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

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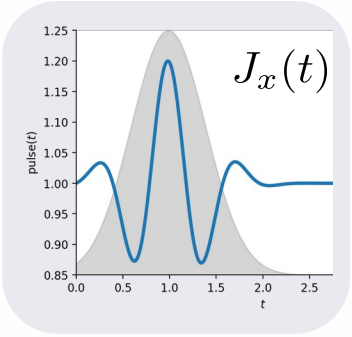
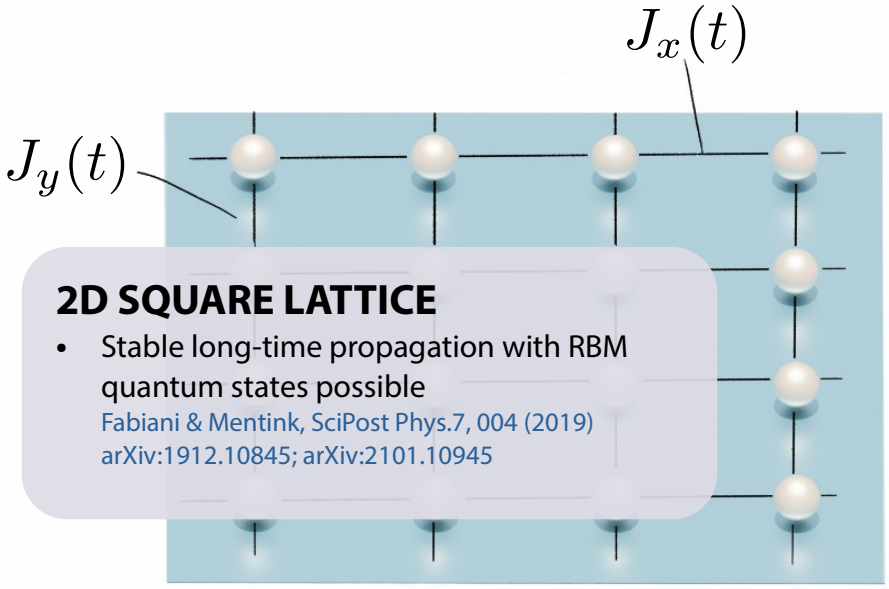
Damian Hofmann[1] Giammarco Fabiani[2]
Johan Mentink[2] Giuseppe Carleo[3] Michael A. Sentef[1]

[1] Max Planck Institute for the Structure and Dynamics of Matter (MPSD), Hamburg, Germany
[2] Radboud University, Institute for Molecules and Materials, Nijmegen, The Netherlands
[3] Institute of Physics, École Politechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

# Motivation: Dynamics in driven Heisenberg system

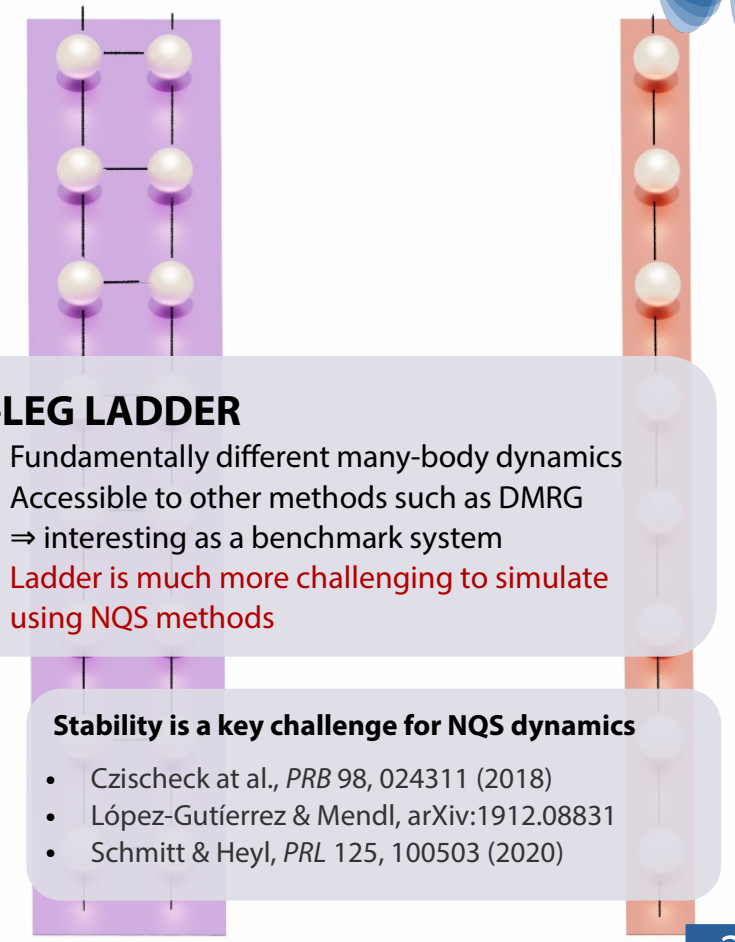
$$\hat{H}(t) = \sum_{\langle i,j \rangle} J_{ij}(t) \hat{S}_i \cdot \hat{S}_j$$




## 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

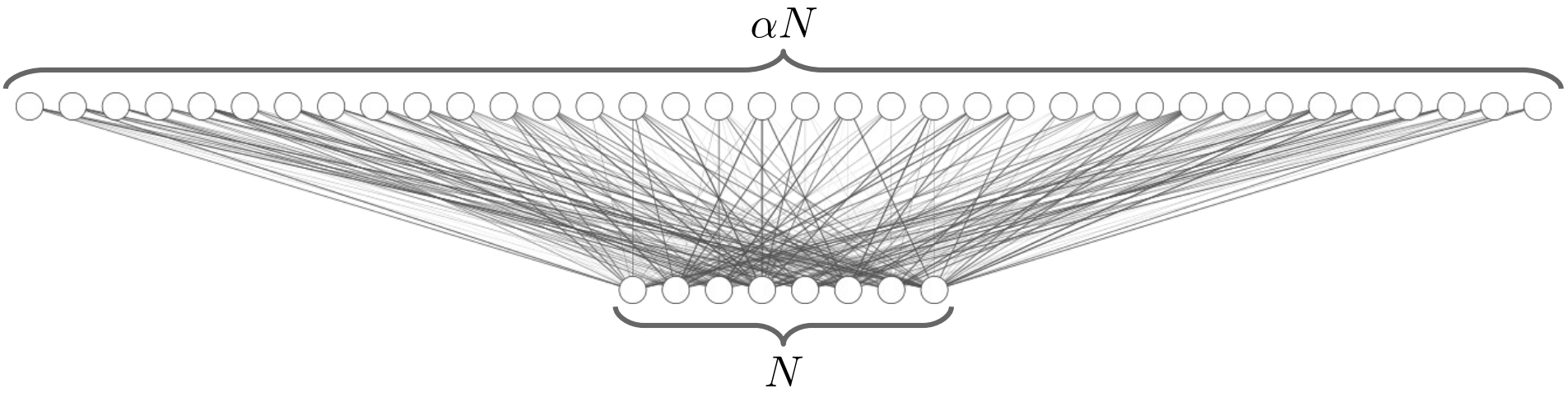
**Stability is a key challenge for NQS dynamics**

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

# Variational *ansatz*: Restricted Boltzmann machine

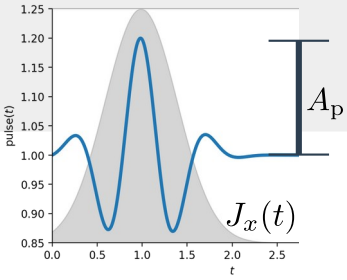
$$\ln \psi_{W,b}(s) = \sum_{j=1}^{\alpha N} \ln \cosh(W s + b)_j$$

- Invariant under lattice translations
- Zero magnetization subspace

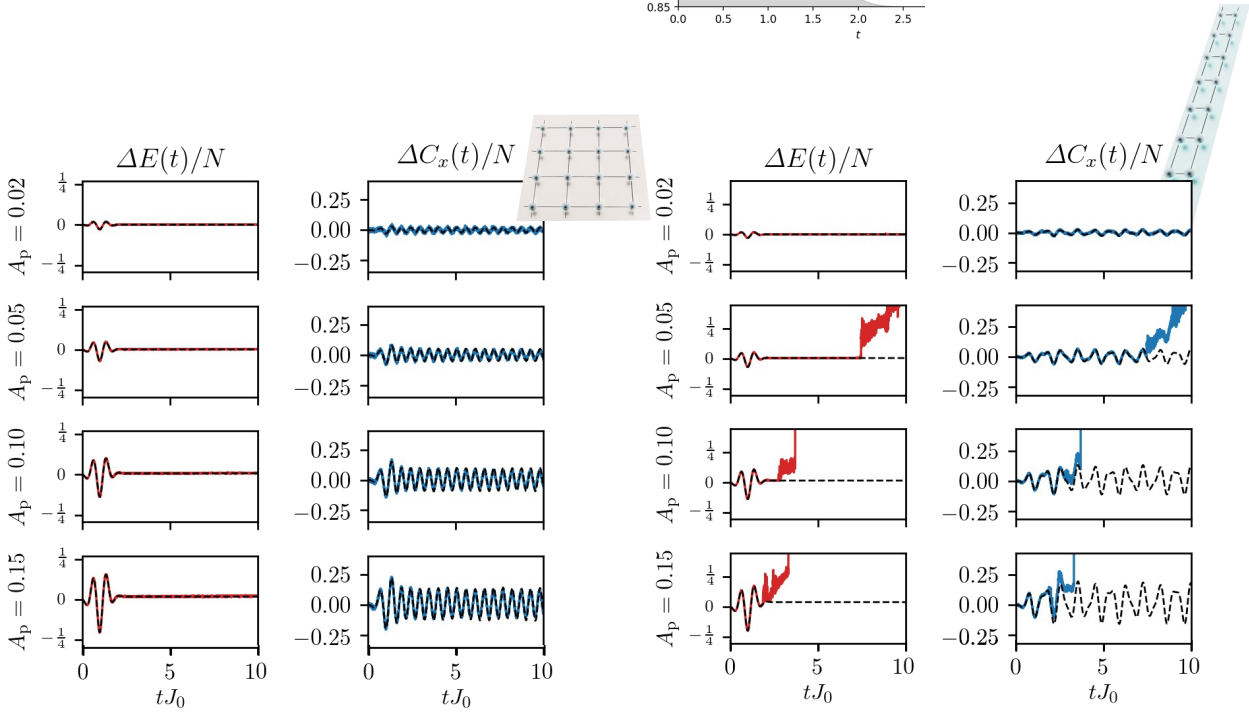



Symmetric RBM architecture – Carleo & Troyer, *Science* 355 (2017)

# Instabilities in time propagation

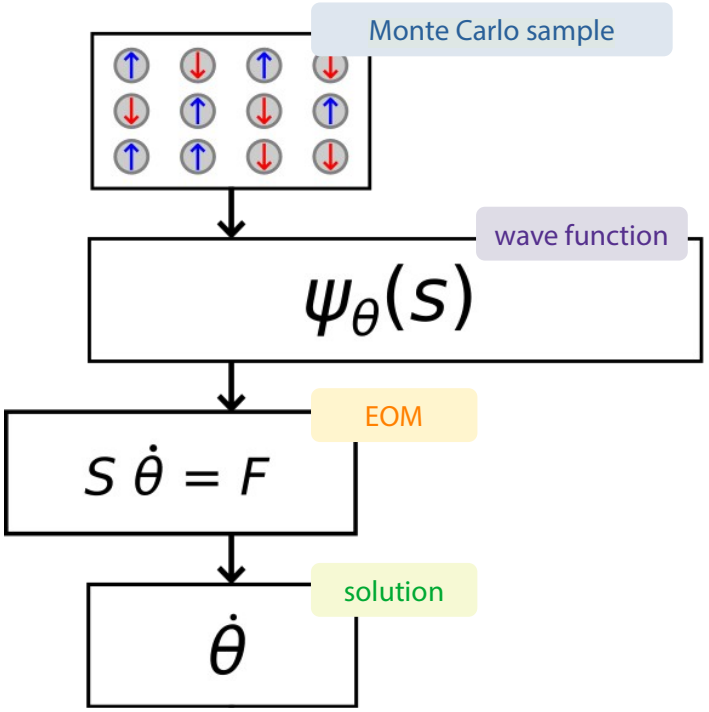



- Propagation using time-dependent variational principle (t-VMC)
- Can exhibit jump instabilities already for weak pulses on the ladder
- Square lattice dynamics are quite stable in comparison
  (for moderate excitation strengths)
- Expressiveness of RBM *ansatz* is not a limiting factor

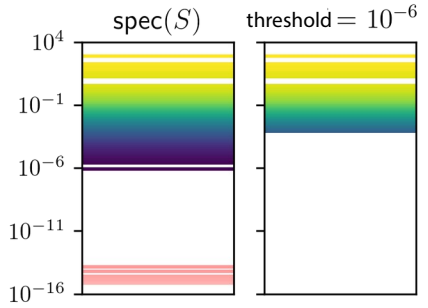


# Stabilization of t-VMC equation of motion

**time-dependent variational Monte Carlo (t-VMC)**




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



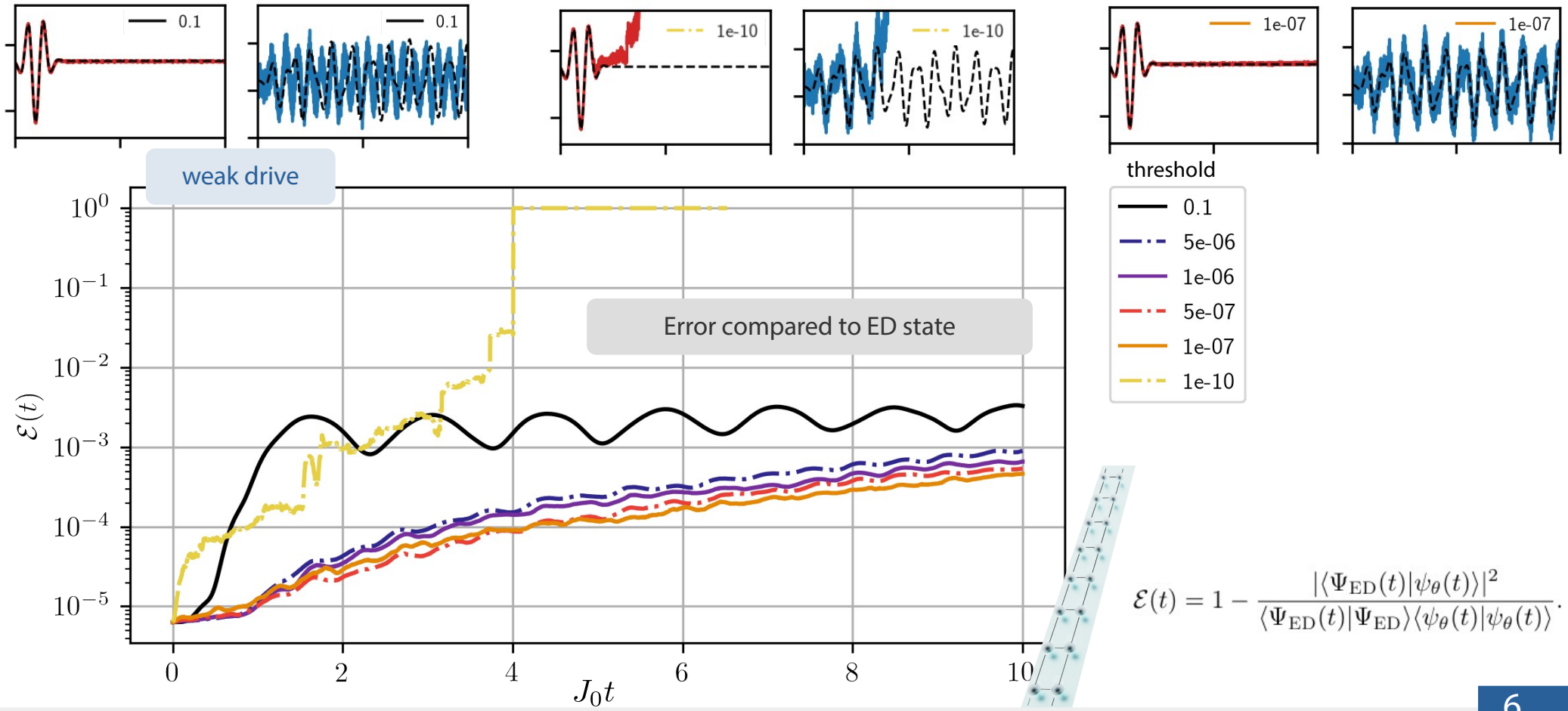

- Equation of motion requires solving linear system
- Typically ill-conditioned ⇒ needs regularization
  - Here: Truncate eigenvalues below threshold

  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)

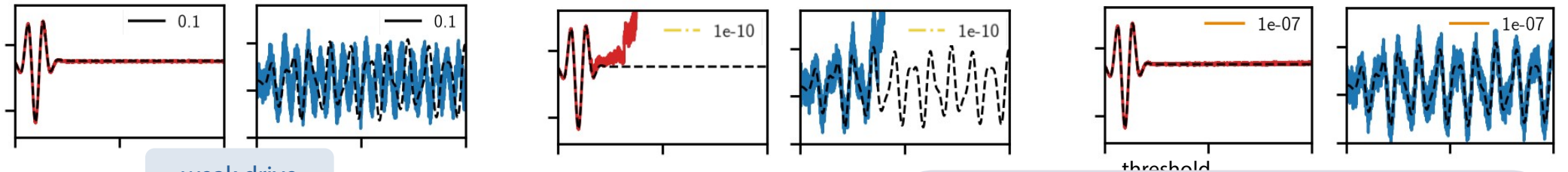
t-VMC – Carleo, Becca, Schiró, Fabrizio, *Sci. Rep.* 2 (2012)

# Threshold dependence of solution quality

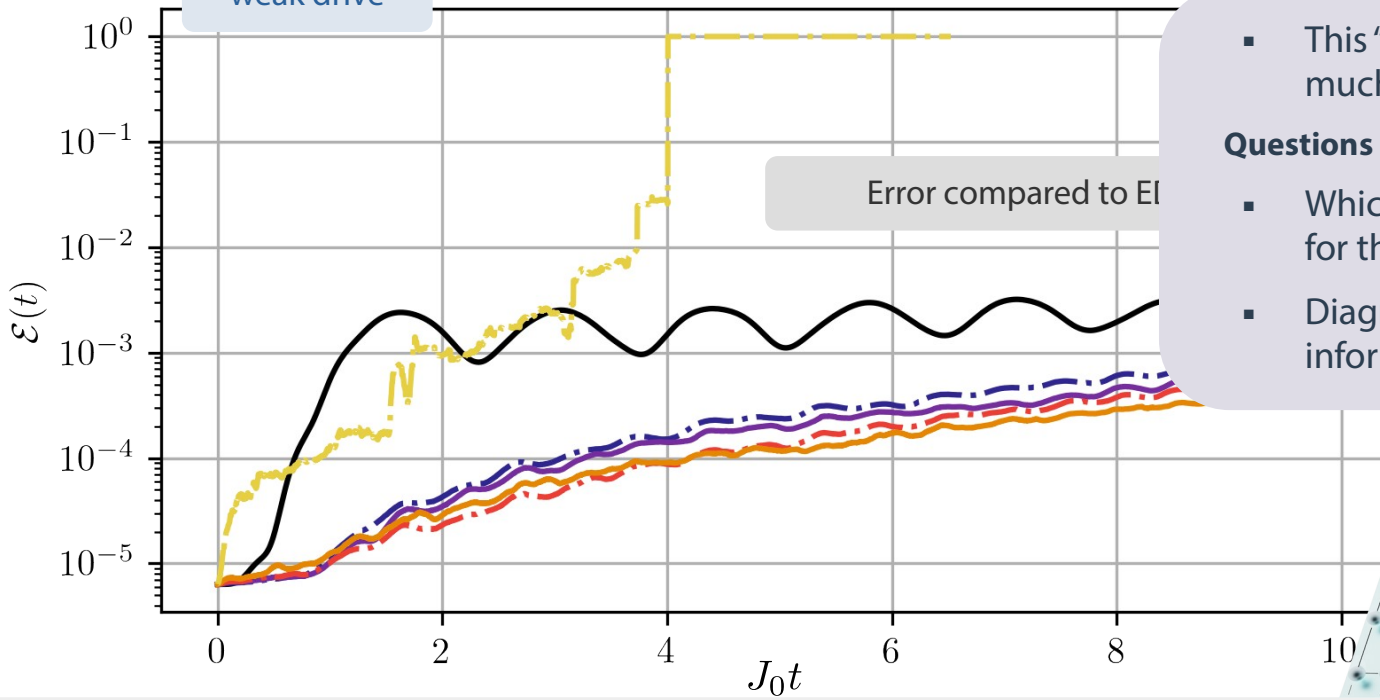



$$\mathcal{E}(t) = 1 - \frac{|\langle \Psi_{\mathrm{ED}}(t) | \psi_\theta(t) \rangle|^2}{\langle \Psi_{\mathrm{ED}}(t) | \Psi_{\mathrm{ED}} \rangle \langle \psi_\theta(t) | \psi_\theta(t) \rangle}.$$

# Threshold dependence of solution quality




weak drive




Error compared to E

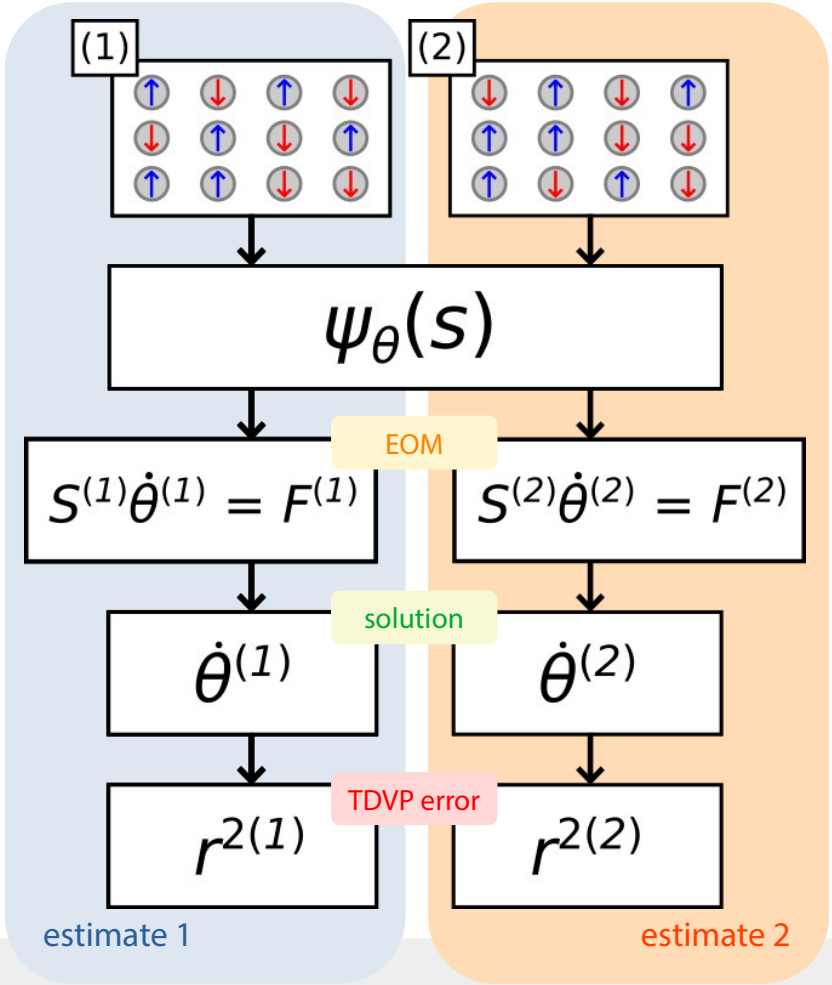
- This "stable regime" of regularization becomes much smaller for higher pulse strength

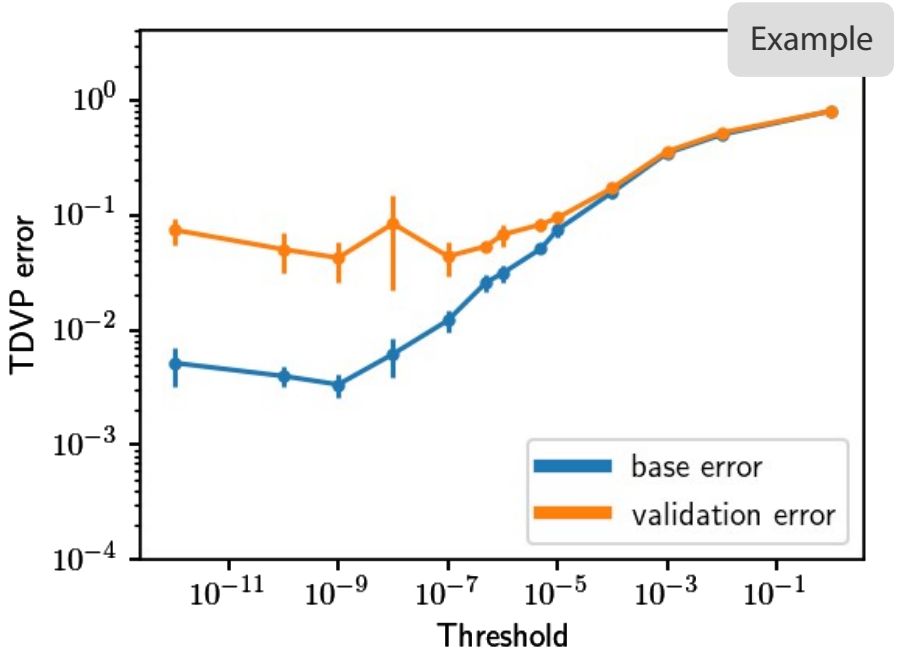
**Questions**

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

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

# Validation error and over-fitting to noise

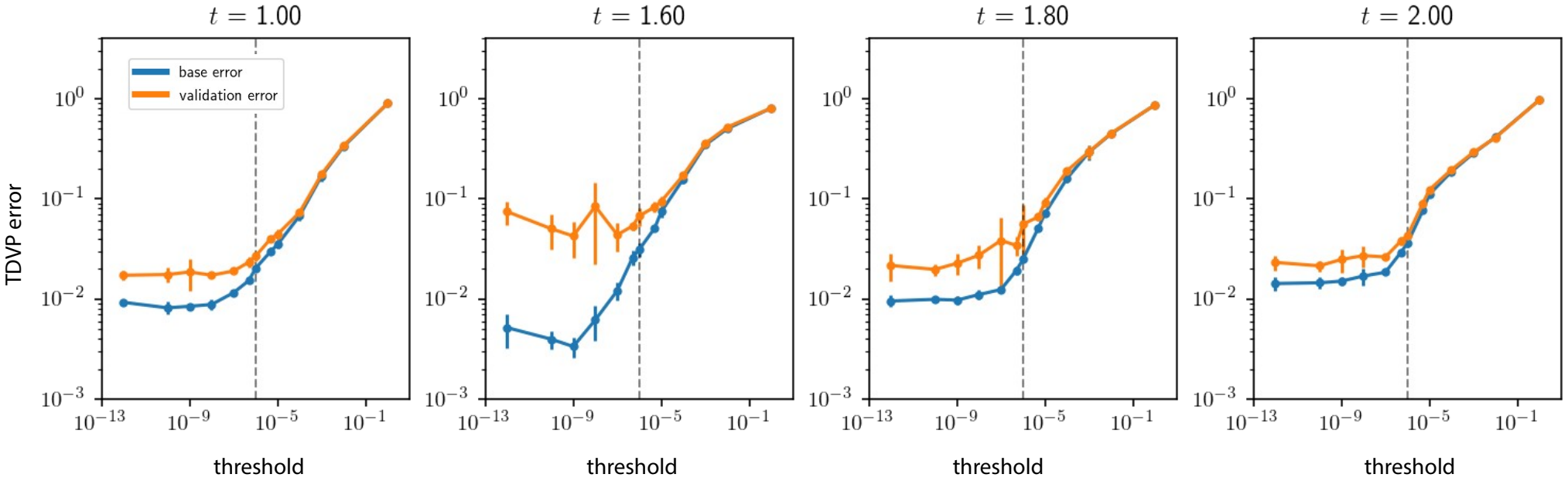


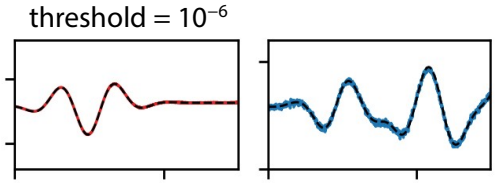



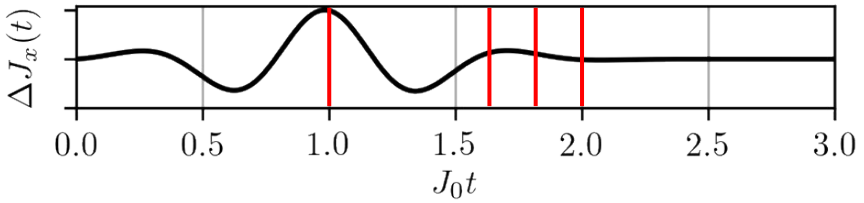

$$r^2_{\text{val}} = r^2[\dot{\theta}^{(2)}, S^{(1)}, F^{(1)}]$$

validation error

# Validation error and over-fitting to noise

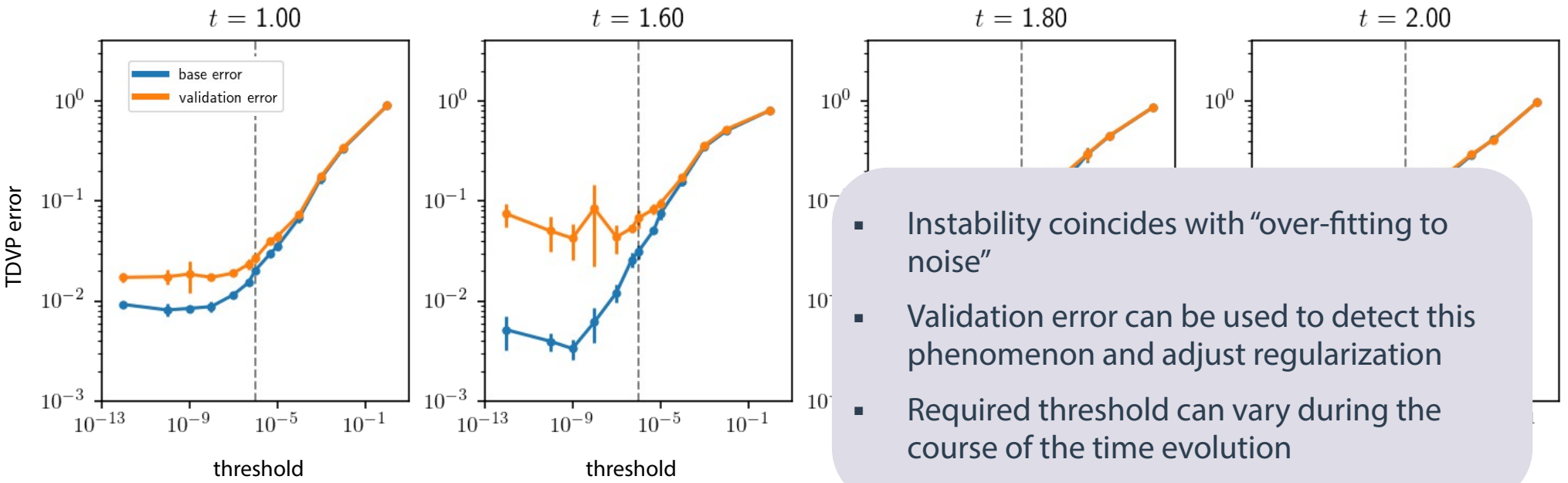


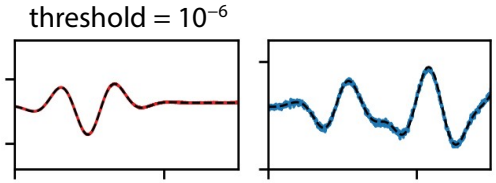



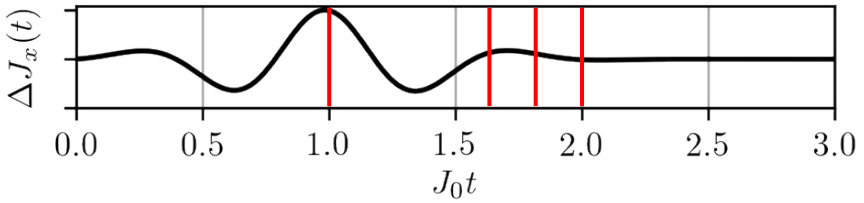

stronger drive

# Validation error and over-fitting to noise




- Instability coincides with "over-fitting to noise"
- Validation error can be used to detect this phenomenon and adjust regularization
- Required threshold can vary during the course of the time evolution

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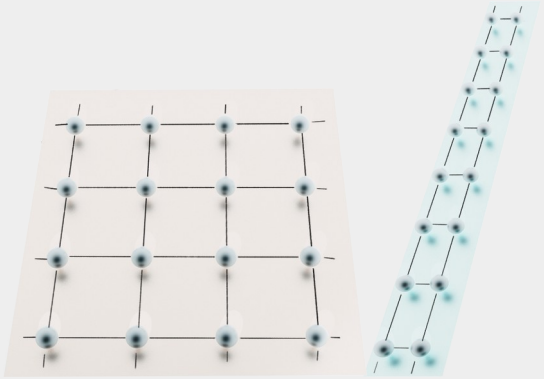
# Summary



mpsd

- Heisenberg ladder is challenging to simulate using RBM quantum states and t-VMC
- Over-fitting to noise is a key source of errors in time-dependent VMC for NQS
- Validation-set TDVP error can help as diagnostic for required fine-tuning of numerical parameters

Thank you for your attention!

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

Net

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

Preprint – in preparation

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[1] *Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany*
[2] *Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands*
[3] *Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland*

Contact – Damian Hofmann
damian.hofmann@mpsd.mpg.de

**The End**