Many-body quantum dynamics simulations with the Ibisco resource

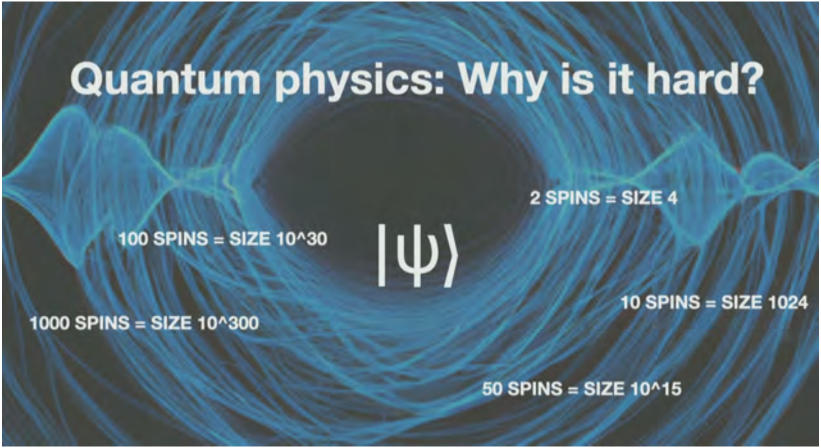
Angelo Russomanno,
Università di Napoli Federico II

April 19 2024

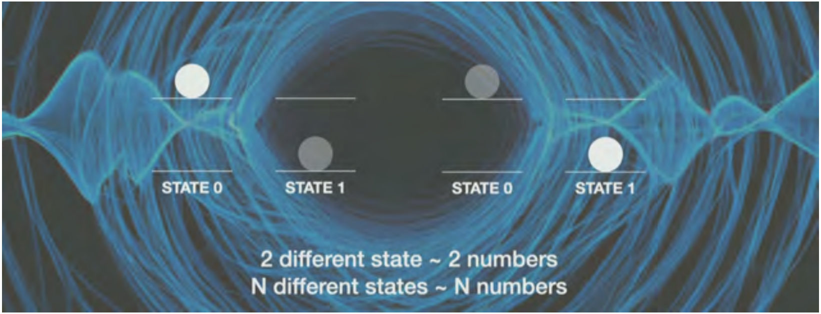
Ig-Nobel prize

Ig-Nobel prize

Deepak Chopra


Quantum physics: Why is it hard?
2 SPINS = SIZE 4
100 SPINS = SIZE 10^30
|ψ⟩
10 SPINS = SIZE 1024
1000 SPINS = SIZE 10^300
50 SPINS = SIZE 10^15

Classical states



Quantum states

Quantum superposition

Quantum states

Quantum superposition

$|0\rangle$

$|1\rangle$

Quantum states

Quantum superposition

$|0\rangle$

$|1\rangle$

Quantum state

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

Quantum states

$|0\rangle$

$|1\rangle$

$|0\rangle$

$|1\rangle$

$$|\psi_{\text{combined}}\rangle = A\,|01\rangle + B\,|00\rangle + C\,|10\rangle + D\,|11\rangle$$

Quantum states

$|0\rangle$

$|1\rangle$

$|0\rangle$

$|1\rangle$

$$|\psi_{\text{combined}}\rangle = A\,|01\rangle + B\,|00\rangle + C\,|10\rangle + D\,|11\rangle$$

L systems $\Longrightarrow$ 2^L complex parameters

Quantum physics is hard

$$2^L$$

Quantum physics is hard

Schrödinger eq.

$$i\,|\dot{\Psi}\rangle = \underbrace{\hat{H}}_{2^L \times 2^L!}\,|\Psi\rangle$$

2^L

Quantum physics is hard

2^L

Schrödinger eq.

$$i\,|\dot{\Psi}\rangle = \underbrace{\hat{H}}_{2^L\times 2^L!}\,|\Psi\rangle$$

Expectation

$$A = \langle\Psi|\hat{A}|\Psi\rangle$$

Quantum physics is hard

2^L

Schrödinger eq.

$$i\,|\dot{\Psi}\rangle = \underbrace{\hat{H}}_{2^L \times 2^L!}\,|\Psi\rangle$$

Expectation

$$A = \langle\Psi|\hat{A}|\Psi\rangle$$

Measure

$$|\Psi\rangle \to |A_n\rangle \qquad p_n = |\,\langle A_n|\Psi\rangle\,|^2$$

Quantum physics is hard

2^L

Schrödinger eq.

$$i\,|\dot{\Psi}\rangle = \underbrace{\hat{H}}_{2^L \times 2^L!}\,|\Psi\rangle$$

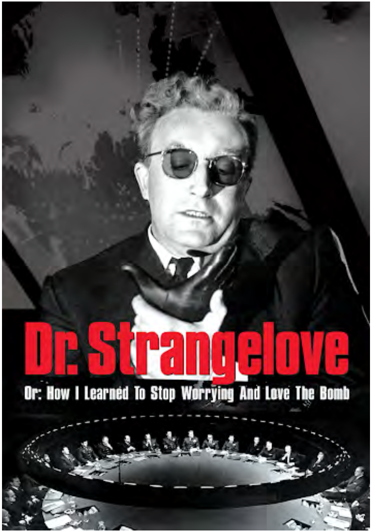
Expectation

$$A = \langle\Psi|\hat{A}|\Psi\rangle$$

POVM Measure

$$|\Psi\rangle \to \frac{\hat{K}_n|\Psi\rangle}{\langle\Psi|\hat{K}_n^\dagger\hat{K}_n|\Psi\rangle} \qquad p_n = \langle\Psi|\hat{K}_n^\dagger\hat{K}_n|\Psi\rangle$$

How I learned to stop worrying and love the hardness

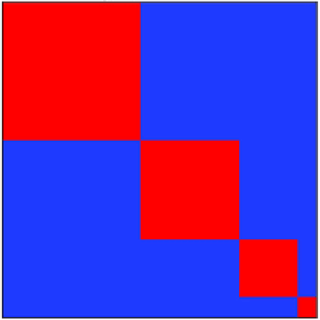


How I learned to stop worrying and love the hardness

Computational resouces

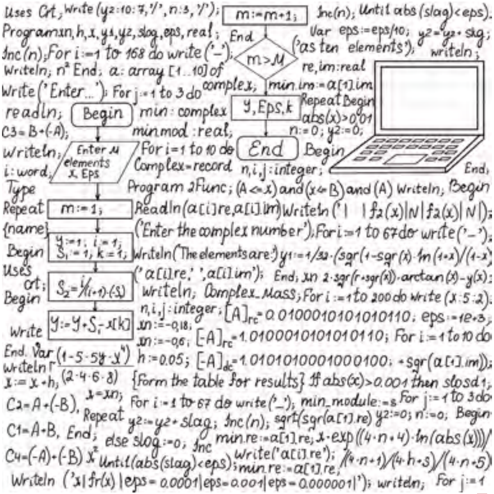
How I learned to stop worrying and love the hardness

Symmetries



How I learned to stop worrying and love the hardness

Algorithms



Publications using Ibisco

- Angelo Russomanno, Giulia Piccitto, Davide Rossini,
  Entanglement transitions and quantum bifurcations under continuous long-range monitoring,
  Physical Review B, **108**, 104313 (2023).
- Martina Minutillo, Procolo Lucignano, Gabriele Campagnano, and Angelo Russomanno,
  Kitaev ring threaded by a magnetic flux: Topological gap, Anderson localization of quasiparticles, and divergence of supercurrent derivative,
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  The impact of different unravelings in a monitored system of free fermions,
  arXiv:2402.06597 (2024).

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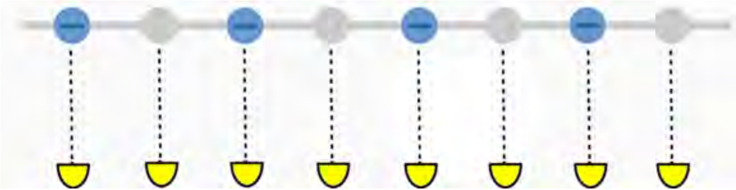
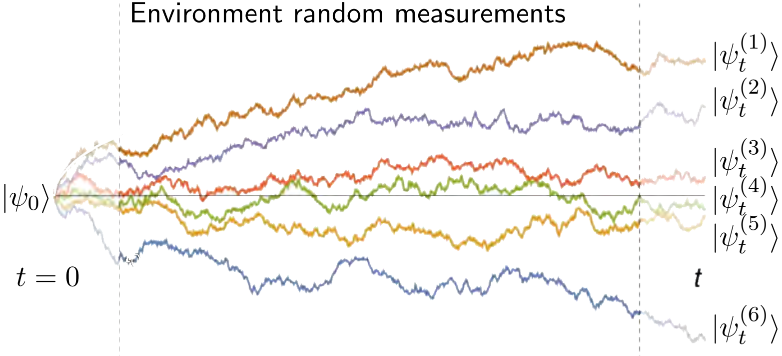
Effect of a classical environment

Environment random measurements



Quantum trajectories

"Brownian motion"

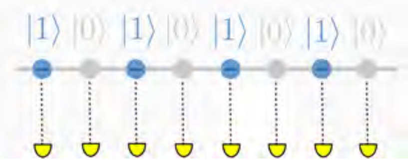


Huge parallelization using MPI

Coupling to an environment (monitored dynamics)

fermionic Hamiltonian

$$\hat{H} = \frac{1}{2}\sum_{j=1}^{L}(\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j)$$



$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -i[\hat{H},\rho_t] + \gamma\sum_{j=1}^{L}\hat{n}_j\rho_t\hat{n}_j - \frac{1}{2}\{\hat{n}_j,\rho_t\}$$

Lindblad equation

$$\hat{n}_i^2 = \hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$$

Coupling to an environment (monitored dynamics)

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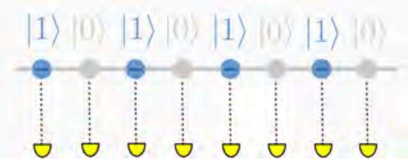

$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -i[\hat{H}, \rho_t] + \gamma \sum_{j=1}^{L} \hat{n}_j \rho_t \hat{n}_j - \frac{1}{2}\{\hat{n}_j, \rho_t\}$ Lindblad equation

$\hat{n}_i^2 = \hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$

Quantum state diffusion unraveling $\overline{|\psi_t\rangle \langle\psi_t|} = \rho_t$

$$\mathrm{d}\,|\psi_t\rangle = -i\hat{H}\mathrm{d}t\,|\psi_t\rangle + \underbrace{\sum_{i=1}^{L}\left(\sqrt{\gamma}[\hat{n}_i - \langle\hat{n}_i\rangle_t]\mathrm{d}W_t^i - \frac{\gamma}{2}[\hat{n}_i - \langle\hat{n}_i\rangle_t]^2\mathrm{d}t\right)}_{\text{Non-Hermitian stochastic quadratic Hamiltonian}}|\psi_t\rangle$$

Coupling to an environment (monitored dynamics)

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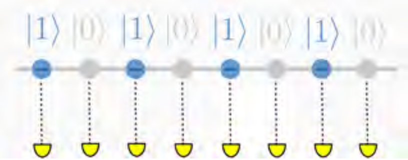

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -i[\hat{H},\rho_t] + \gamma\sum_{j=1}^{L}\hat{n}_j\rho_t\hat{n}_j - \frac{1}{2}\{\hat{n}_j,\rho_t\}$$ Lindblad equation

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Quantum state diffusion unraveling $\overline{|\psi_t\rangle\langle\psi_t|} = \rho_t$

Gaussian (Wiener process) $\langle \mathrm{d}W_t^i \mathrm{d}W_{t'}^j\rangle = \delta(t-t')\delta_{i\,j}\mathrm{d}t$

$$\mathrm{d}|\psi_t\rangle = -i\hat{H}\mathrm{d}t|\psi_t\rangle + \sum_{i=1}^{L}\left(\sqrt{\gamma}[\hat{n}_i - \langle\hat{n}_i\rangle_t]\,\overbrace{\mathrm{d}W_t^i} - \frac{\gamma}{2}[\hat{n}_i - \langle\hat{n}_i\rangle_t]^2\mathrm{d}t\right)|\psi_t\rangle$$

Non-Hermitian stochastic quadratic Hamiltonian

Coupling to an environment (monitored dynamics)

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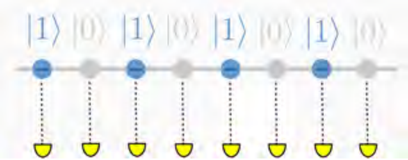

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$|\psi_t\rangle$ Slater determinant (discretize time and multiply $L \times L$ matrices)

Coupling to an environment (monitored dynamics)

Trotterize

$$|\psi(t+\delta t)\rangle \propto \mathrm{e}^{\sum_j \left[\delta W_t^j + (2\langle \hat{n}_j \rangle_t - 1)\gamma \delta t\right] \hat{n}_j} \mathrm{e}^{-i\hat{H}\delta t} |\psi(t)\rangle + \mathcal{O}(\gamma^2 \delta t^2)$$

- Slater determinant $|\psi_t\rangle = \prod_k \left(\sum_j U_{j\,k}(t)\hat{c}_j^\dagger\right)|0\rangle$
  $U_{j\,k}(t)$ $L \times L/2$, $U^\dagger U = \mathbf{1}_{N\times N}$.

Coupling to an environment (monitored dynamics)

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- Dissipative step $U(t) \to V = MU(t)$ with
  $M_{j\,k} = \delta_{j\,k}\,\mathrm{e}^{\delta W_t^j + (2\langle \hat{n}_j\rangle_t - 1)\gamma\delta t}$.

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- Unitary step $V \to V' = \mathrm{e}^{-ih\delta t} V$ with $h_{k\,l} = \frac{1}{2}(\delta_{k\,l+1} + \delta_{k\,l-1})$.

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- Get $U(t+\delta t)$ with QR decomposition of V' (orthonormalization that keeps constant the correlation matrix $C = UU^\dagger$).

Coupling to an environment (monitored dynamics)

Trotterize

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  Study $\langle \hat{n}_j\rangle_t$
- Unitary step $V \to V' = \mathrm{e}^{-ih\delta t}V$ with $h_{k\,l} = \frac{1}{2}(\delta_{k\,l+1} + \delta_{k\,l-1})$.
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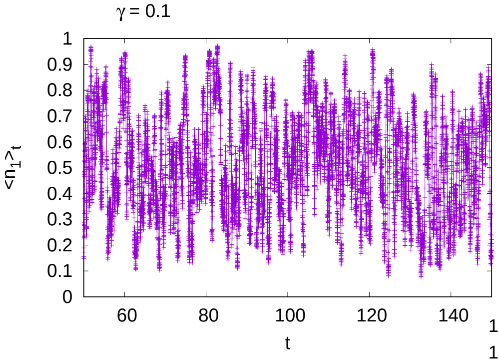
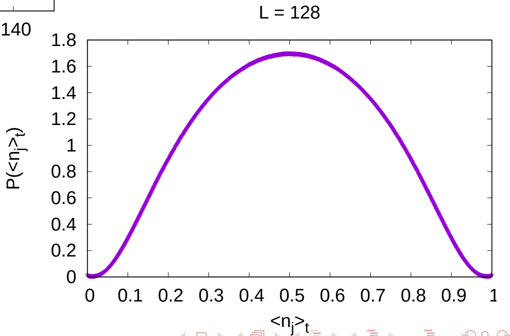
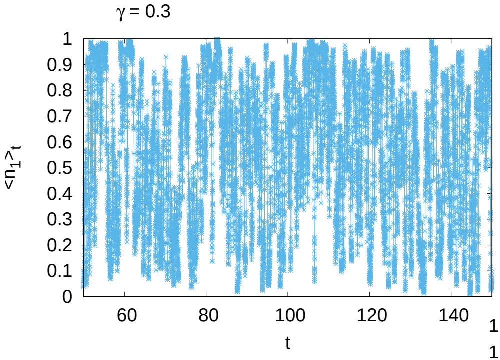


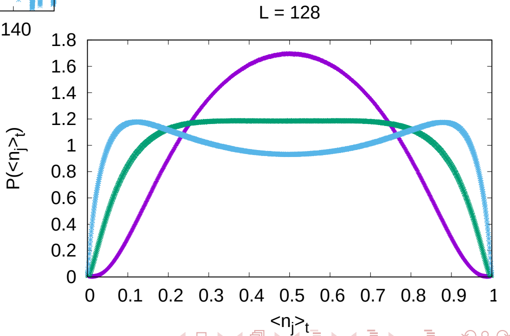
Unimodal distribution

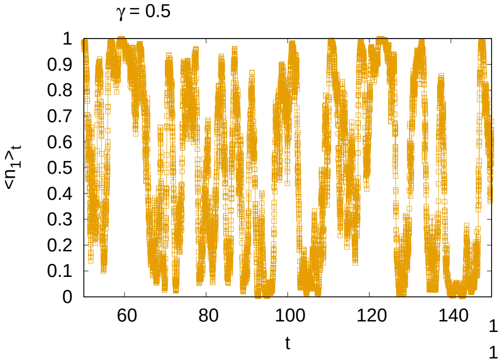




Unimodal distribution

Bimodal distribution





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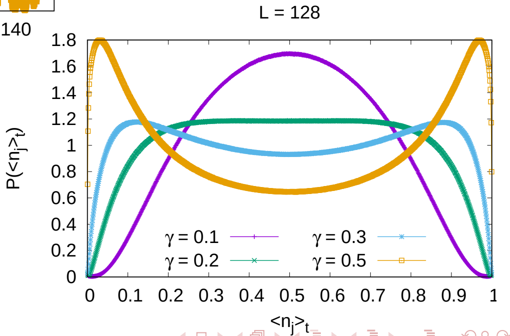
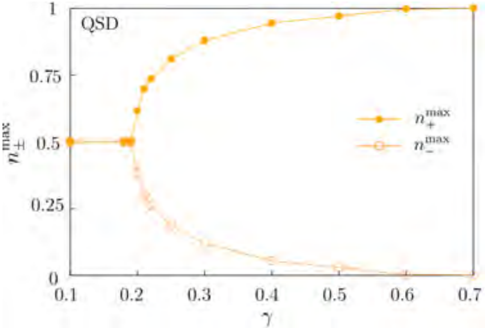


"Quantum bifurcation"



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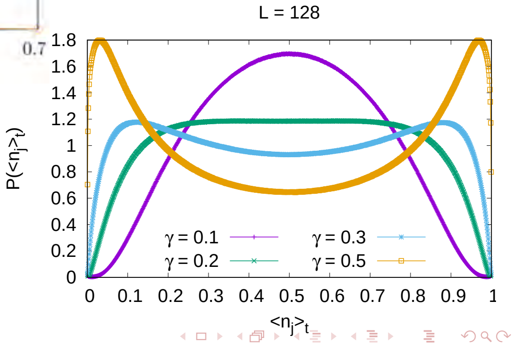

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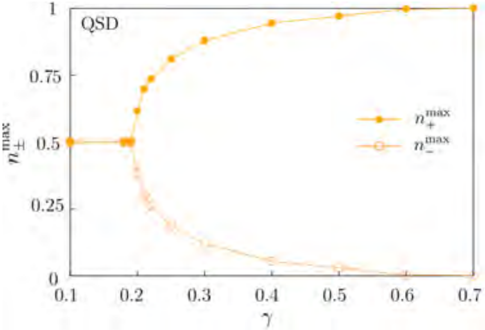


Unimodal distribution

Bimodal distribution

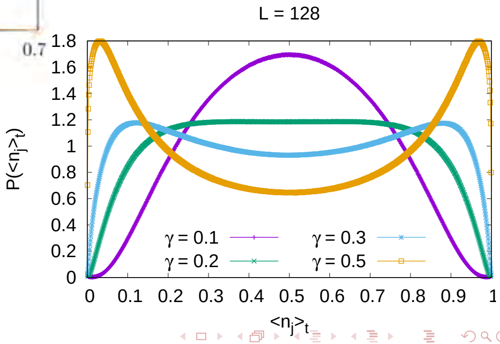
Classical bifurcation
(2^{nd} order transition)

Landau free energy $P \sim \mathrm{e}^{-\mathcal{F}}$

Metropolis algorithm

classical finite-size 2D Ising

magnetization distribution



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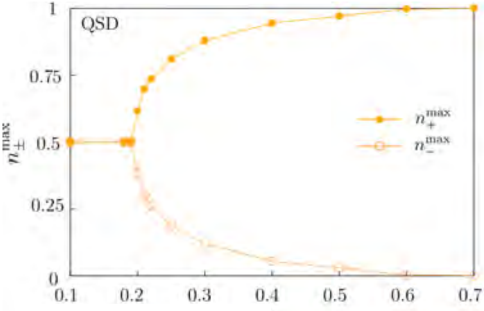
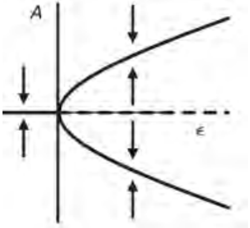


$$\tau_0\, d_t A = \varepsilon A - g A^3 + \cdots$$



Classical bifurcation in nonlinear dynamics

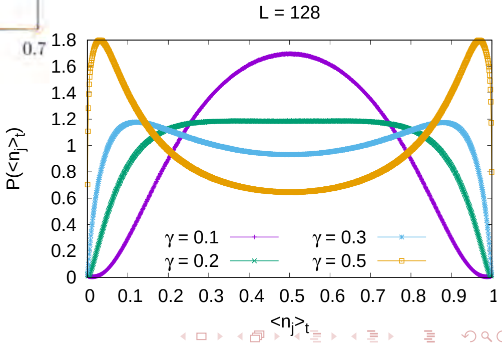
Classical bifurcation
(2nd order transition)

Landau free energy $P \sim \mathrm{e}^{-\mathcal{F}}$

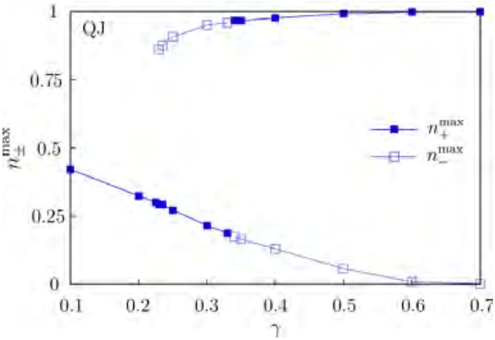
Metropolis algorithm

classical finite-size 2D Ising

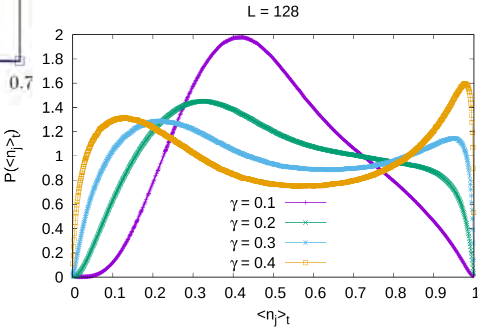
magnetization distribution



Different (quantum-jump) unraveling

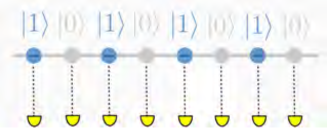


Classical analog
(1^{st} order transition)



Let's get nonintegrable

$$\hat{H} = \sum_{j=1}^{L} \left[\frac{J}{2} \left(\hat{\sigma}_j^{+} \hat{\sigma}_{j+1}^{-} + \text{H. c.} \right) + \frac{V}{4} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + \frac{W}{2} (-1)^j \hat{\sigma}_j^z \right]$$



$$\begin{aligned} |\psi_{t+\delta t}\rangle &= (\mathbf{1} - i\hat{H}\delta t) |\psi_t\rangle \\ &+ \sum_l \left[\delta\xi_l(t) \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right) - \frac{\gamma}{2} \delta t \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right)^2 \right] |\psi_t\rangle + \mathcal{O}(\gamma^2 \delta t^2) \end{aligned}$$

$\overline{\delta\xi_j(t)\delta\xi_l(t')} = \delta_{j\,l}\delta_{t\,t'}\delta t$ Gaussian uncorrelated

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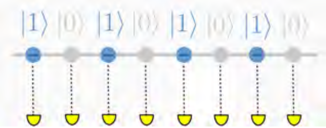

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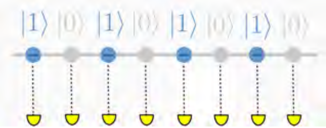
Trotterize

$$|\psi_{t+\delta t}\rangle = \mathcal{N} \mathrm{e}^{-i\hat{H}\delta t} \mathrm{e}^{\sum_l \left[\delta\xi_l(t) \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right) - \gamma \delta t \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right)^2 \right]} |\psi_t\rangle + \mathcal{O}(\gamma^2 \delta t^2)$$

Let's get nonintegrable

$$\hat{H} = \sum_{j=1}^{L} \left[\frac{J}{2} \left(\hat{\sigma}_j^+ \hat{\sigma}_{j+1}^- + \text{H. c.} \right) + \frac{V}{4} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + \frac{W}{2} (-1)^j \hat{\sigma}_j^z \right]$$



$$\begin{aligned} |\psi_{t+\delta t}\rangle &= (\mathbf{1} - i\hat{H}\delta t)\,|\psi_t\rangle \\ &+ \sum_l \left[\delta\xi_l(t) \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right) - \frac{\gamma}{2} \delta t \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right)^2 \right] |\psi_t\rangle + \mathcal{O}(\gamma^2 \delta t^2) \end{aligned}$$

$\overline{\delta\xi_j(t)\delta\xi_l(t')} = \delta_{j\,l}\delta_{t\,t'}\delta t$ Gaussian uncorrelated

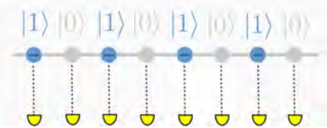
Trotterize

$$|\psi_{t+\delta t}\rangle = \mathcal{N} \mathrm{e}^{-i\hat{H}\delta t} \mathrm{e}^{\sum_l \left[\delta\xi_l(t) \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right) - \gamma \delta t \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right)^2 \right]} |\psi_t\rangle + \mathcal{O}(\gamma^2 \delta t^2)$$

Rotation symmetry along $z \Longrightarrow \hat{S}_z = \frac{1}{2} \sum_l \hat{\sigma}_l^z$ conserved

Let's get nonintegrable

$$\hat{H} = \sum_{j=1}^{L} \left[\frac{J}{2} \left(\hat{\sigma}_j^+ \hat{\sigma}_{j+1}^- + \text{H. c.} \right) + \frac{V}{4} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + \frac{W}{2} (-1)^j \hat{\sigma}_j^z \right]$$



$$\begin{aligned} |\psi_{t+\delta t}\rangle &= (\mathbf{1} - i\hat{H}\delta t)\,|\psi_t\rangle \\ &+ \sum_l \left[\delta\xi_l(t) \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right) - \frac{\gamma}{2}\delta t \left(\hat{\sigma}_l^z - \langle \sigma_l^z \rangle_t \right)^2 \right] |\psi_t\rangle + \mathcal{O}(\gamma^2 \delta t^2) \end{aligned}$$

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Rotation symmetry along $z \Longrightarrow \hat{S}_z = \frac{1}{2}\sum_l \hat{\sigma}_l^z$ conserved

Restrict to block with $S_z = 0 \Longrightarrow \dim \mathcal{H}_L = \binom{L}{L/2}$

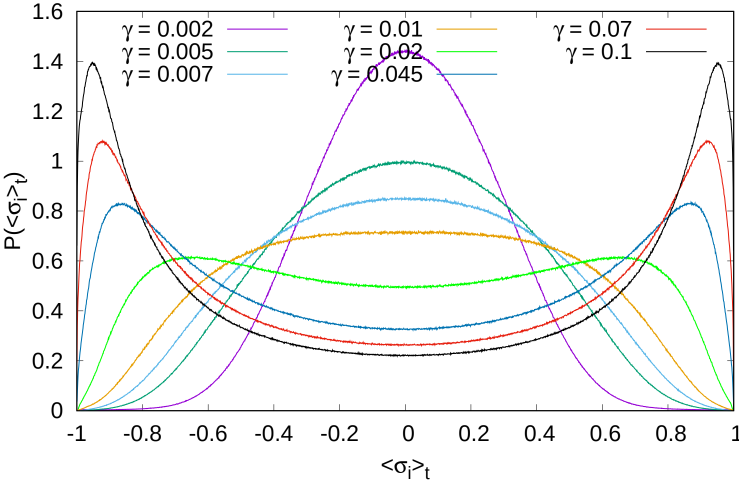
Krylov algorithm

ACM Trans. Math. Softw. 24 (1) (1998) 130–156 (Expokit)

J. Chem. Phys. 85, 5870–5876 (1986)

- $|\Psi'\rangle = \mathrm{e}^{-i\hat{H}\delta t} |\Psi\rangle$.
- Write the subspace $\mathrm{Span}\{|\Psi\rangle, \hat{H}|\Psi\rangle, \hat{H}^2|\Psi\rangle, \ldots, \hat{H}^M|\Psi\rangle\}$ ($\hat{H}$ sparse).
- Expand the Hamiltonian in this basis (truncate).
- Converges even for $M \simeq 20$.

Quantum bifurcation



Localization properties

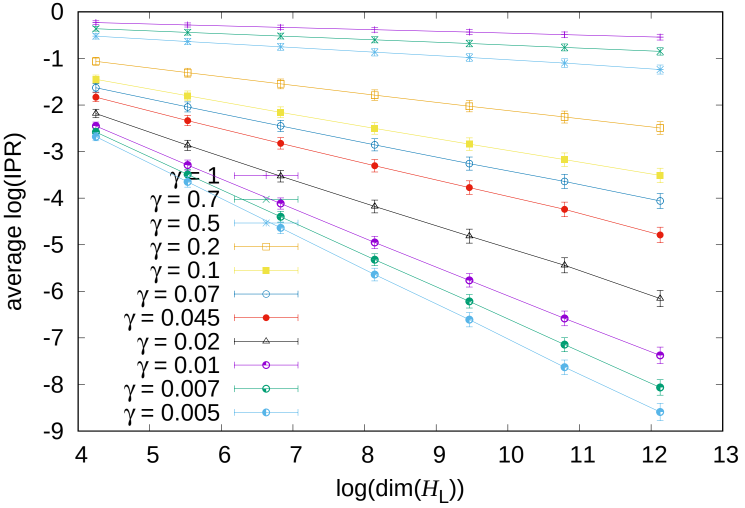
- Inverse participation ratio IPR $= \sum_{\{s_j\}} |\langle\{s_j\}| |\Psi_t\rangle\rangle|^4$.
- $|\{s_j\}\rangle$ classical spin configurations $\hat{\sigma}_l^z |\{s_j\}\rangle = s_l |\{s_j\}\rangle$.
- IPR ~ 1 localized.
- IPR $\sim 1/\dim \mathcal{H}_L$ fully delocalized.

Localization properties

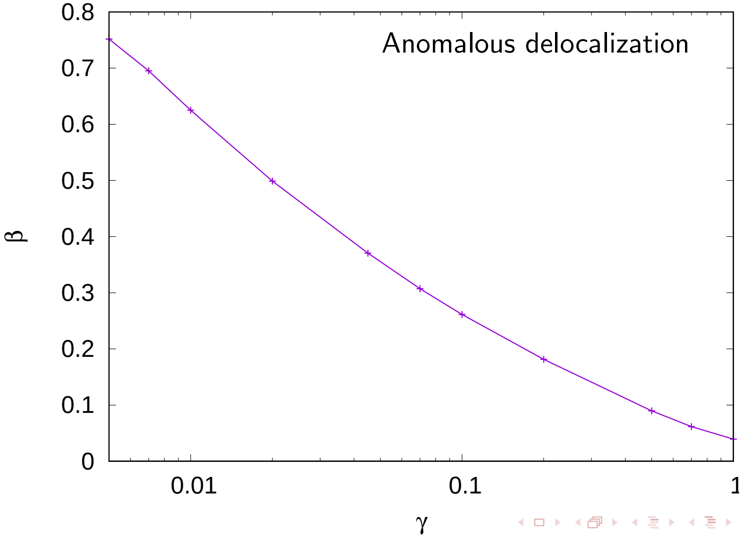
- Inverse participation ratio $\overline{\log(\text{IPR})} = \overline{\log\left(\sum_{\{s_j\}} |\langle\{s_j\}|\,|\Psi_t\rangle\rangle|^4\right)}$ (average over time and realizations).
- $|\{s_j\}\rangle$ classical spin configurations $\hat{\sigma}_l^z\,|\{s_j\}\rangle = s_l\,|\{s_j\}\rangle$.
- $\overline{\log(\text{IPR})} \sim 0$ localized.
- $\overline{\log(\text{IPR})} \sim -\log\dim\mathcal{H}_L$ fully delocalized.
- $\overline{\log(\text{IPR})} \sim -\beta\log\dim\mathcal{H}_L$ with $0 < \beta < 1$ anomalously delocalized.

Localization properties

Linear fit $\overline{\log(\mathrm{IPR})} \sim -\beta \log \dim \mathcal{H}_L$



Localization properties



Future challenges

- Matrix product states and robustness of Many-Body localization to local heating.
- Neural network states and QAOA dynamics.

Thank you for your attention!