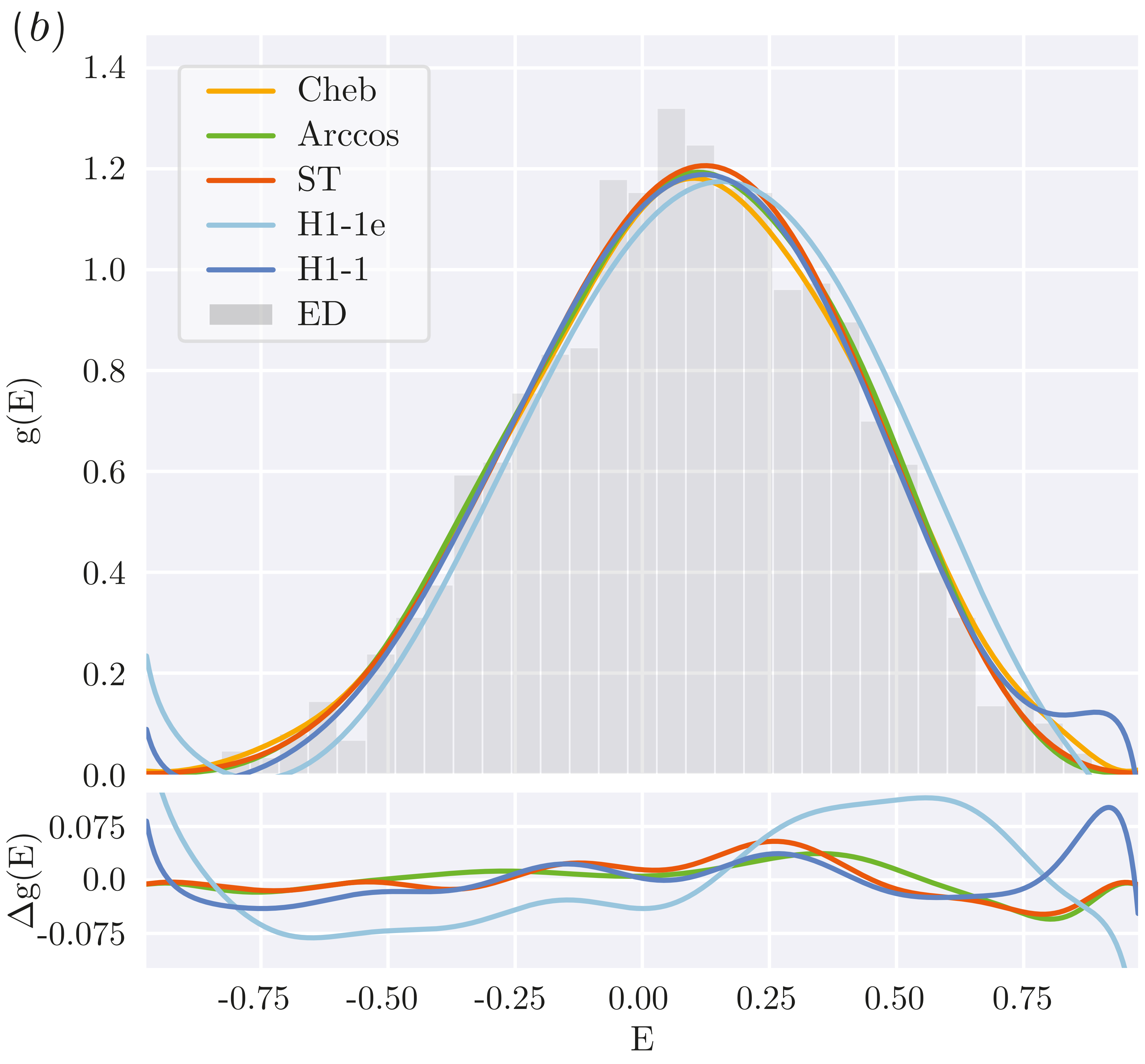
A related work using Quantinuum H1-1 (20-qubit) device

Summer *et al.*, arXiv:2303.13476

All-to-all connection



12-site XYZ model



erations on a many-qubit register. We emphasise that the accuracy of our hardware results has been limited primarily by financial constraints, and not by fundamental resource scalings nor even by noise on the H1-1 device.

Summary

A quantum-classical hybrid method for microcanonical ensembles is proposed

Microcanonical TPQ state

Random state ↓

$$|\psi_{\tau,r}(E)\rangle = [\hat{G}_\tau(E)]^{\frac{1}{2}}|\phi_r\rangle$$

Gaussian (center E, width $\sim 1/\tau$)

$$\hat{G}_\tau(E) = \mathrm{e}^{-(\hat{\mathscr{H}}-E)^2\tau^2}$$

Density matrix

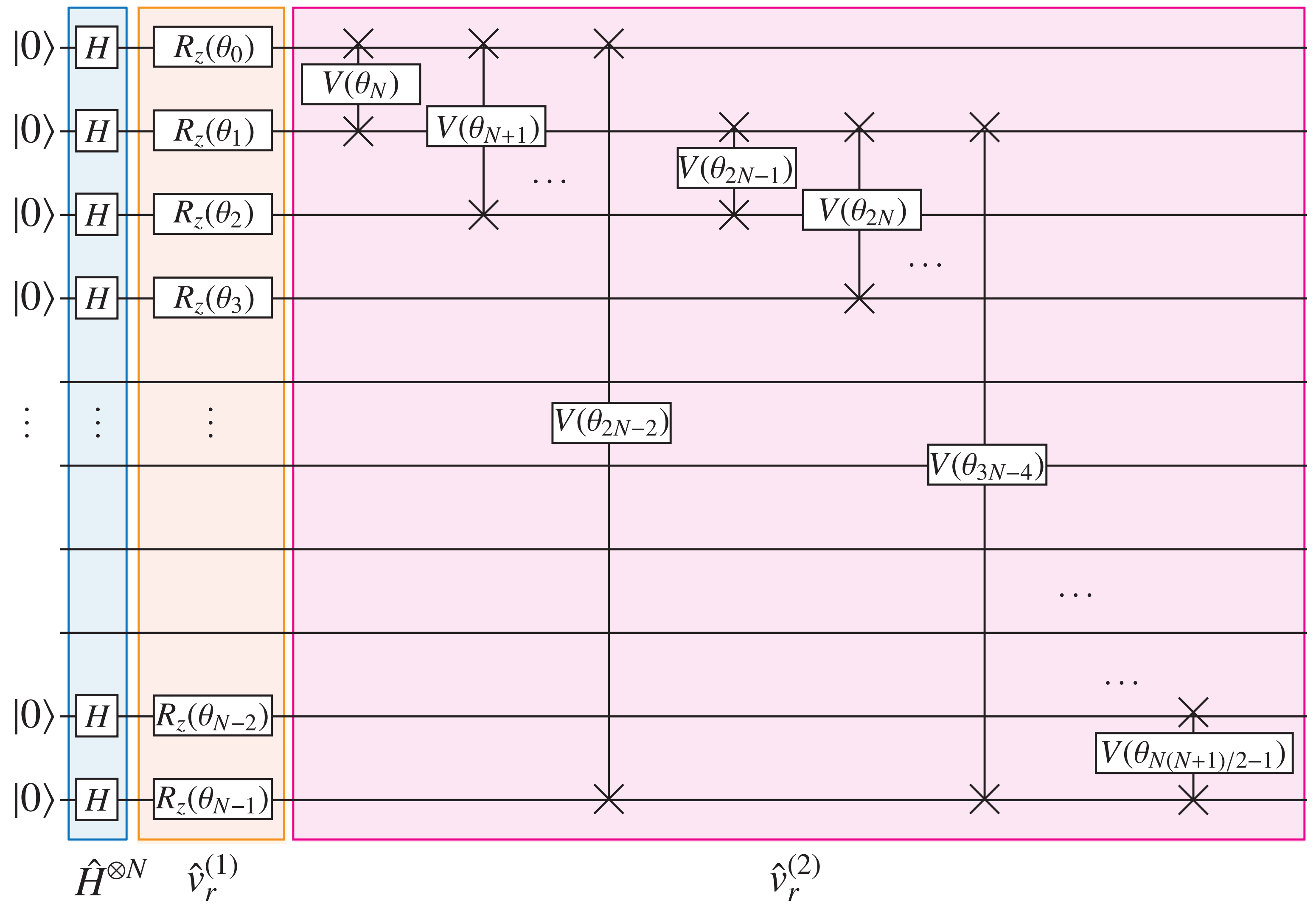
$$\hat{\rho}_{\mathrm{mic},\tau}(E) \equiv \frac{\hat{G}_\tau(E)}{\mathrm{Tr}\left[\hat{G}_\tau(E)\right]}$$

Requirements for random states $|\phi_r\rangle$

- Statistical average of $\langle\phi_r|\hat{X}|\phi_r\rangle$ coincides with $\mathrm{Tr}[\hat{X}]/D$.
- Covariance $\mathrm{Cov}(x, y)$ decreases exponentially in N.

Diagonal-unitary 2-design

Quantum circuit reproducing the properties of the random phase states up to 2nd statistical moments.



$|\phi_r\rangle$ can be prepared with $O(N^2)$ 2 qubit gates

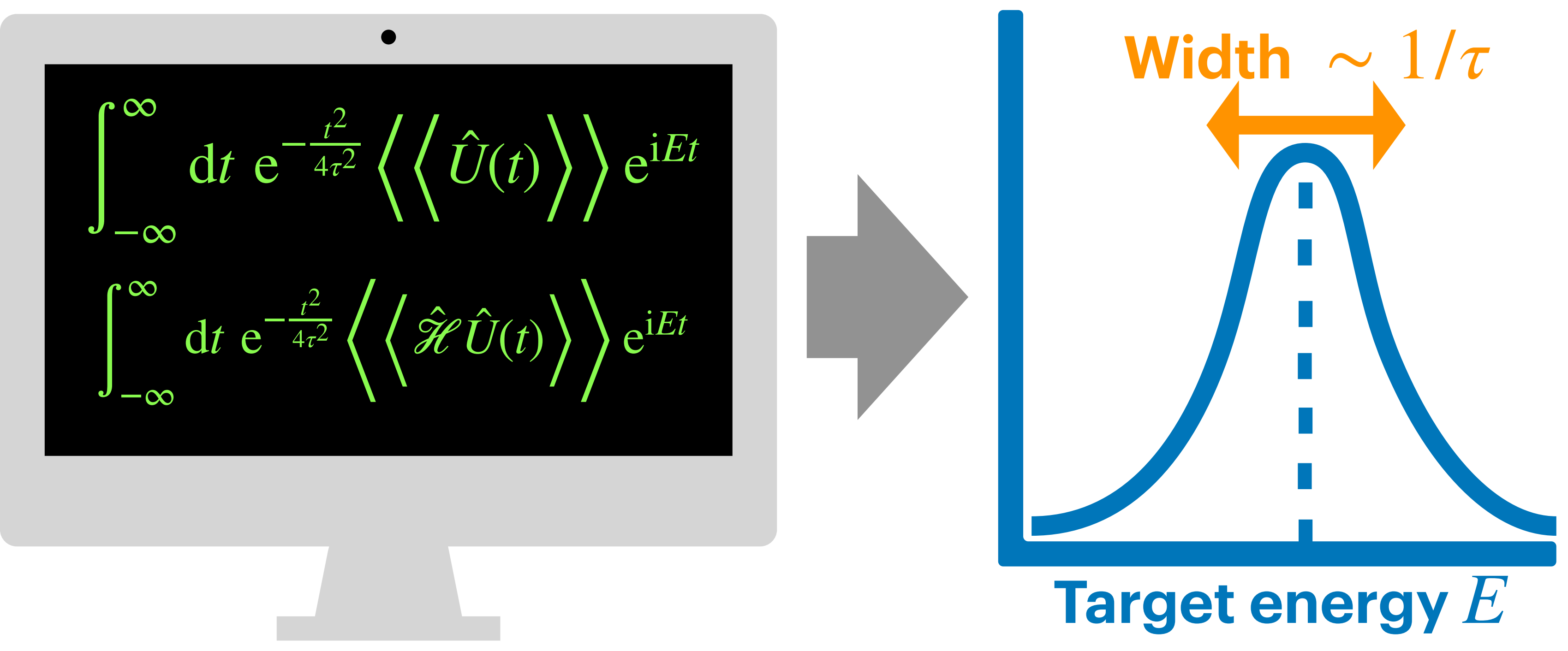
Thermodynamic quantities

- $S_\tau(E) = \ln \mathrm{Tr}[\hat{G}_\tau(E)]$
- $\beta_\tau(E) = \partial_E S_\tau(E) = 2\tau^2\left(\mathscr{E}_\tau(E) - E\right)$
- $\mathscr{E}_\tau(E) = \mathrm{Tr}\left[\hat{\rho}_{\mathrm{mic},\tau}(E)\hat{\mathscr{H}}\right] = \dfrac{\mathrm{Tr}[\hat{\mathscr{H}}\hat{G}_\tau(E)]}{\mathrm{Tr}[\hat{G}_\tau(E)]}$

Gaussian as a sum of time-evolution operators

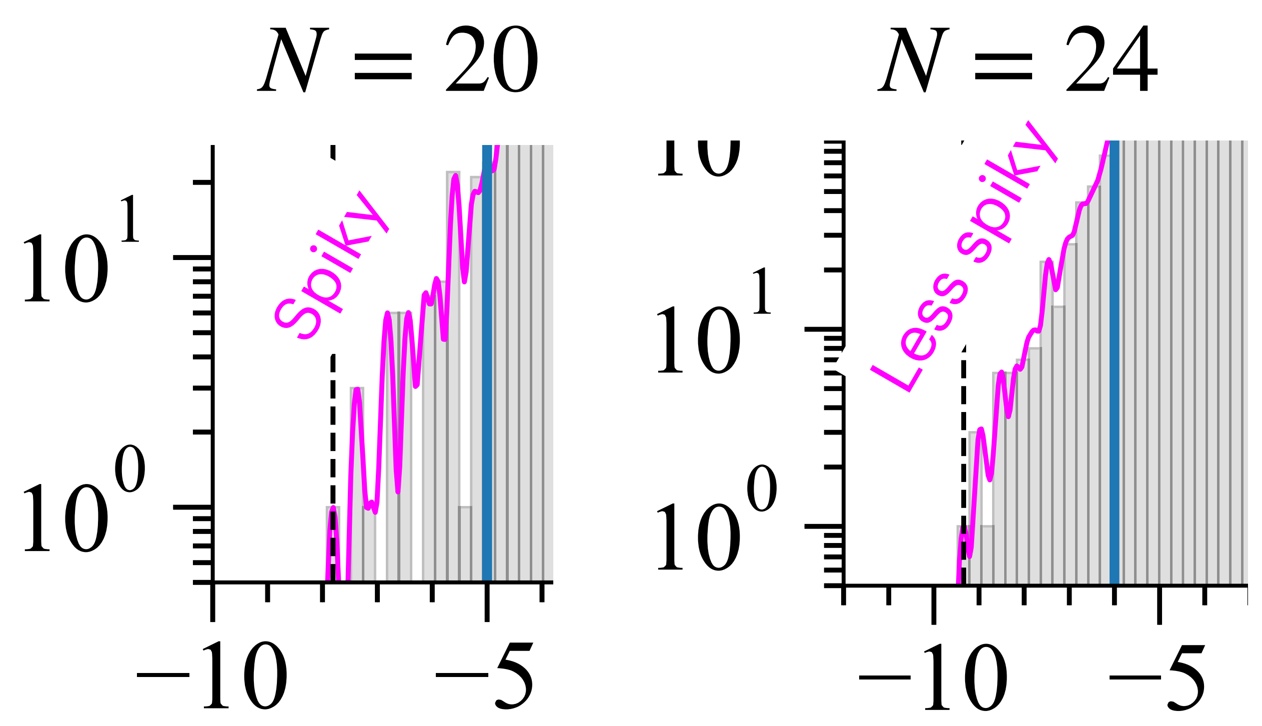
$$\hat{G}_\tau(E) = \frac{1}{2\sqrt{\pi}\tau}\int_{-\infty}^{\infty}\mathrm{d}t\mathrm{e}^{-\frac{t^2}{4\tau^2}}\mathrm{e}^{\mathrm{i}Et}\hat{U}(t),\quad \hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{\mathscr{H}}t}$$

"FT from **time-evolved** states to **energy-resolved** states"



Evaluate $\langle\phi_r|\hat{U}(t)|\phi_r\rangle$ and $\langle\phi_r|\hat{\mathscr{H}}\hat{U}(t)|\phi_r\rangle$ on QC and classically sum and integrate over r and t.

Classical simulation



- 2-designs are important to obtain thermodynamic quantities with a fixed number R of samples.
- The method becomes more relevant for energy windows with the larger number of states.

Quantum simulation

Work in progress