Title: Data-enhanced variational Monte Carlo for Rydberg atom arrays

Speakers: Stefanie Czischek

Collection: Quantum Criticality: Gauge Fields and Matter

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Abstract: Rydberg atom arrays are programmable quantum simulators capable of preparing interacting qubit systems in a variety of quantum states. However, long experimental state preparation times limit the amount of measurement data that can be generated at reasonable timescales, posing a challenge for the reconstruction and characterization of quantum states. Over the last years, neural networks have been explored as a powerful and systematically tuneable ansatz to represent quantum wavefunctions. These models can be efficiently trained from projective measurement data or through Hamiltonian-guided variational Monte Carlo. In this talk, I will compare the data-driven and Hamiltonian-driven training procedures to reconstruct ground states of two-dimensional Rydberg atom arrays. I will discuss the limitations of both approaches and demonstrate how pretraining on a small amount of measurement data can significantly reduce the convergence time for a subsequent variational optimization of the wavefunction.

Data-enhanced variational Monte Carlo for Rydberg atom arrays

Stef Czischek

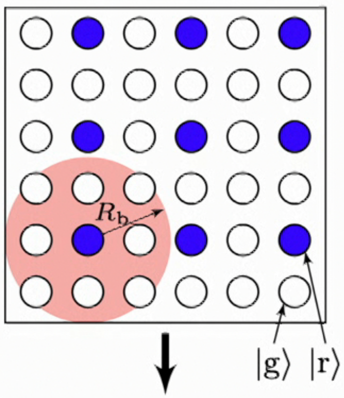
Quantum Criticality: Gauge Fields and Matter

May 18, 2022

UNIVERSITY OF WATERLOO

PIQUIL

Rydberg atom arrays

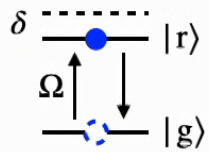


Projective measurement

$|\boldsymbol{\sigma}\rangle = |\mathrm{g\ r\ g} \dots \mathrm{g\ g}\rangle$

$N = L \times L$

atoms on
square lattice



$\hat{\sigma}_i^x = |\mathrm{g}\rangle_i \langle \mathrm{r}|_i$

$\hat{n}_i = |\mathrm{r}\rangle_i \langle \mathrm{r}|_i$

van der Waals interaction:
penalize two excitations within R_b
(Rydberg blockade)

$$V_{ij} = \frac{\Omega R_b^6}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^6}$$

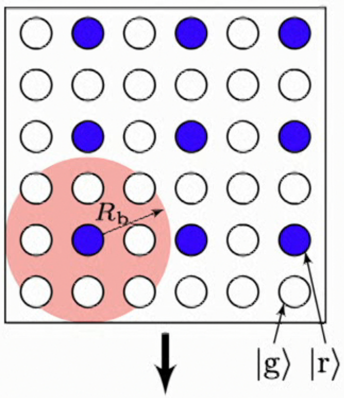
$$\hat{H} = -\frac{\Omega}{2}\sum_{i=1}^{N} \hat{\sigma}_i^x - \delta \sum_{i=1}^{N} \hat{n}_i + \sum_{i,j} V_{ij} \hat{n}_i \hat{n}_j$$

Laser driving:
detuning δ, Rabi frequency Ω

Stefanie.Czischek@uOttawa.ca

[SC, et al., PRB **105**, 205108 (2022)]

Rydberg atom arrays



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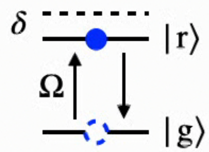

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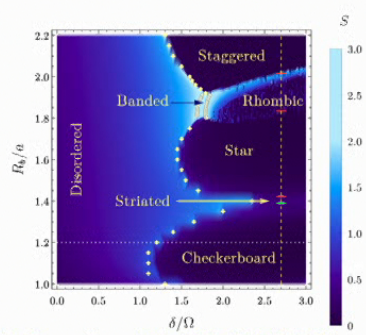
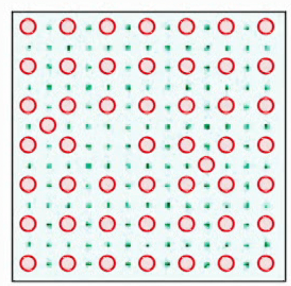
Laser driving:
detuning δ, Rabi frequency Ω

- various phases of matter
- well-controlled experimental realizations



[R. Samajdar et al., PRL **124** (2020)]



[S. Ebadi et al., Nature **595** (2021)]

[G. Semeghini et al., Science 374 (2021)]
[R. Samajdar et al., PNAS 118 (2021)]
[M. Kalinowski et al., PRB **105** (2022)]
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[E. Merali et al., arXiv:2107.0076 (2021)]

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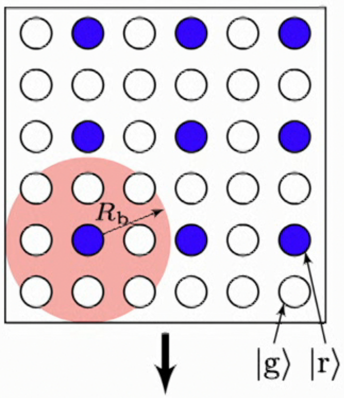

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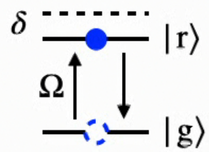

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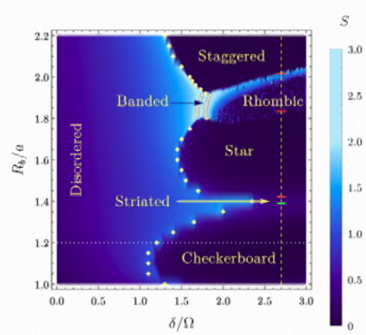
Laser driving:
detuning δ, Rabi frequency Ω

- various phases of matter
- well-controlled experimental realizations

BUT: long state preparation times



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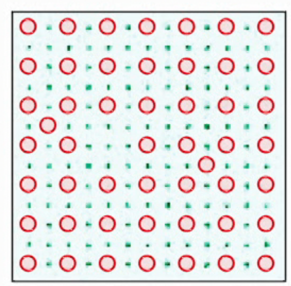

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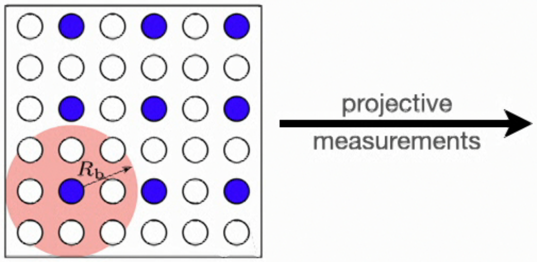
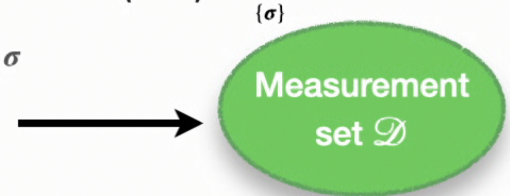
Quantum State Reconstruction



$$(\,\text{-}1 \;\; 1 \;\; \text{-}1 \;\; 1 \;\; \text{-}1 \;\; 1 \; \cdots \; \text{-}1 \;\; \text{-}1\,) = \boldsymbol{\sigma}$$

$$|\Psi\rangle = |\bigcirc\bullet\bigcirc\bullet\bigcirc\bullet\cdots\bigcirc\bigcirc\rangle$$

$$\left\langle \mathcal{O}_{\text{diag}} \right\rangle = \sum_{\{\boldsymbol{\sigma}\}} \mathcal{O}_{\text{diag}}(\boldsymbol{\sigma})\,\Psi(\boldsymbol{\sigma})\Psi(\boldsymbol{\sigma})^*$$

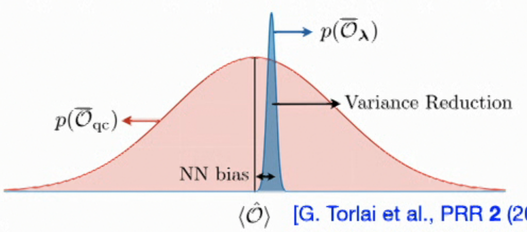


$$p_{\mathcal{D}}(\boldsymbol{\sigma}) \approx \Psi(\boldsymbol{\sigma})\Psi^*(\boldsymbol{\sigma})$$

Ground states of stoquastic Hamiltonians:

$$\Psi(\boldsymbol{\sigma}) \in \mathbb{R} \quad \Rightarrow \quad \Psi(\boldsymbol{\sigma}) \approx \sqrt{p_{\mathcal{D}}(\boldsymbol{\sigma})}$$

- Tomographically reconstruct quantum state from finite measurement set
  - Generate more measurement data



[G. Torlai et al., PRR **2** (2020)]

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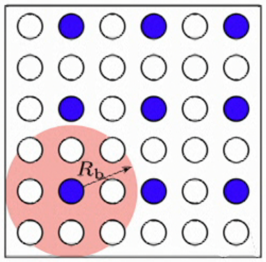
[SC, et al., PRB **105**, 205108 (2022)]

Quantum State Reconstruction



projective measurements

$$(-1 \;\; 1 \;\; -1 \;\; 1 \;\; -1 \;\; 1 \;\cdots\; -1 \;\; -1) = \boldsymbol{\sigma}$$

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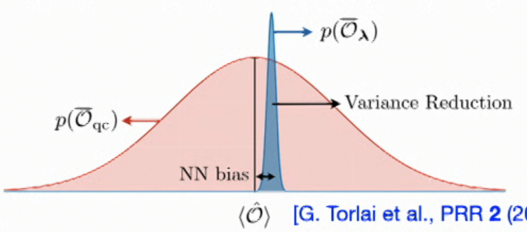


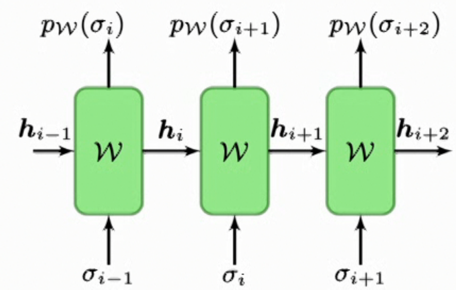
[G. Torlai et al., PRR **2** (2020)]

RNN quantum states:

$$p_{\text{RNN}}(\boldsymbol{\sigma}; \mathscr{W}) \approx \Psi(\boldsymbol{\sigma})\Psi(\boldsymbol{\sigma})^*$$

Tune expressivity via N_{h} hidden units

[M. Hibat-Allah et al., PRR **2** (2020)]



[SC, et al., PRB **105**, 205108 (2022)]

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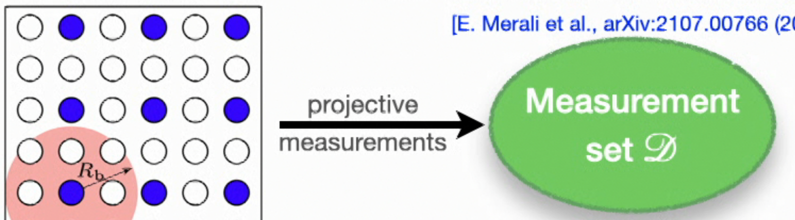
Data-based Rydberg state reconstruction

$N = L \times L$ atoms

10^5 measurements to estimate H_{QMC}

[E. Merali et al., arXiv:2107.00766 (2021)]



$p_{\mathscr{D}}(\boldsymbol{\sigma})$

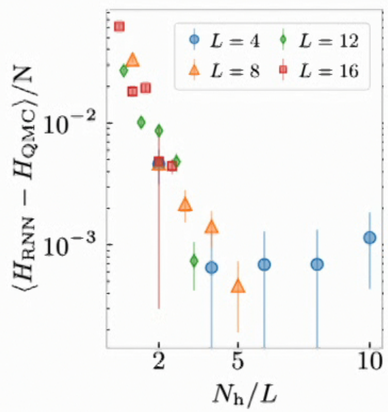
$$\hat{H} = -\frac{\Omega}{2}\sum_{i=1}^{N}\hat{\sigma}_i^x - \delta\sum_{i=1}^{N}\hat{n}_i + \sum_{i,j}V_{ij}\hat{n}_i\hat{n}_j$$

stoquastic

$$V_{ij} = \frac{\Omega R_b^6}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^6} = \frac{7}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^6} \qquad \Omega = \delta = 1$$

$$p_{\mathrm{RNN}}(\boldsymbol{\sigma}; \mathscr{W}) \approx p_{\mathscr{D}}(\boldsymbol{\sigma})$$

Training:
Minimize Kullback-Leibler divergence



Train on full dataset:
Network can reconstruct the state

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[SC, et al., PRB **105**, 205108 (2022)]

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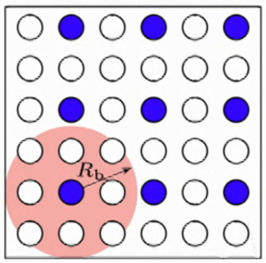

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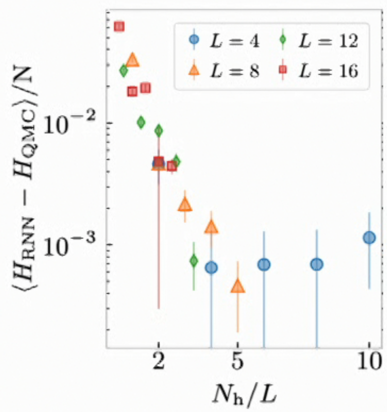

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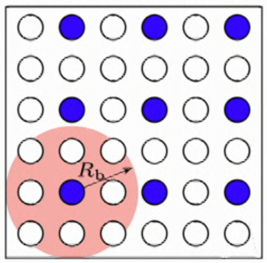

projective measurements → Measurement set $\mathscr{D}$

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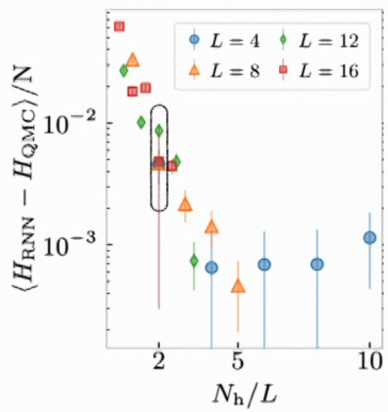

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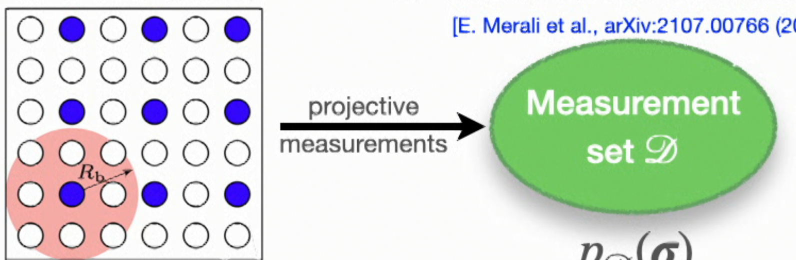

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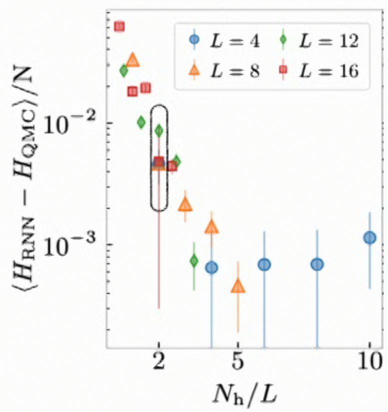
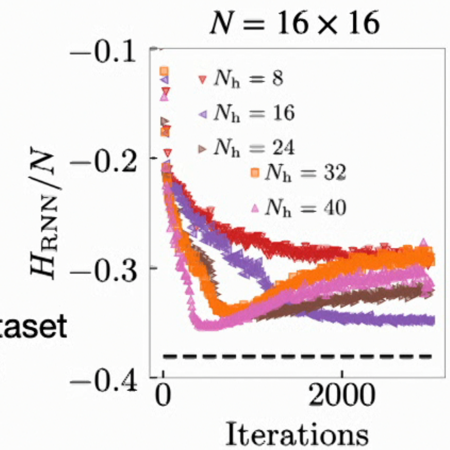


Train on full dataset:
Network can reconstruct the state

Train on limited dataset (10^3 samples):
Overfitting



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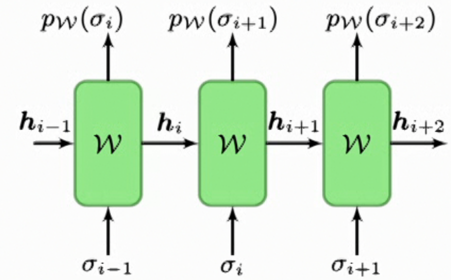
[SC, et al., PRB **105**, 205108 (2022)]

Variational Monte Carlo

- Find ground state via energy minimization
- Training:
  Minimize local energy $H_{\mathrm{RNN}} = \langle \Psi_{\mathscr{W}} | \hat{H} | \Psi_{\mathscr{W}} \rangle$
  evaluated on N_s RNN samples



$$\Psi_{\mathscr{W}}(\boldsymbol{\sigma}) = \langle \Psi_{\mathscr{W}} | \boldsymbol{\sigma} \rangle = \sqrt{p_{\mathrm{RNN}}(\boldsymbol{\sigma}; \mathscr{W})}$$

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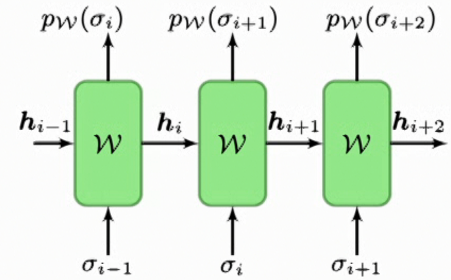

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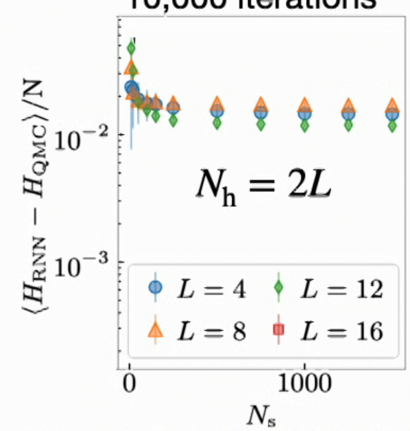
10,000 iterations



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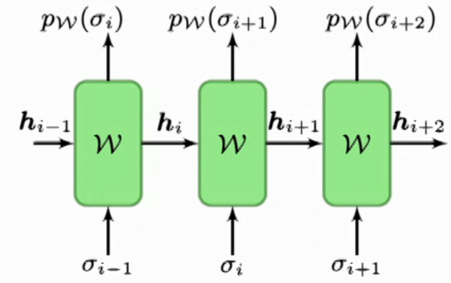

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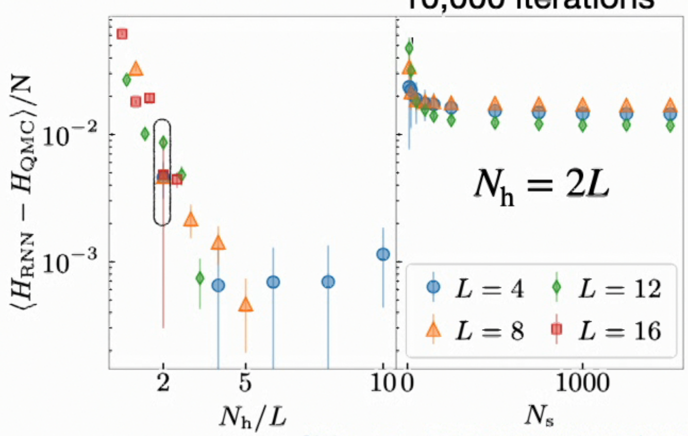

[SC, et al., PRB **105**, 205108 (2022)]

Network expressivity is not the bottleneck!
Limited by convergence times...

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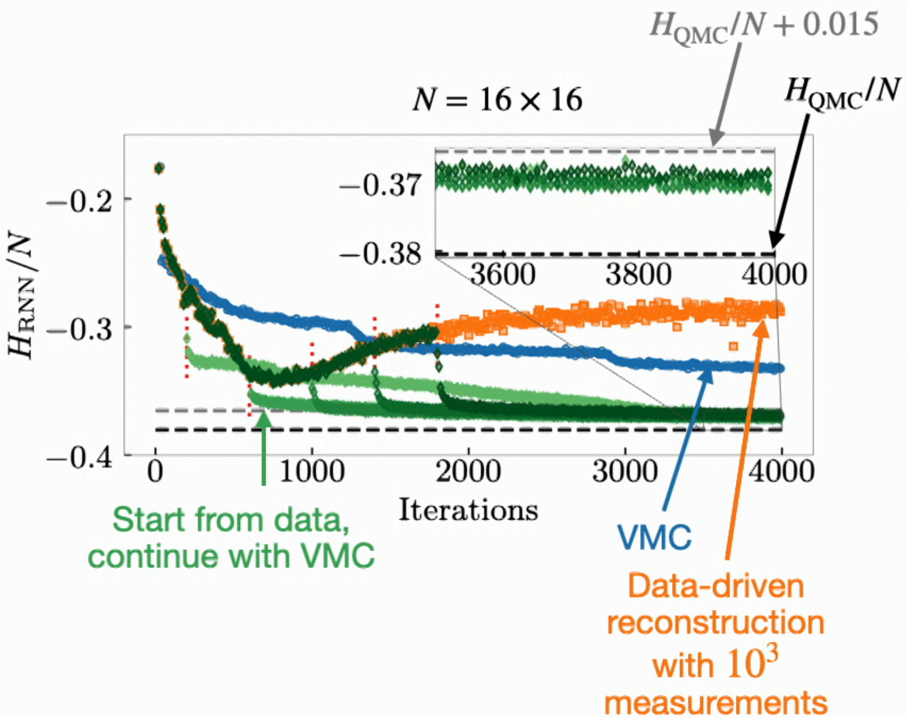
Data-enhanced variational Monte Carlo



- Data-driven reconstruction
- Followed by Hamiltonian-driven VMC

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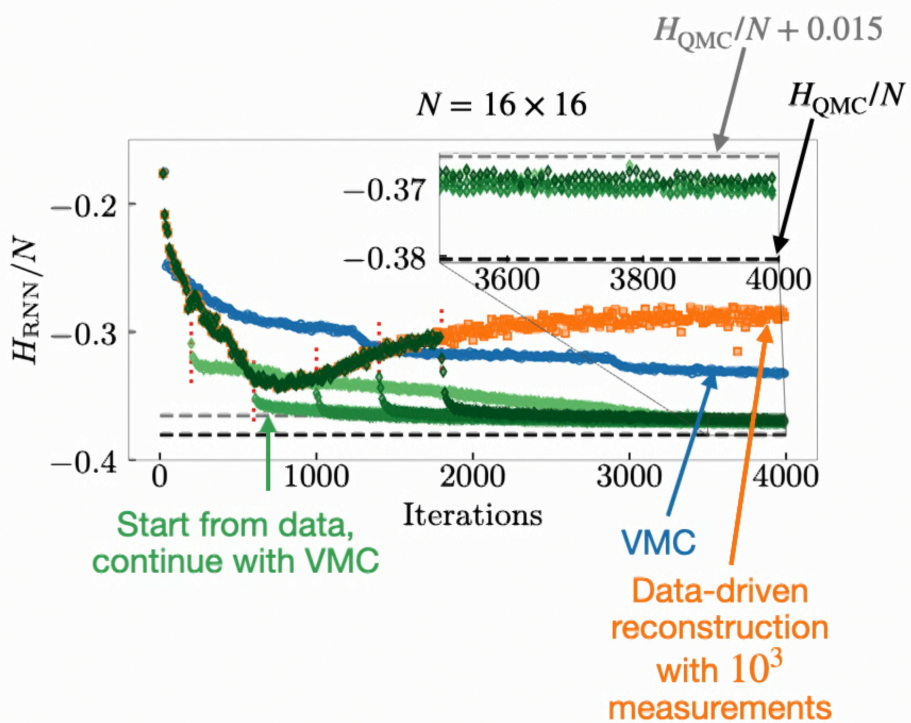

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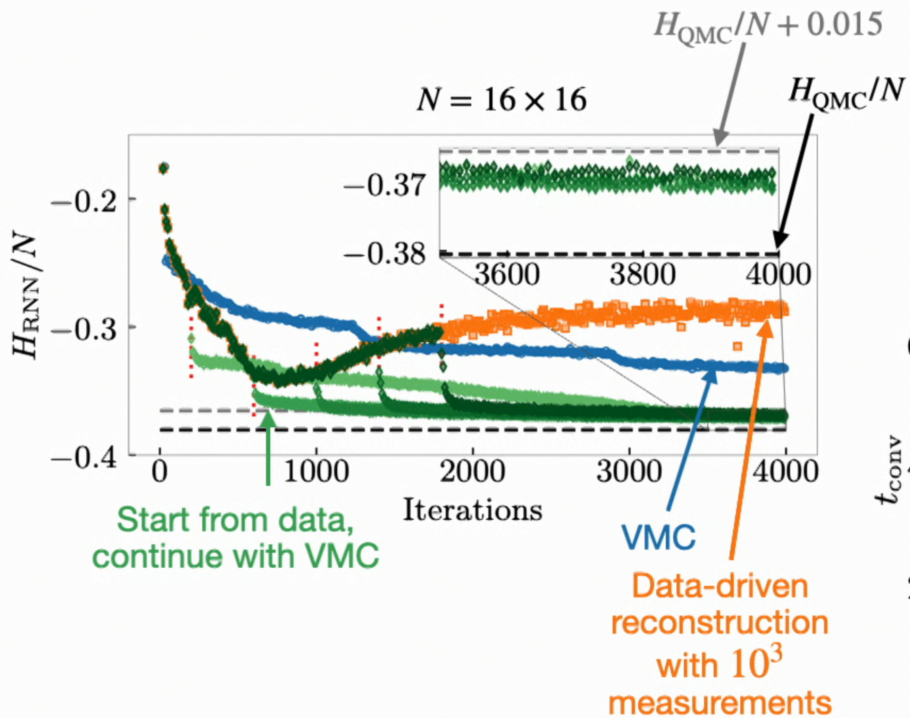

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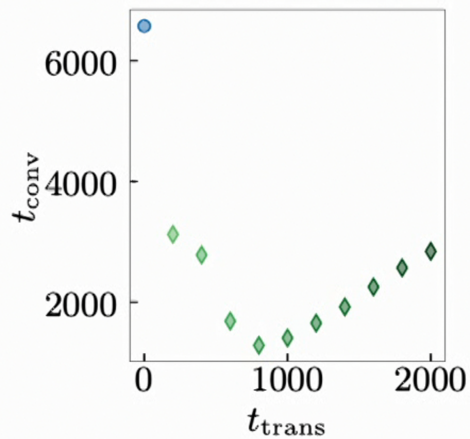

Independent of t_{trans} we can always significantly reduce the convergence time!

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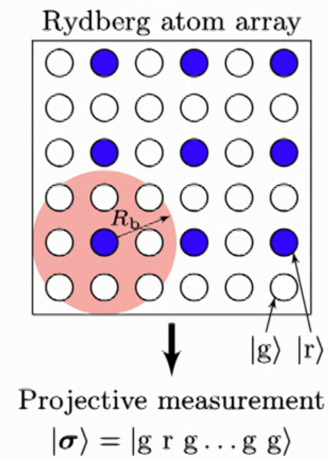
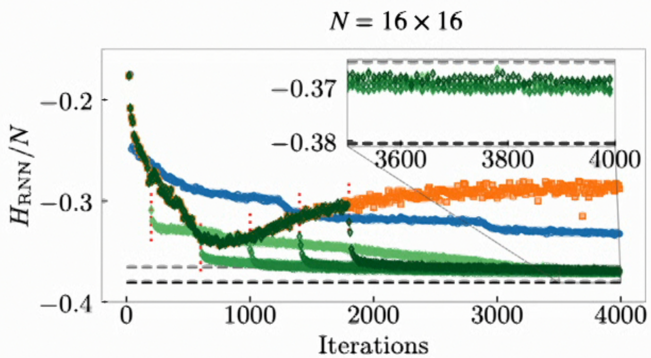
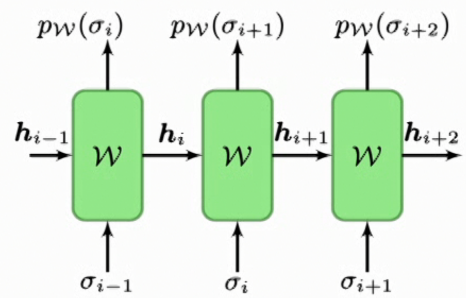
[SC, et al., PRB **105**, 205108 (2022)]

Summary & Outlook

- Data-driven training: large amount of data
- Hamiltonian-driven training: slow convergence
- Data-enhanced VMC gives significant improvement with limited data







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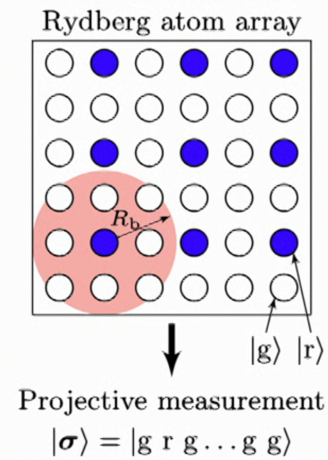
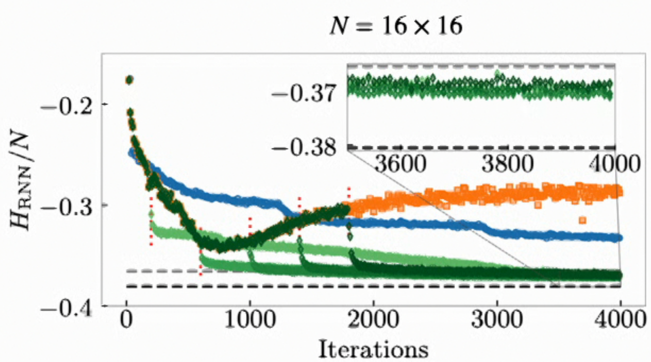
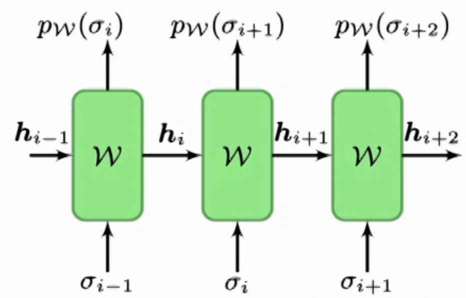
[SC, et al., PRB **105**, 205108 (2022)]

Summary & Outlook

- Data-driven training: large amount of data
- Hamiltonian-driven training: slow convergence
- Data-enhanced VMC gives significant improvement with limited data







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