arXiv:2105.01054

mpsd

Challenges for simulating quantum spin dynamics in two dimensions by neural network quantum states

SPICE DPEQM Workshop

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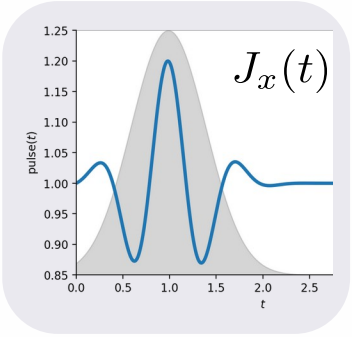
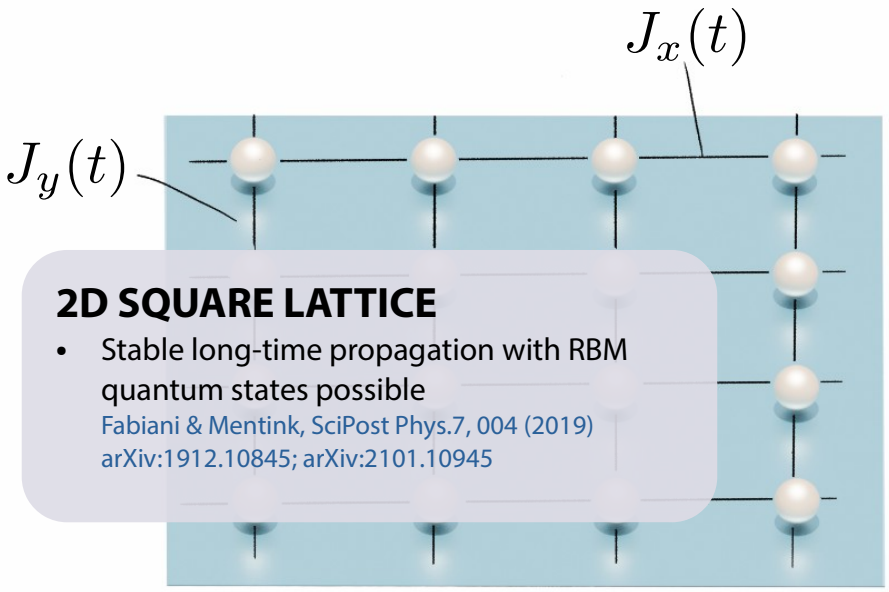
Motivation: Dynamics in driven Heisenberg system

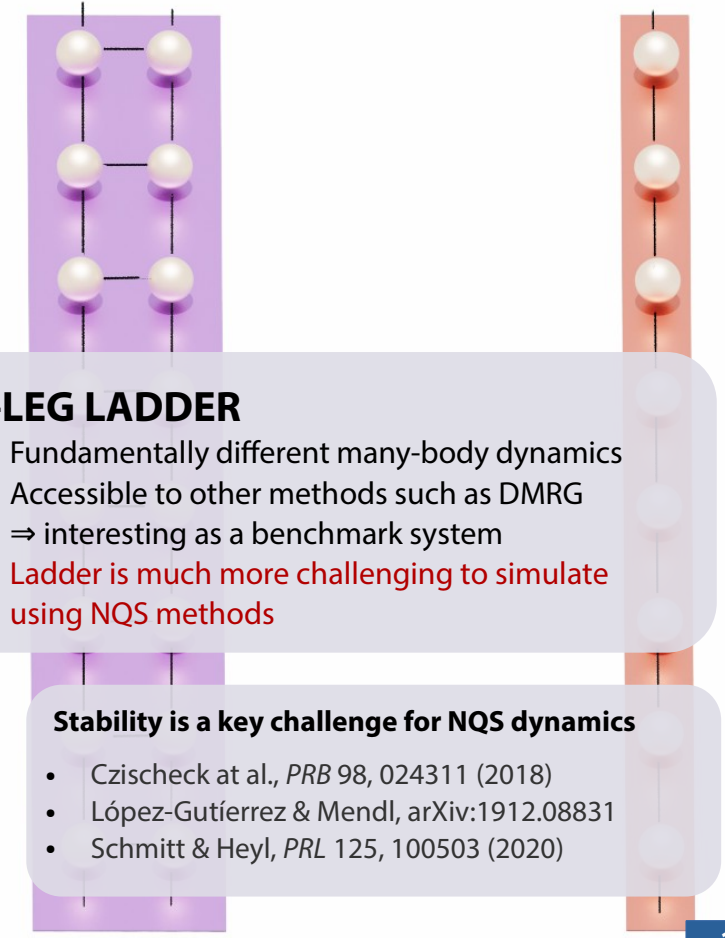
$$\hat{H}(t) = \sum_{\langle i,j \rangle} J_{ij}(t) \hat{S}_i \cdot \hat{S}_j$$





2D SQUARE LATTICE

- Stable long-time propagation with RBM quantum states possible
  Fabiani & Mentink, SciPost Phys.7, 004 (2019)
  arXiv:1912.10845; arXiv:2101.10945



2-LEG LADDER

- Fundamentally different many-body dynamics
- Accessible to other methods such as DMRG
- ⇒ interesting as a benchmark system
- Ladder is much more challenging to simulate using NQS methods

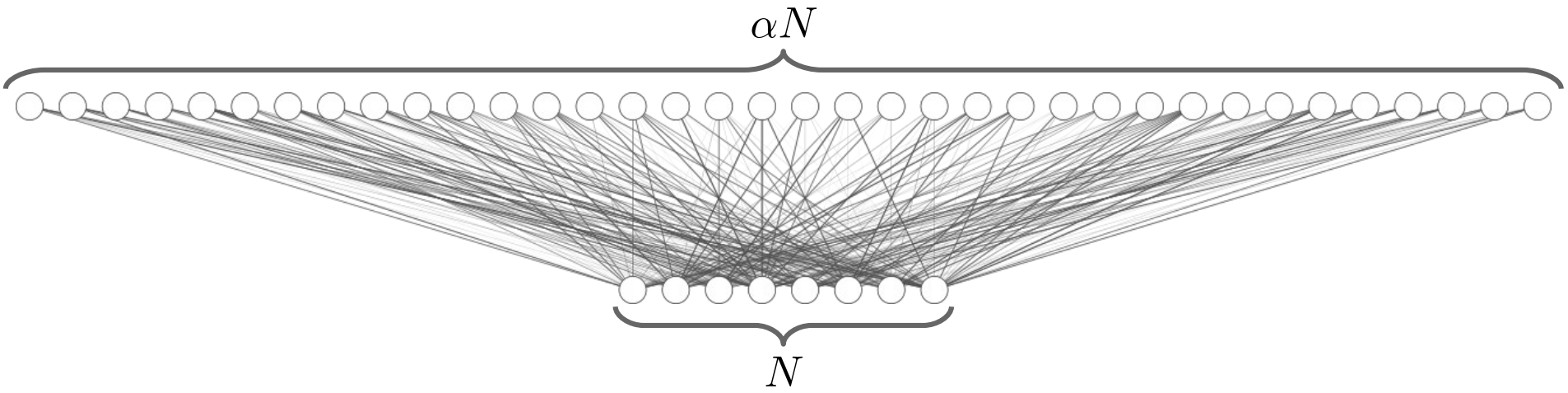
Stability is a key challenge for NQS dynamics

- Czischeck at al., *PRB* 98, 024311 (2018)
- López-Gutíerrez & Mendl, arXiv:1912.08831
- Schmitt & Heyl, *PRL* 125, 100503 (2020)

Variational *ansatz*: Restricted Boltzmann machine

$$\ln \psi_{W,b}(s) = \sum_{j=1}^{\alpha N} \ln \cosh(W s + b)_j$$

- Invariant under lattice translations
- Zero magnetization subspace



Symmetric RBM architecture – Carleo & Troyer, *Science* 355 (2017)

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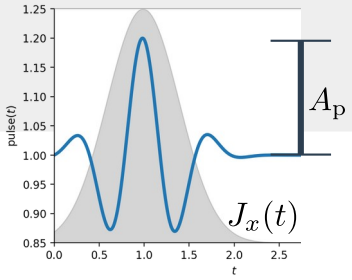
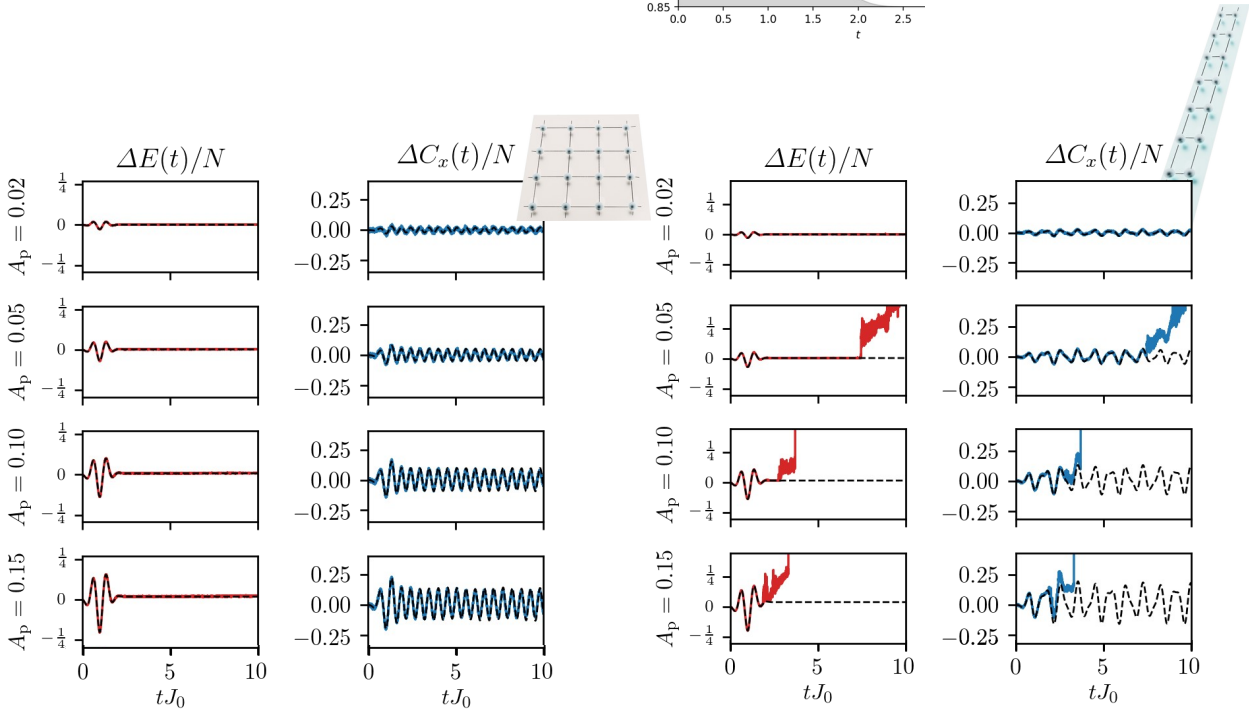
Instabilities in time propagation



- Propagation using time-dependent variational principle (t-VMC)
- Can exhibit jump instabilities already for weak pulses on the ladder
- Square lattice dynamics are quite stable in comparison
  (for moderate excitation strengths)
- Expressiveness of RBM *ansatz* is not a limiting factor



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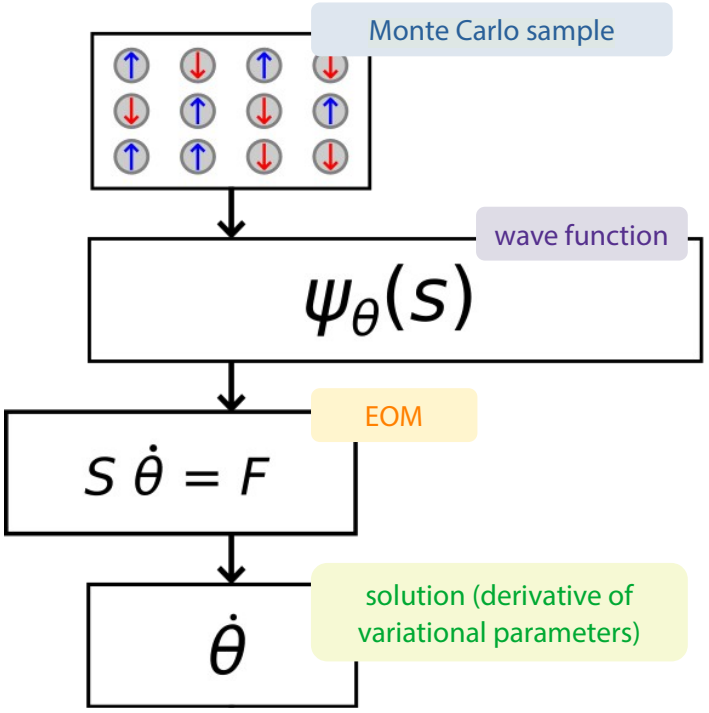
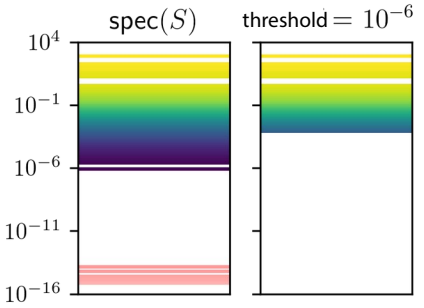
Stabilization of t-VMC equation of motion

time-dependent variational Monte Carlo (t-VMC)



$$S \cdot \dot{\theta} = -\mathrm{i}\nabla_{\theta^*}\langle \hat{H} \rangle$$



- Equation of motion requires solving linear system
- Typically ill-conditioned ⇒ needs regularization
  - Here: Truncate eigenvalues below threshold

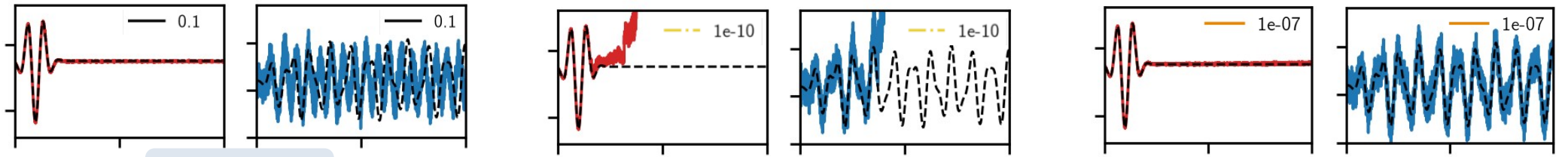
  requires tuning of hyper parameters
- Other regularization methods typically require adjustment of hyper-parameters as well
  - Shift diagonal elements (squeezes spectrum)
  - Truncate equation based on gradient noise

Schmitt & Heyl, *PRL* 125, 100503 (2020)

t-VMC – Carleo, Becca, Schiró, Fabrizio, *Sci. Rep.* 2 (2012)

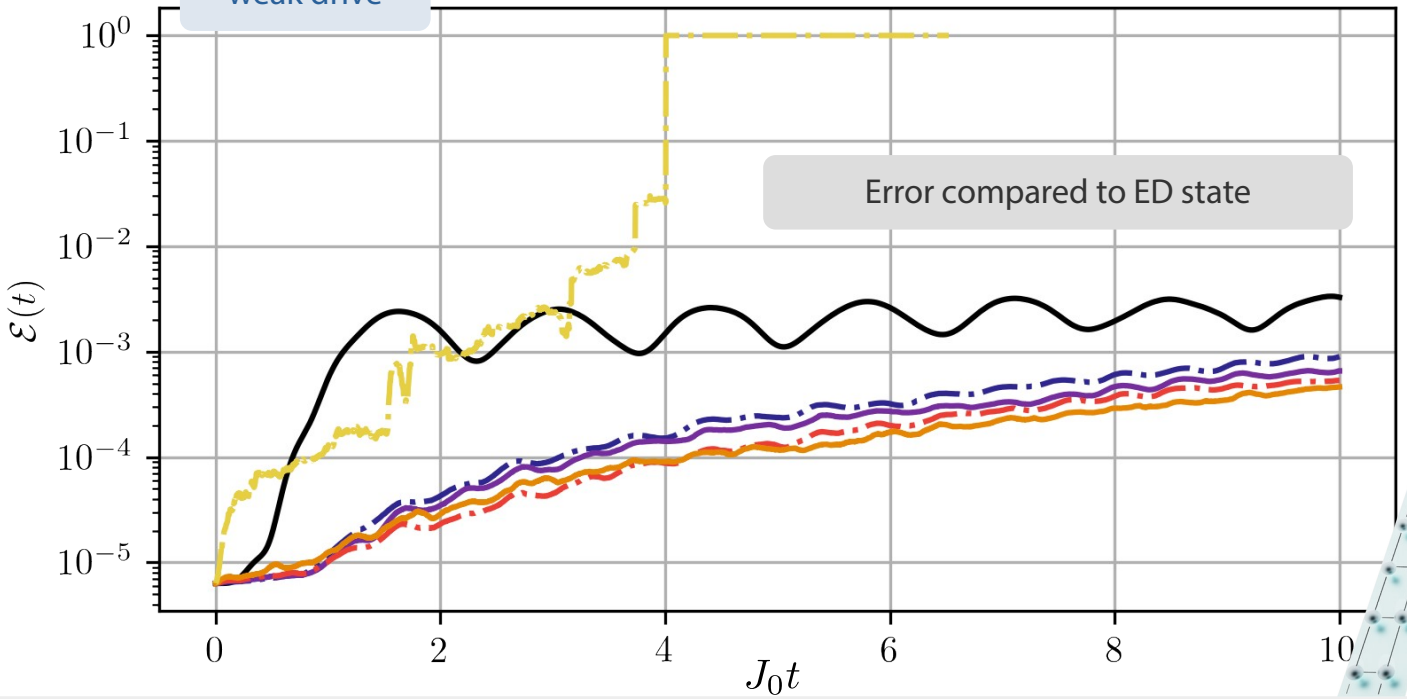
arXiv:2105.01054

Threshold dependence of solution quality



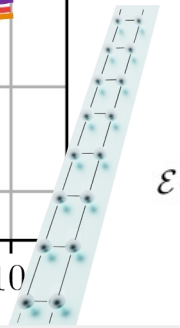
weak drive

Error compared to ED state



threshold

- 0.1
- 5e-06
- 1e-06
- 5e-07
- 1e-07
- 1e-10



$$\mathcal{E}(t) = 1 - \frac{|\langle \Psi_{\mathrm{ED}}(t) | \psi_\theta(t) \rangle|^2}{\langle \Psi_{\mathrm{ED}}(t) | \Psi_{\mathrm{ED}} \rangle \langle \psi_\theta(t) | \psi_\theta(t) \rangle}.$$

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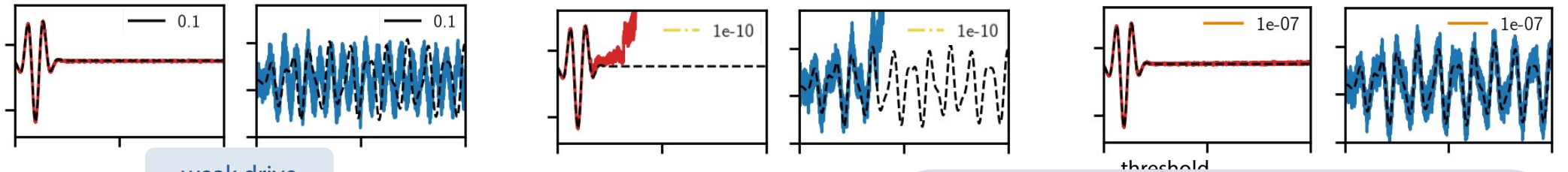
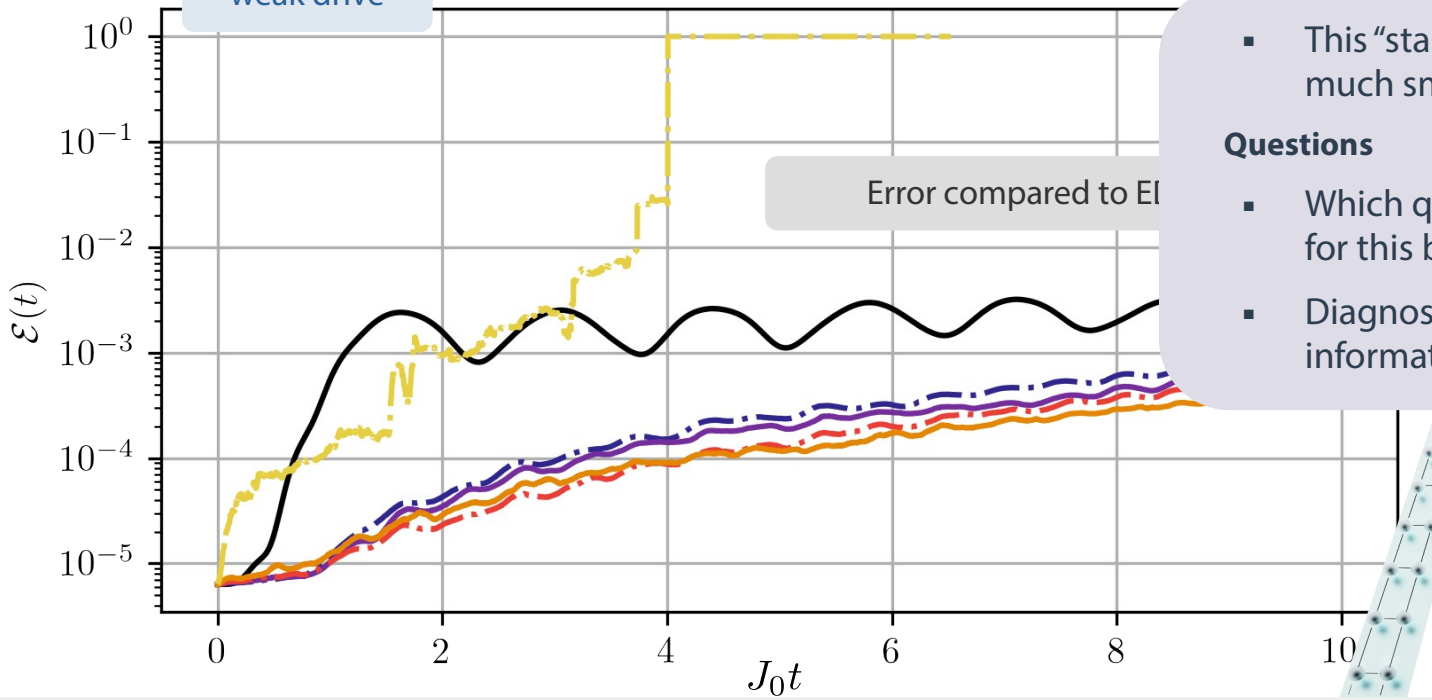
Threshold dependence of solution quality



weak drive



Error compared to E

- This "stable regime" of regularization becomes much smaller for higher pulse strength

Questions

- Which quantity can be used as a diagnostic for this behavior?
- Diagnostic should be accessible with information available in VMC

$$\mathcal{E}(t) = 1 - \frac{|\langle \Psi_{\mathrm{ED}}(t) | \psi_\theta(t) \rangle|^2}{\langle \Psi_{\mathrm{ED}}(t) | \Psi_{\mathrm{ED}} \rangle \langle \psi_\theta(t) | \psi_\theta(t) \rangle}.$$

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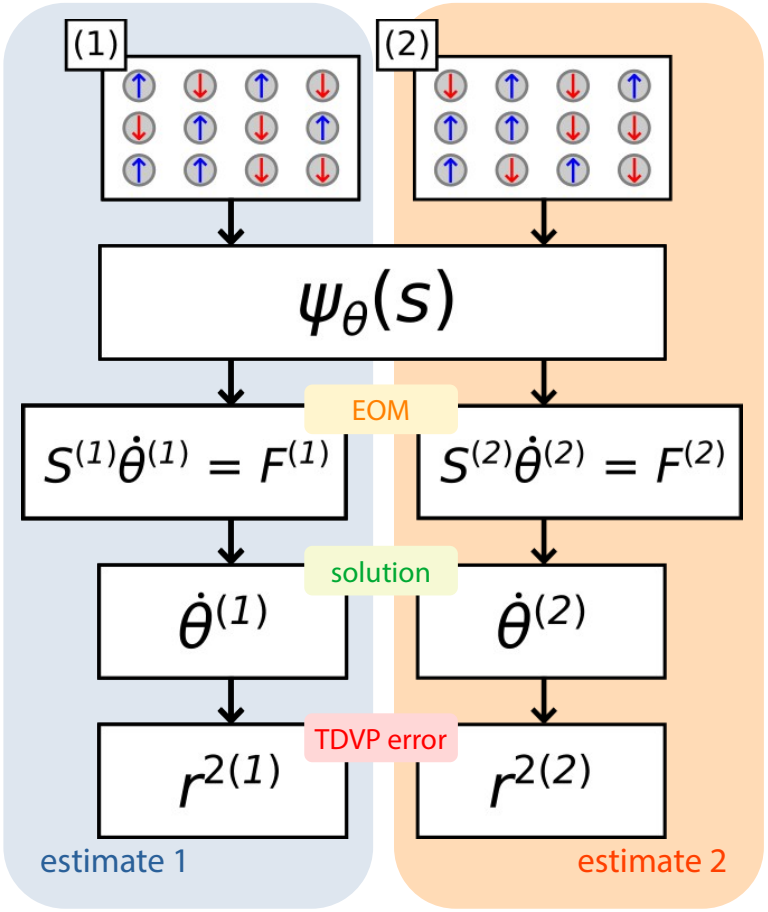
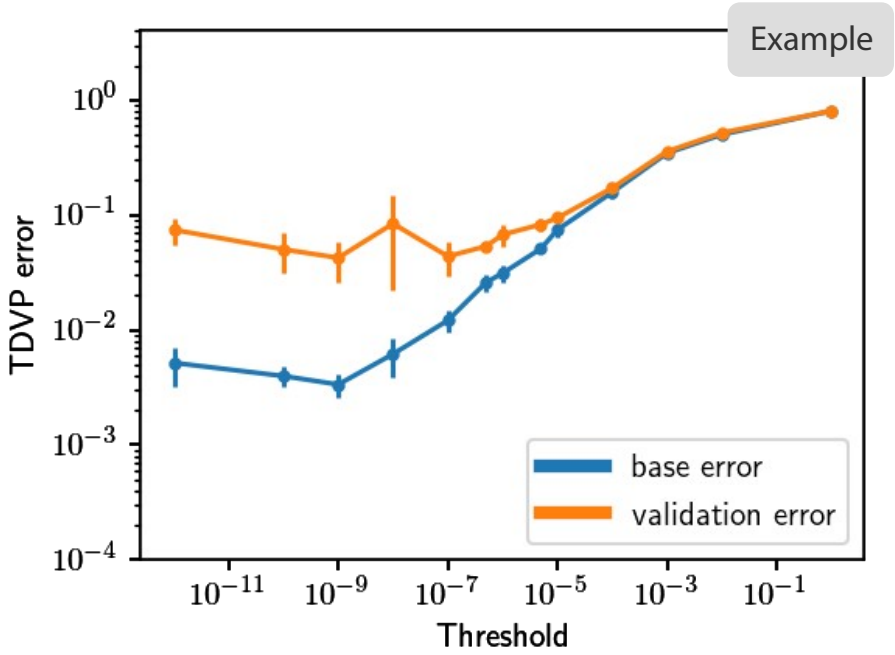
Validation error and over-fitting to noise





$$r^2_{\text{val}} = r^2[\dot{\theta}^{(2)}, S^{(1)}, F^{(1)}]$$

validation error

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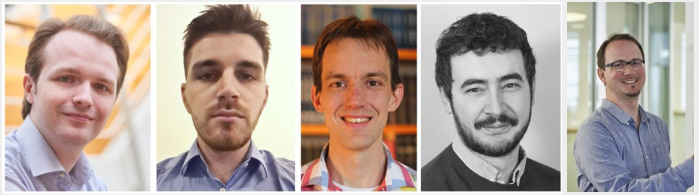
Summary

Thank you for your attention!

- Heisenberg ladder is challenging to simulate using RBM quantum states and t-VMC
- Stochastic noise in t-VMC can lead to jump-type instabilities when combined with a susceptible equation of motion
- Over-fitting to noise is a key problem in time-dependent VMC for NQS
- Validation-set TDVP error can help as diagnostic for required fine-tuning of numerical parameters

DH, Fabiani, Mentink, Carleo, Sentef – arXiv:2105.01054



Software – NetKet framework
Carleo, Choo, Hofmann, et al.
SoftwareX 10, 100311 (2019)
https://www.netket.org

Software – ULTRAFAST code
Fabiani & Mentink
SciPost Phys. 7, 004 (2019)
https://github.com/ultrafast-code/ULTRAFAST

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