Combining data-driven and Hamiltonian-driven training for learning Quantum Ground States

Schuyler Moss

September 12th, 2022

UNIVERSITY OF WATERLOO

PI QUANTUM INTELLIGENCE LAB

International Conference on Recent Progress in Many-Body Theories XXI

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Stefanie Czischek, **M. Schuyler Moss**, et al. Phys. Rev. B **105**, 205108 – Published 9 May 2022

https://arxiv.org/abs/2203.04988

Ejaaz Merali (Not Pictured)

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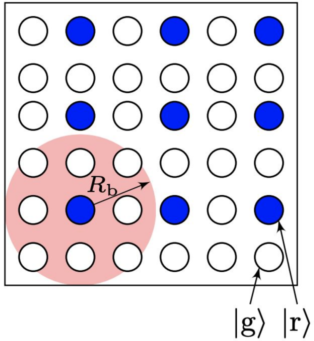
Learning Quantum Ground states

Of what?

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



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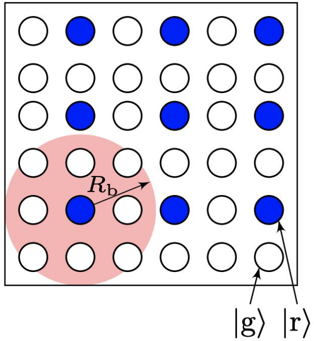
$$\hat{\sigma}_i^x = |g\rangle_i\langle r|_i + |r\rangle_i\langle g|_i$$

“spin flip”
(off diagonal)



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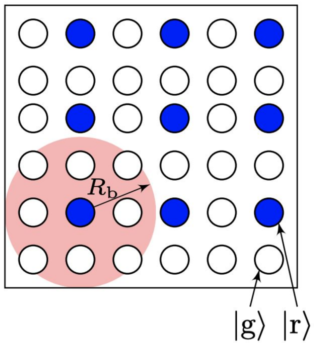
$$\hat{n}_i = |r\rangle_i\langle r|_i$$

occupation operator
(diagonal)



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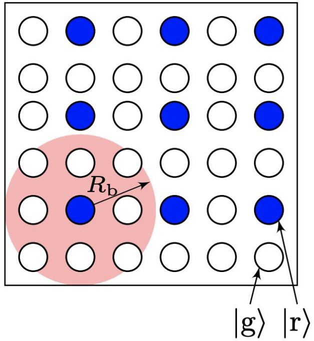

$$V_{ij} = \frac{\Omega R_b^6}{|\mathbf{r}_i - \mathbf{r}_j|^6}$$

Van der Waals potential

Learning Quantum Ground states

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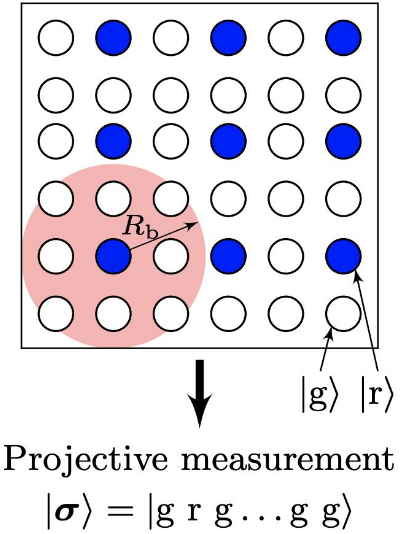

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Learning Quantum Ground states

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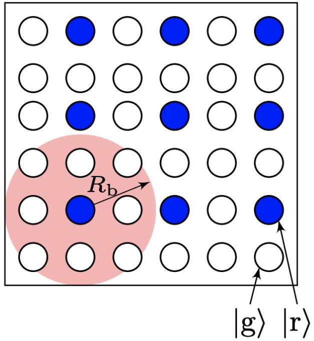

Rydberg Basis:

- Hamiltonian is Stoquastic
- Measurements in this basis are informationally complete

Learning Quantum Ground states

Of what?

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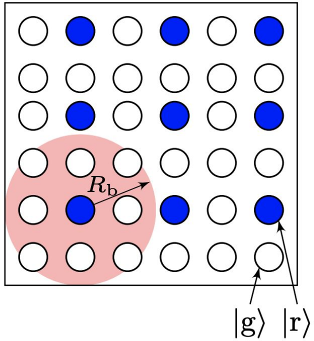
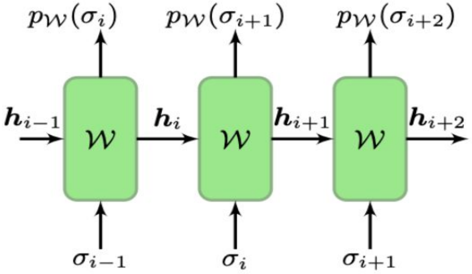


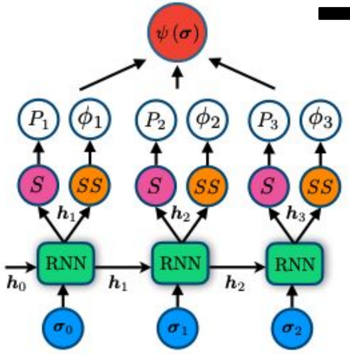
With what?



where $\quad \Psi_{\mathcal{W}}(\boldsymbol{\sigma}) = \sqrt{\prod_i p_{\mathcal{W}}(\sigma_i)}$

Hibat-Allah et. al. Recurrent neural network wave functions. *Physical Review Research*, *2*(2), p.023358.

Aside #1 on RNN Wavefunctions



$$|\Psi\rangle = \sum_{\sigma} \exp(i\phi(\sigma))\sqrt{P(\sigma)}|\sigma\rangle$$

$$\phi(\sigma) = \sum_{n=1}^{N} \phi_n$$

$$P(\sigma) \equiv \prod_{n=1}^{N} P_n$$

Hibat-Allah et. al. Recurrent neural network wave functions. *Physical Review Research*, *2*(2), p.023358.

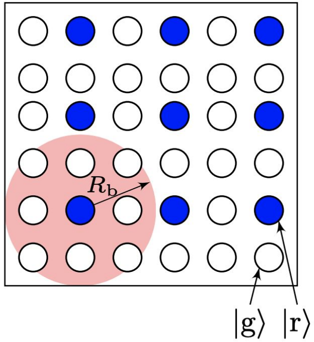
Not limited to Stoquastic Hamiltonians!!!!

Aside #2 on RNN Wavefunctions

The many nice properties:

- Autoregressive Neural Network
  - Chain rule of probabilities: $$P(x_1, x_2, ..., x_N) = \prod_i^N p(x_i | x_{j<i})$$
  - Efficient sampling
  - Encodes a ***normalized*** probability distribution

- Natural interpretation for lattice systems



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Hamiltonian-Driven

Carleo, Giuseppe, and Matthias Troyer. "Solving the quantum many-body problem with artificial neural networks." *Science* 355.6325 (2017): 602-606.

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$$\downarrow$$

$$H_{\mathrm{RNN}} = \frac{\langle\Psi_{\mathcal{W}}|\hat{H}|\Psi_{\mathcal{W}}\rangle}{\langle\Psi_{\mathcal{W}}|\Psi_{\mathcal{W}}\rangle}$$

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$$H_{\text{RNN}} = \frac{\sum_{\sigma} |\langle \Psi_{\mathcal{W}} | \sigma \rangle|^2 \frac{\langle \sigma | \hat{H} | \Psi_{\mathcal{W}} \rangle}{\langle \sigma | \Psi_{\mathcal{W}} \rangle}}{\sum_{\sigma'} |\langle \Psi_{\mathcal{W}} | \sigma' \rangle|^2}$$

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$$H_{\mathrm{RNN}} = \frac{\sum_\sigma \boxed{|\langle \Psi_{\mathcal{W}}|\sigma\rangle|^2} \frac{\langle \sigma|\hat{H}|\Psi_{\mathcal{W}}\rangle}{\langle \sigma|\Psi_{\mathcal{W}}\rangle}}{\boxed{\sum_{\sigma'} |\langle \Psi_{\mathcal{W}}|\sigma'\rangle|^2}}$$

$P(\sigma)$

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$$H_{\text{loc}}(\sigma)$$

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$$H_{\mathrm{RNN}} = \sum_{\sigma} P(\sigma)H_{\mathrm{loc}}(\sigma)$$

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$$H_{\mathrm{RNN}} = \sum_{\sigma} P(\sigma) H_{\mathrm{loc}}(\sigma)$$

$$H_{RNN} \approx \frac{1}{N_s}\sum_{\boldsymbol{\sigma}\sim p_{RNN}(\boldsymbol{\sigma};\mathcal{W})} H_{loc}(\boldsymbol{\sigma})$$

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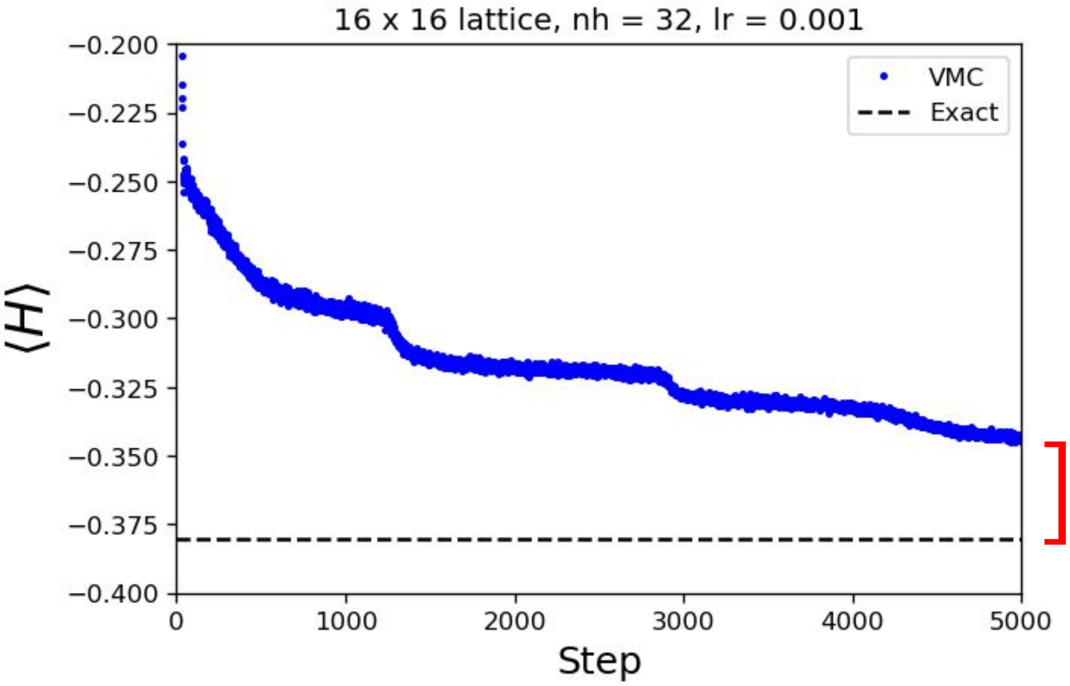
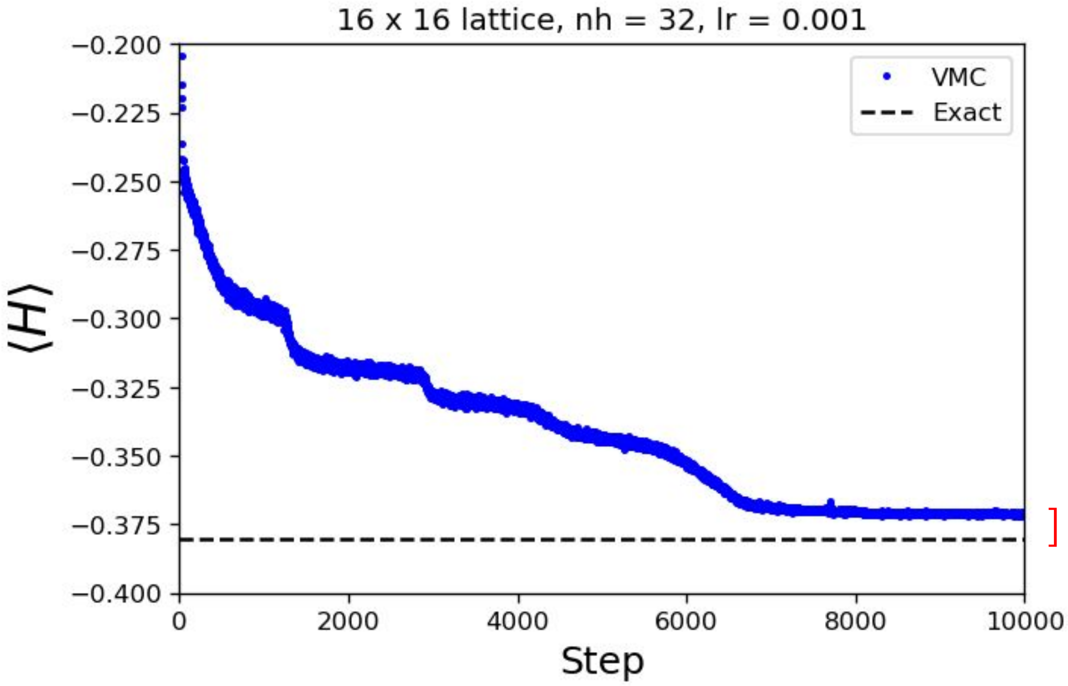
Optimization Challenges (variational training)



not great…

Optimization Challenges (variational training)



] better… but…

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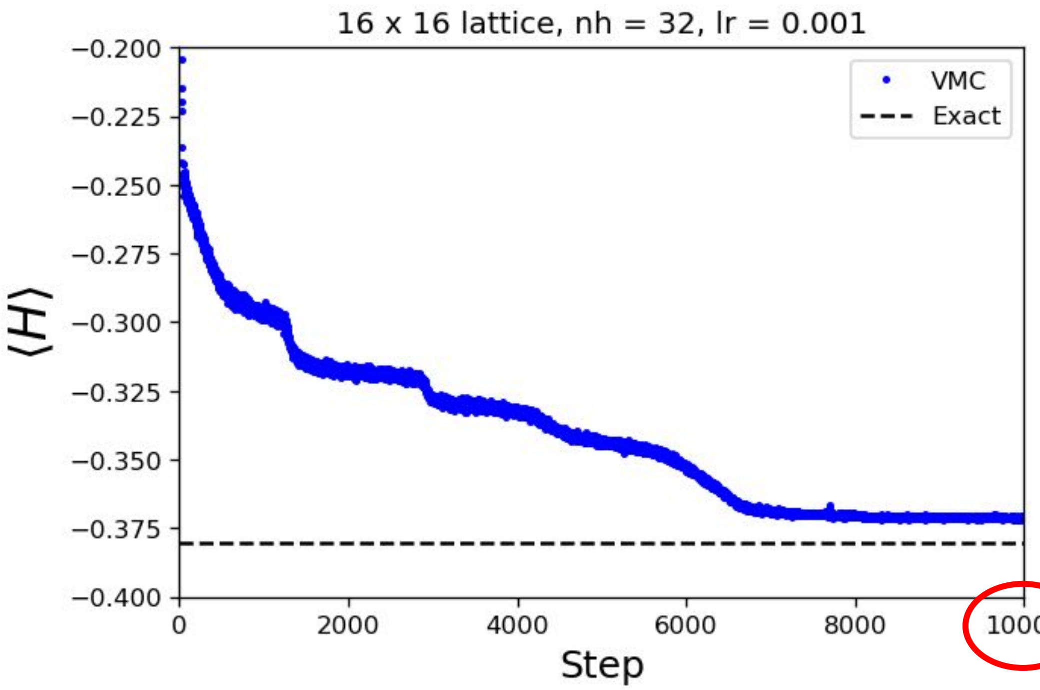
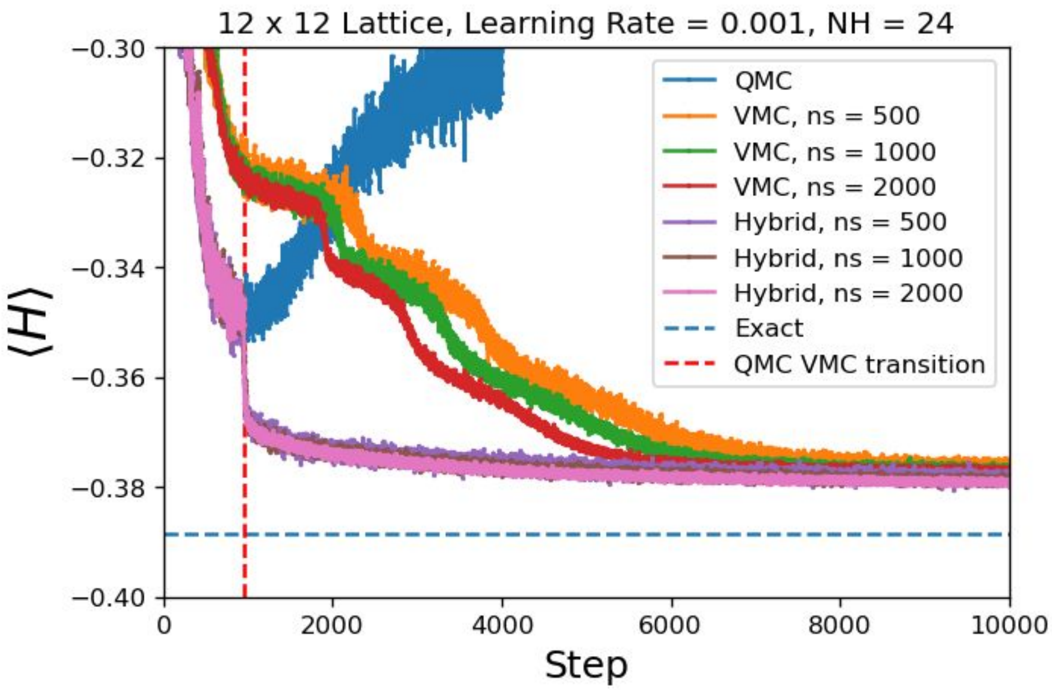


] better… but…

Very long runtime

Aside on Energy Estimation



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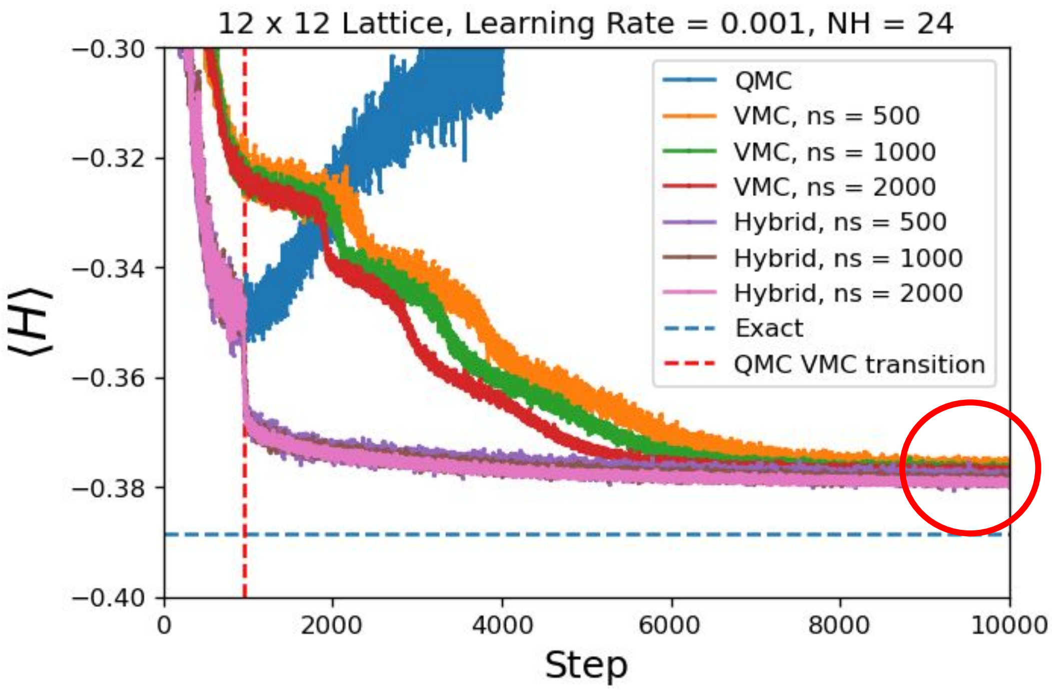
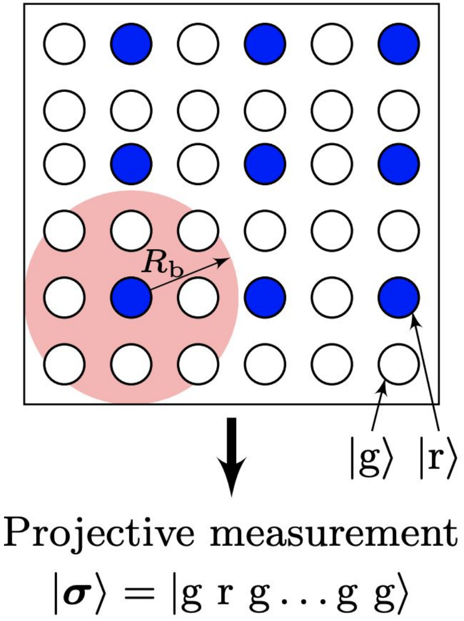


reasonable increases in ns don't result in significant improvements

Data-Driven Training

Torlai *et al.* Neural-network quantum state tomography. *Nature Phys* 14, 447–450 (2018).

Merali, Ejaaz *et al.* "Stochastic series expansion quantum monte carlo for rydberg arrays." *arXiv preprint arXiv:2107.00766* (2021).



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$$\mathcal{L}_{KL}(\mathcal{W}) = \sum_{\{\boldsymbol{\sigma}\}} p_{\mathcal{D}}(\boldsymbol{\sigma}) \log \frac{p_{\mathcal{D}}(\boldsymbol{\sigma})}{p_{RNN}(\boldsymbol{\sigma}; \mathcal{W})}$$

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$$\approx -S_{\mathcal{D}} - \sum_{\boldsymbol{\sigma} \in \mathcal{D}} p_{\mathcal{D}}(\boldsymbol{\sigma}) \log p_{\mathrm{RNN}}(\boldsymbol{\sigma})$$

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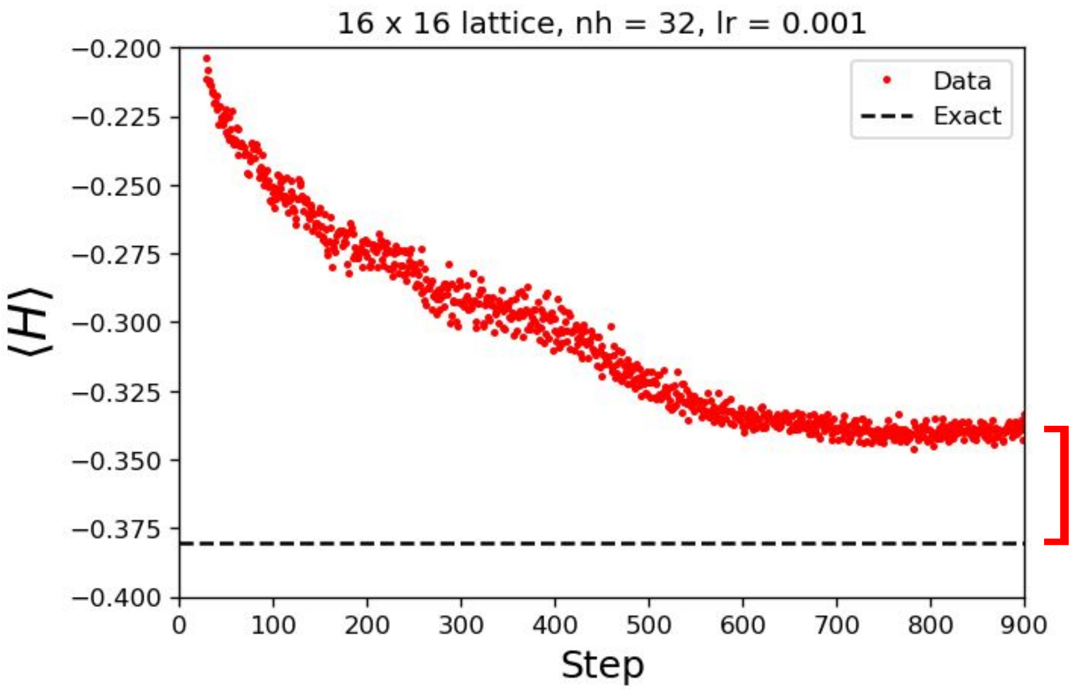
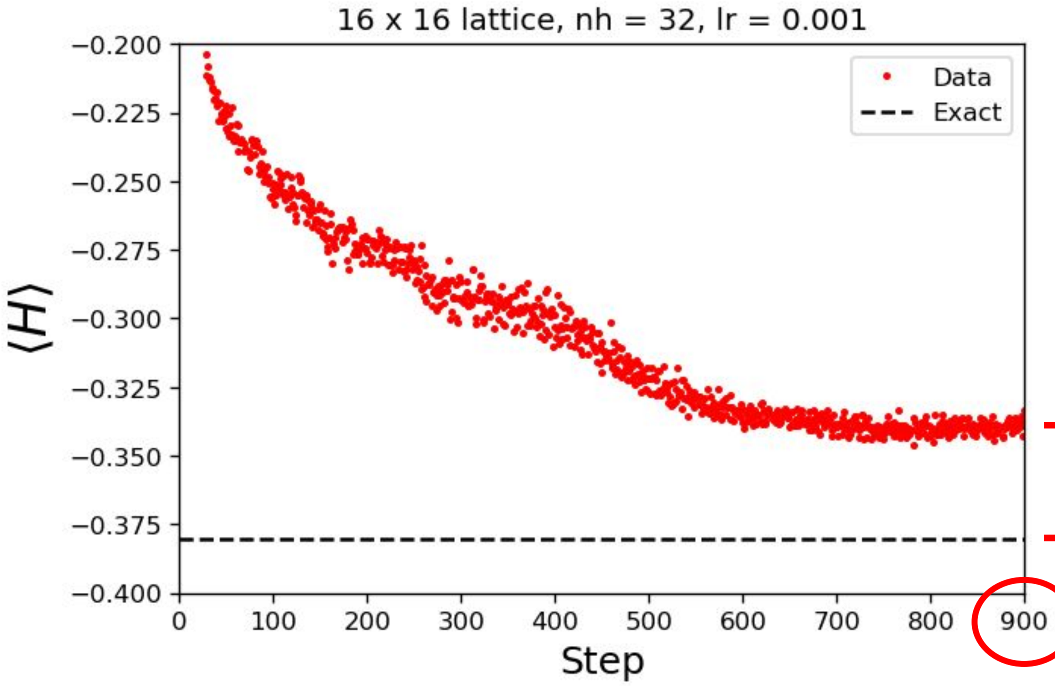
Optimization Challenges (training with data)



Again,
not great…

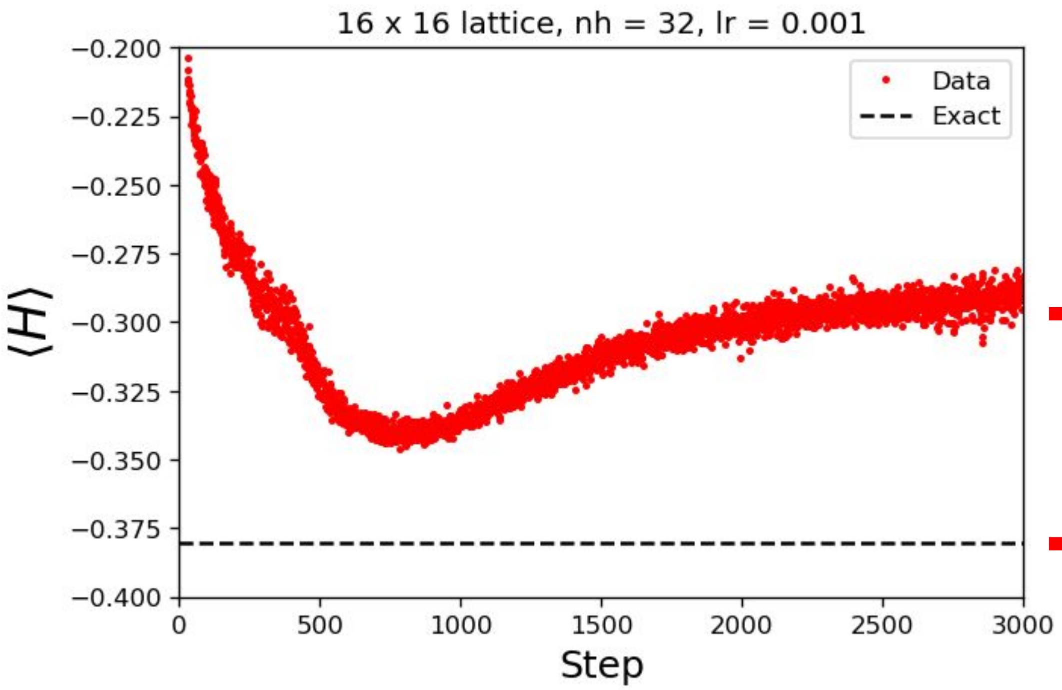
Optimization Challenges (training with data)



Again, not great…

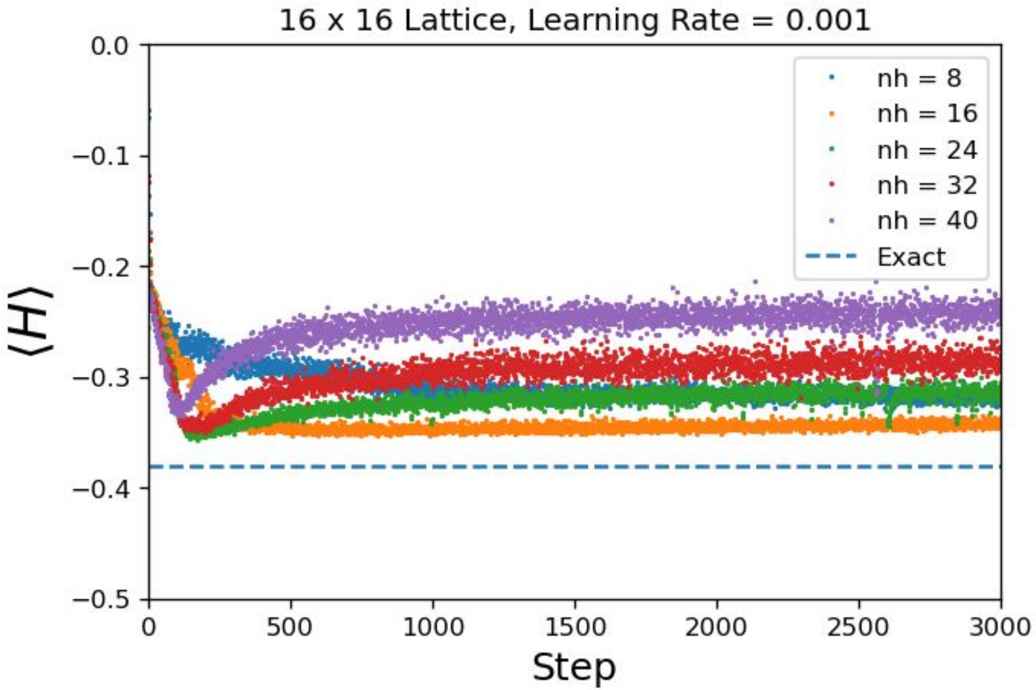
but… much faster.

Optimization Challenges (training with data)



Really bad.

Aside on Overfitting



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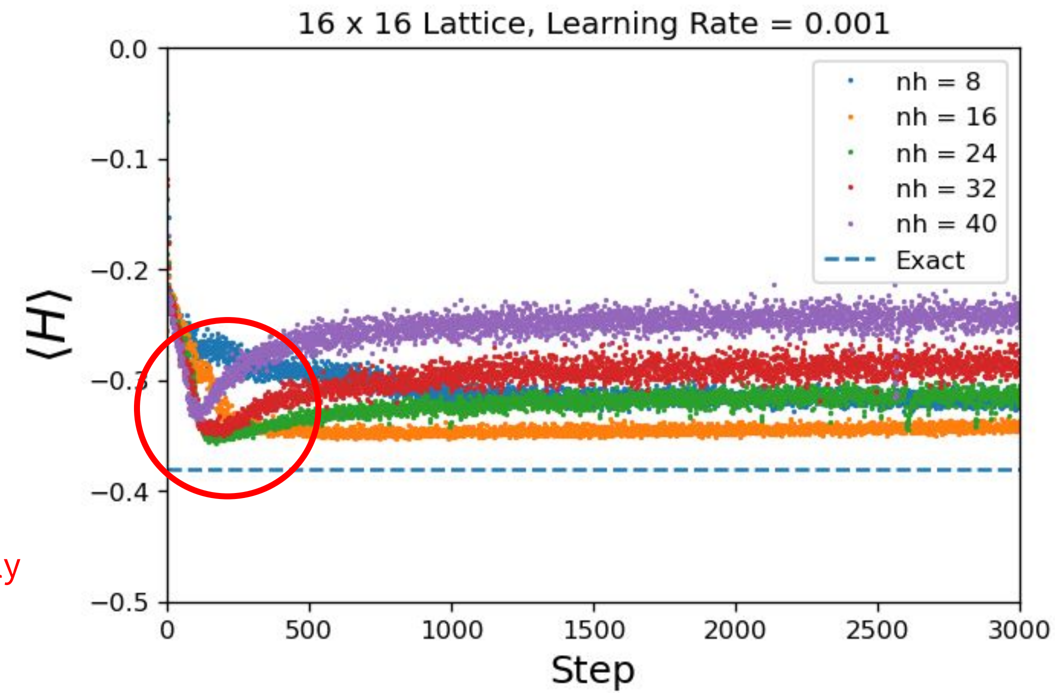
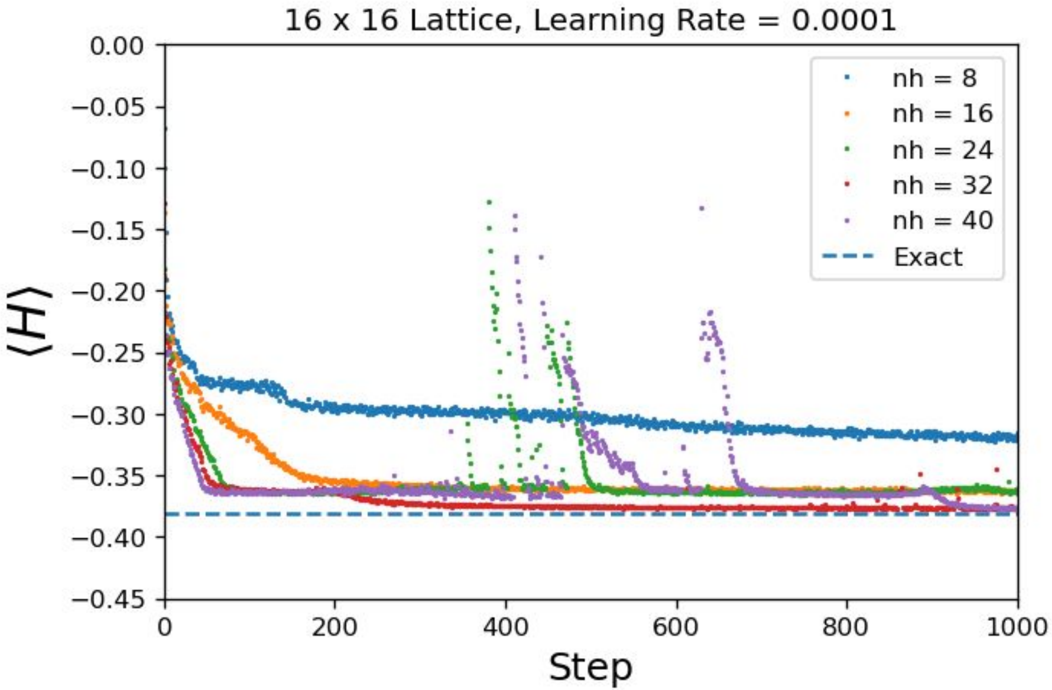


Overfitting occurs consistently

Aside on Expressiveness



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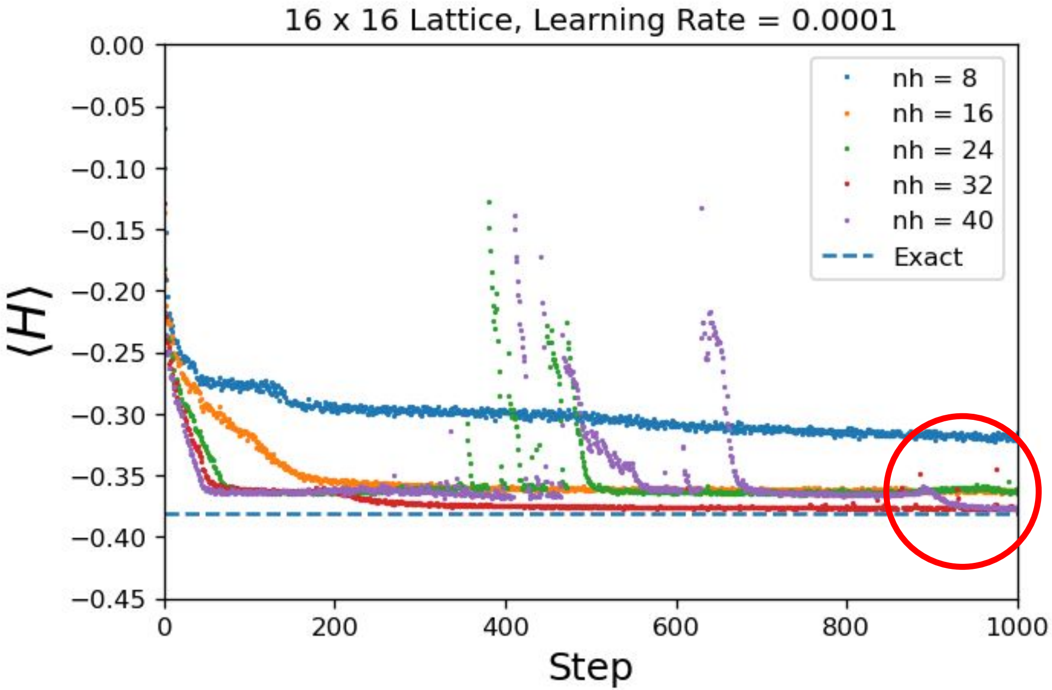
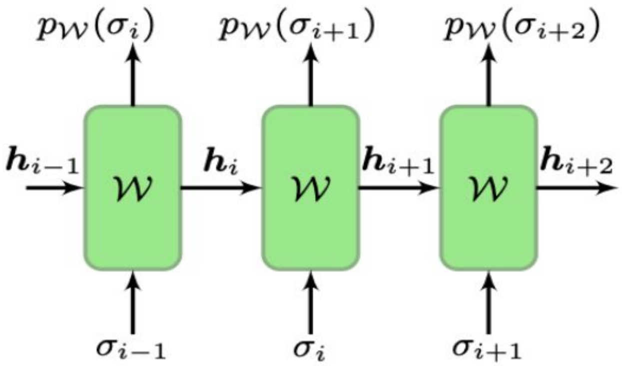


Given the full data set, some system sizes are expressive enough

Proposed Solution



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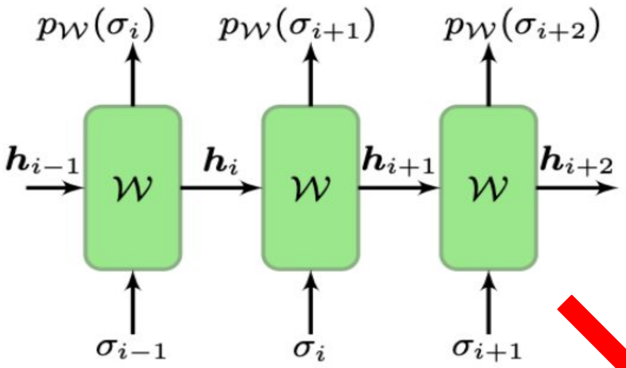
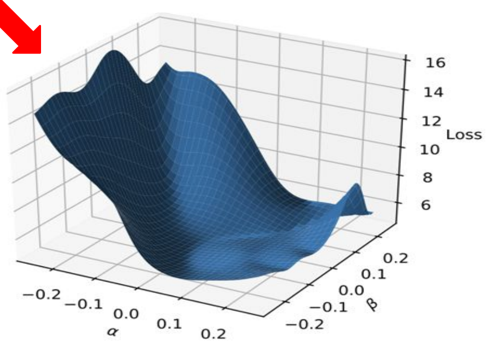


train variationally

Hibat-Allah et. al. Recurrent neural network wave functions. *Physical Review Research*, *2*(2), p.023358.

$$\langle H \rangle$$



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train with data

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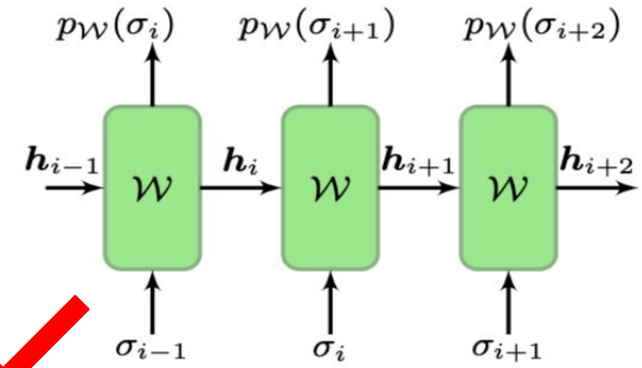

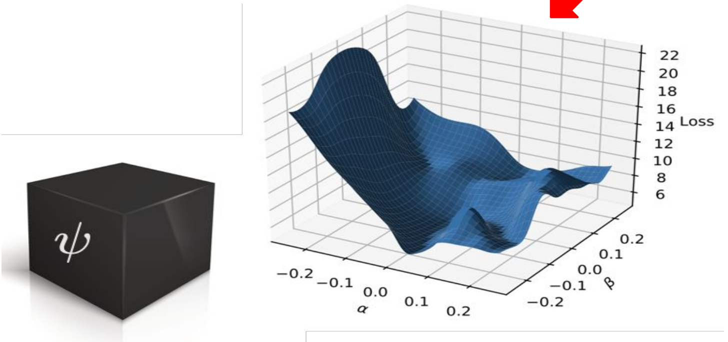

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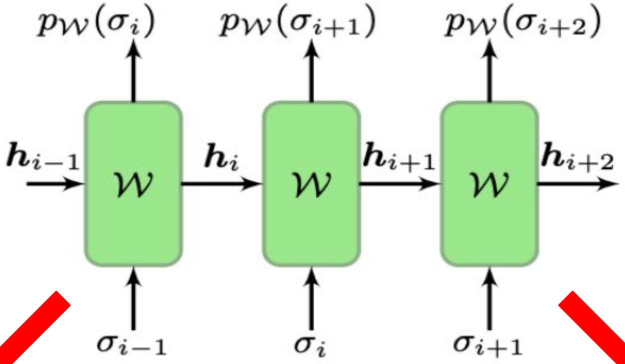

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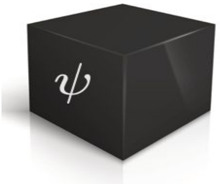

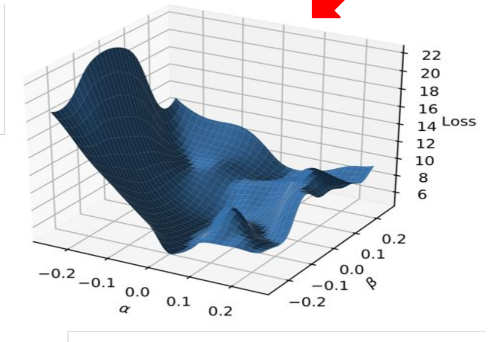

&

??

$\langle H \rangle$

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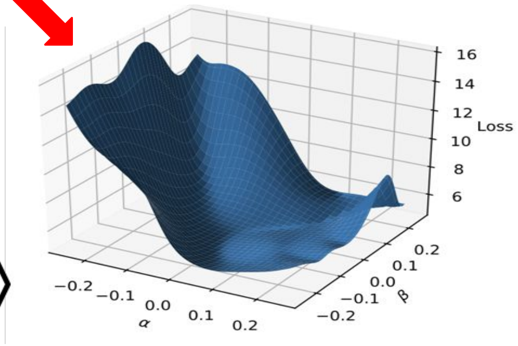
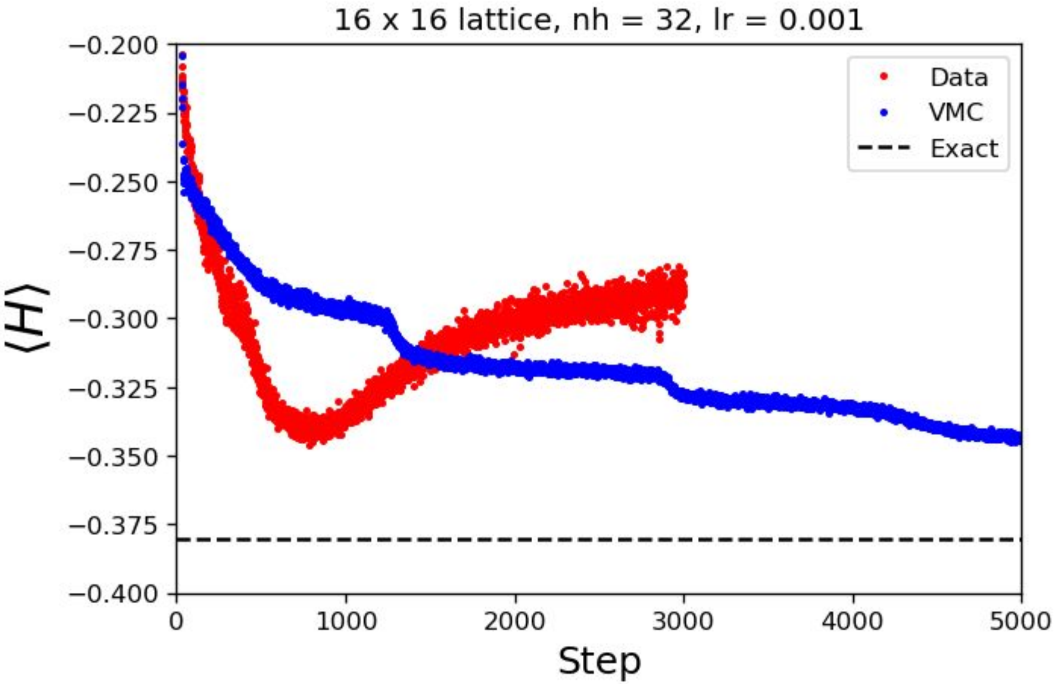


Combining Training Methods



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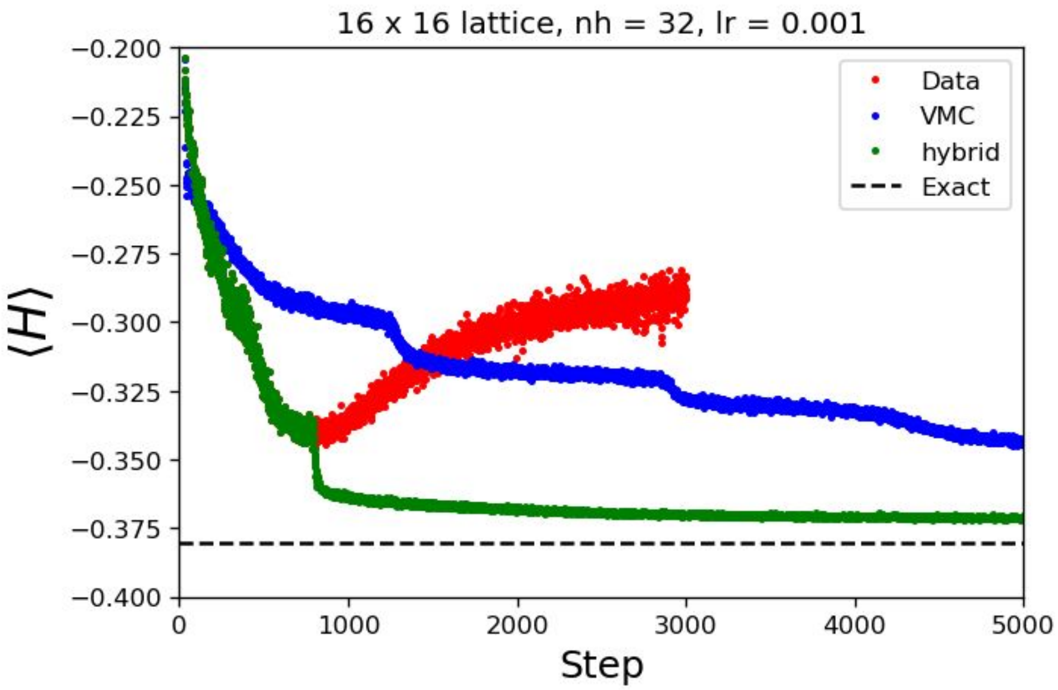

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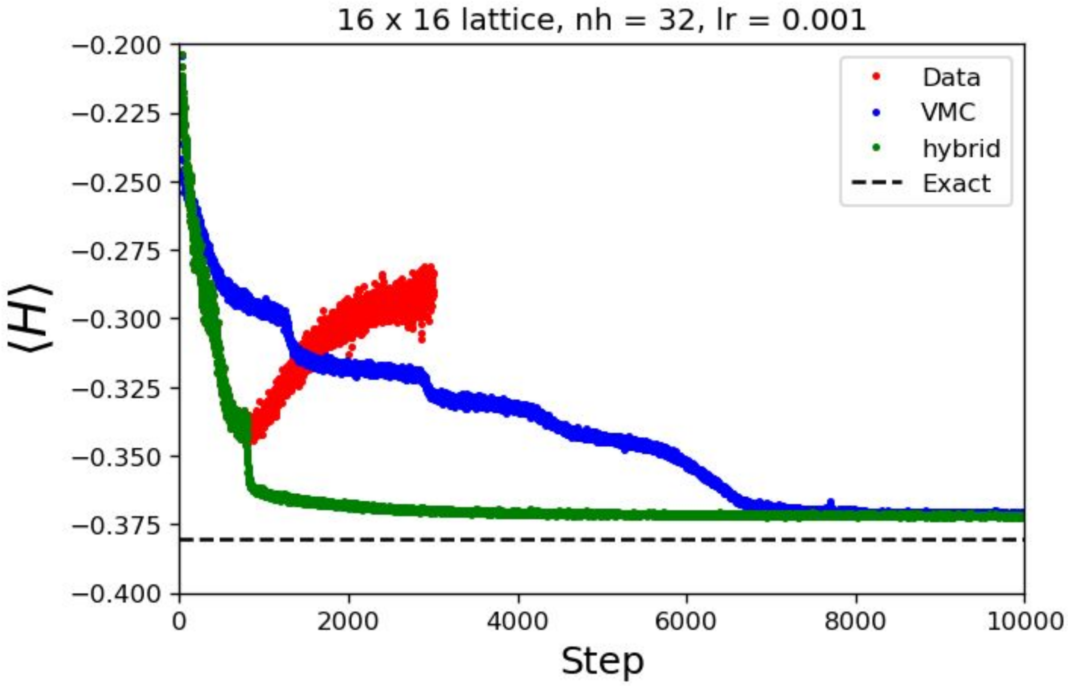
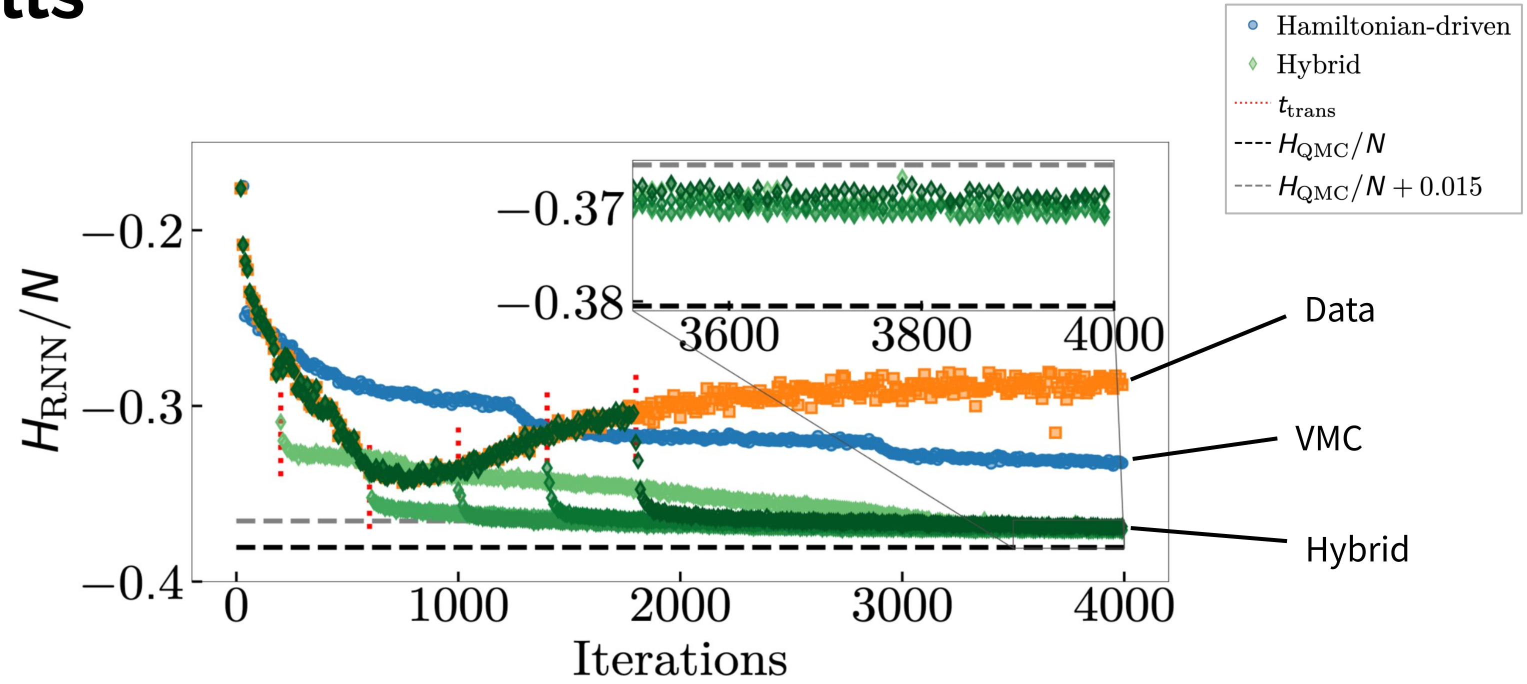
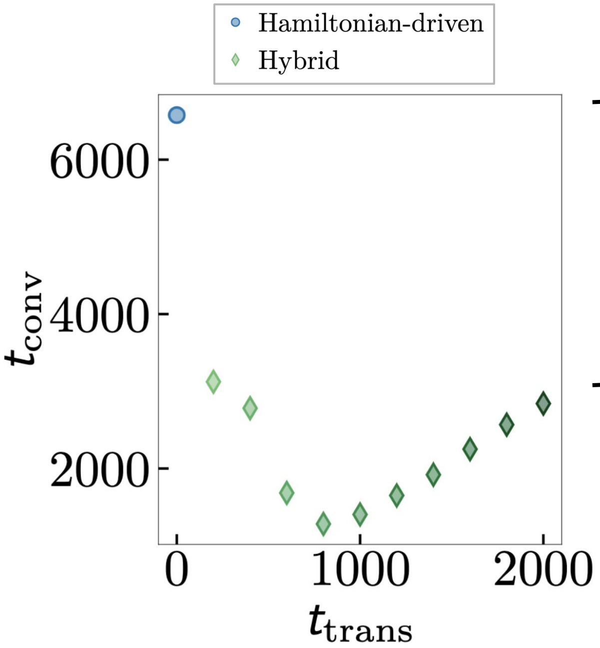


Results



Stefanie Czischek, **M. Schuyler Moss**, et al. Phys. Rev. B **105**, 205108 – Published 9 May 2022

Results



Huge improvement (even for non-optimal transition point)

Stefanie Czischek, **M. Schuyler Moss**, et al. Phys. Rev. B **105**, 205108 – Published 9 May 2022

Conclusions & Open Questions

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Bennewitz, Elizabeth R., et al. "Neural error mitigation of near-term quantum simulations." *Nature Machine Intelligence* 4.7 (2022): 618-624.

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Open Questions:

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