Towards the Optimizer that NQS Deserves

M. Drissi, J.W.T Keeble, J. Rozalén Sarmiento & A. Rios, Phil. Trans. R. Soc. A. 382 (2024)




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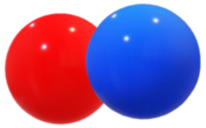
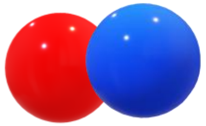
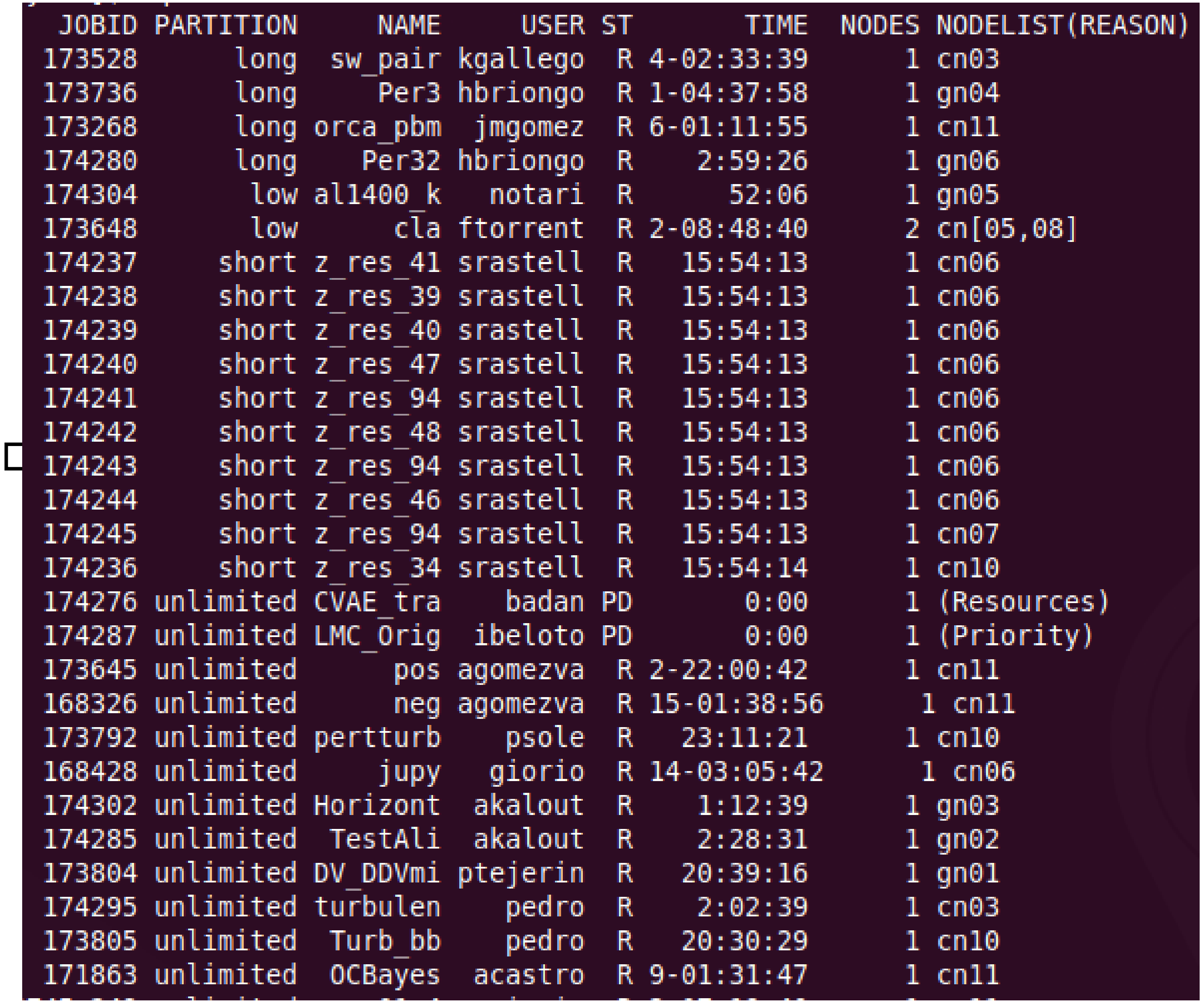
The computation problem



$$\psi_\theta(X, \sigma, \tau)$$

The computation problem





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173268      long orca_pbm  jmgomez  R 6-01:11:55      1 cn11
174280      long    Per32 hbriongo  R    2:59:26      1 gn06
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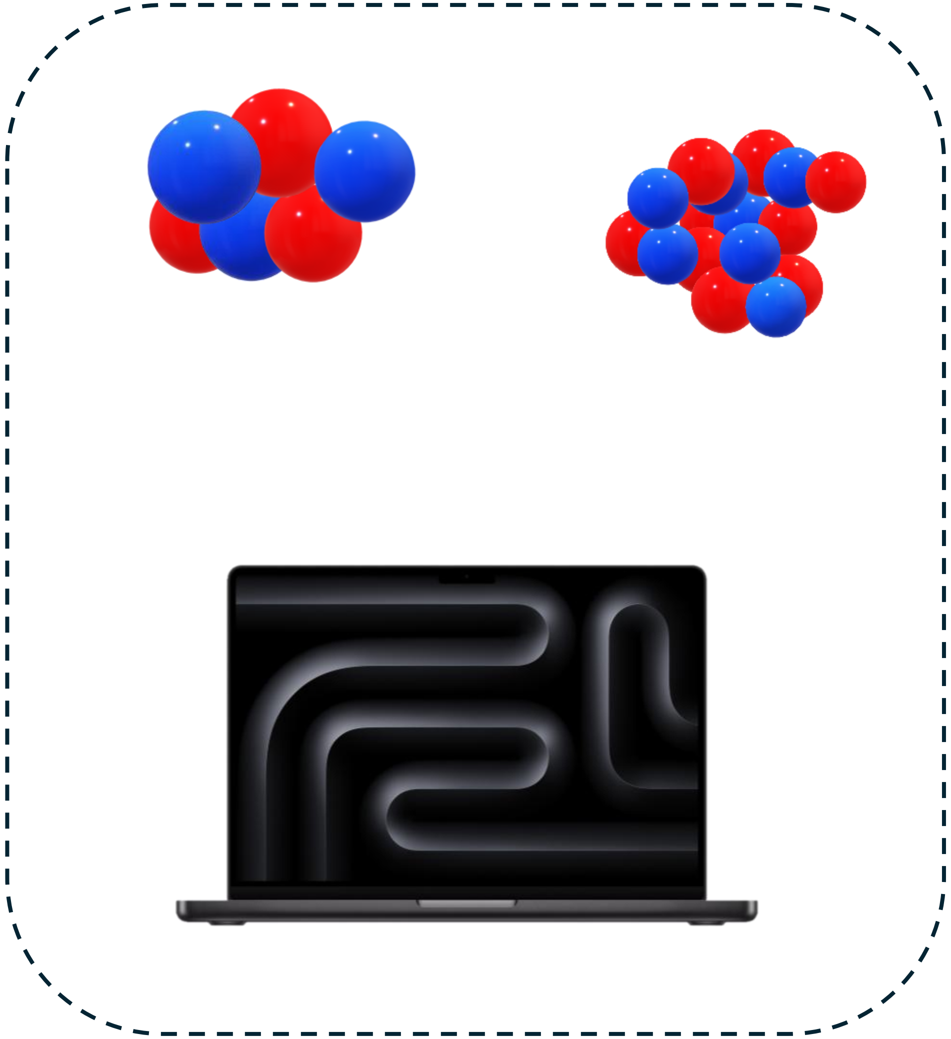
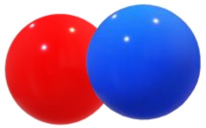
$$\psi_\theta(X, \sigma, \tau)$$

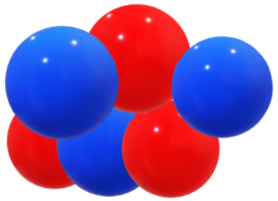
Exponential Scaling Problem

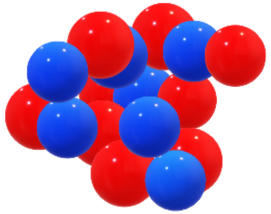
Exponential Scaling Problem

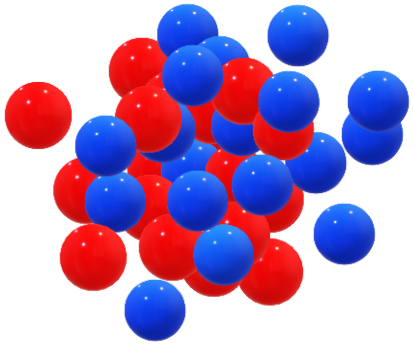


Exponential Scaling Problem



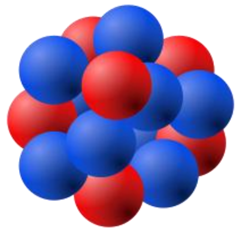






Neural Quantum States

- **Goal:** Solve for the wave function of a nucleus, ψ

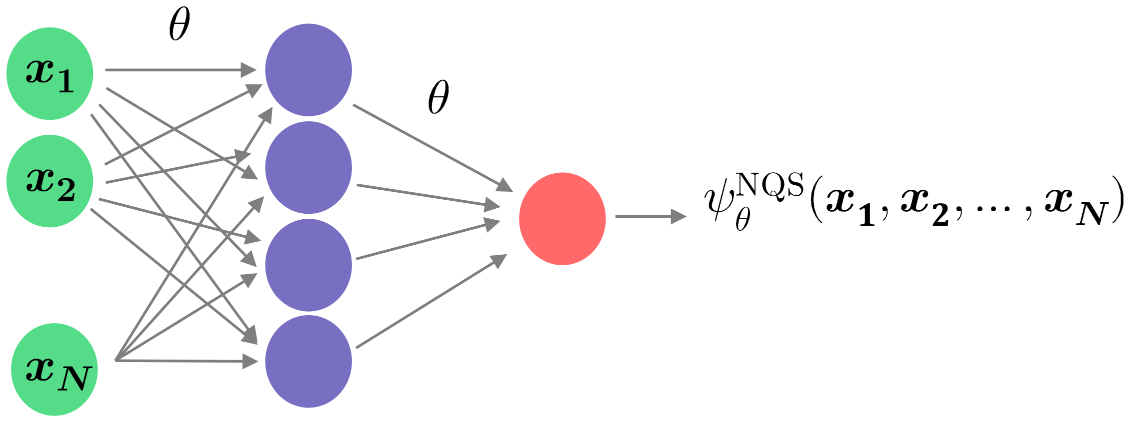


$\longrightarrow |\psi\rangle$

- **How?** Rayleigh-Ritz variational principle

$$\frac{\langle \psi_\theta | \hat{H} | \psi_\theta \rangle}{\langle \psi_\theta | \psi_\theta \rangle} \geq E_{\mathrm{GS}}$$

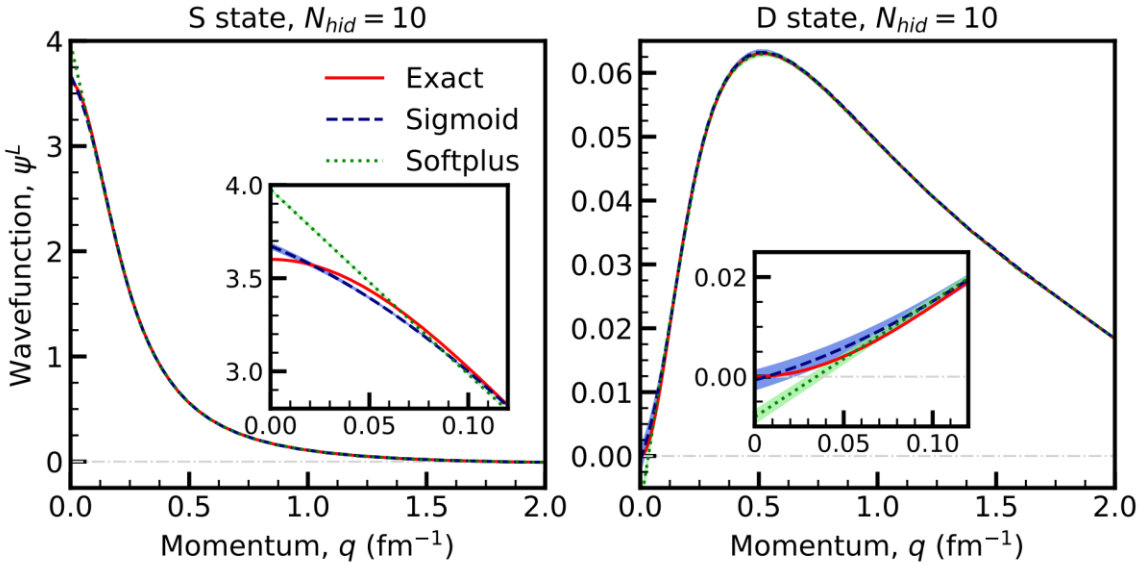
$$|\psi_\theta\rangle = \int |x\rangle \; \psi_\theta(\boldsymbol{x_1}, \boldsymbol{x_2}, \dots, \boldsymbol{x_N}) \mathrm{d}^{3\mathrm{N}} x$$

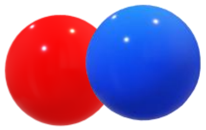


- **NQS Ansatz:** $\psi_{\mathrm{NQS}}(\boldsymbol{x_1}, \boldsymbol{x_2}, \dots, \boldsymbol{x_N}; \boldsymbol{\theta})$

NQS for Nuclei

2020

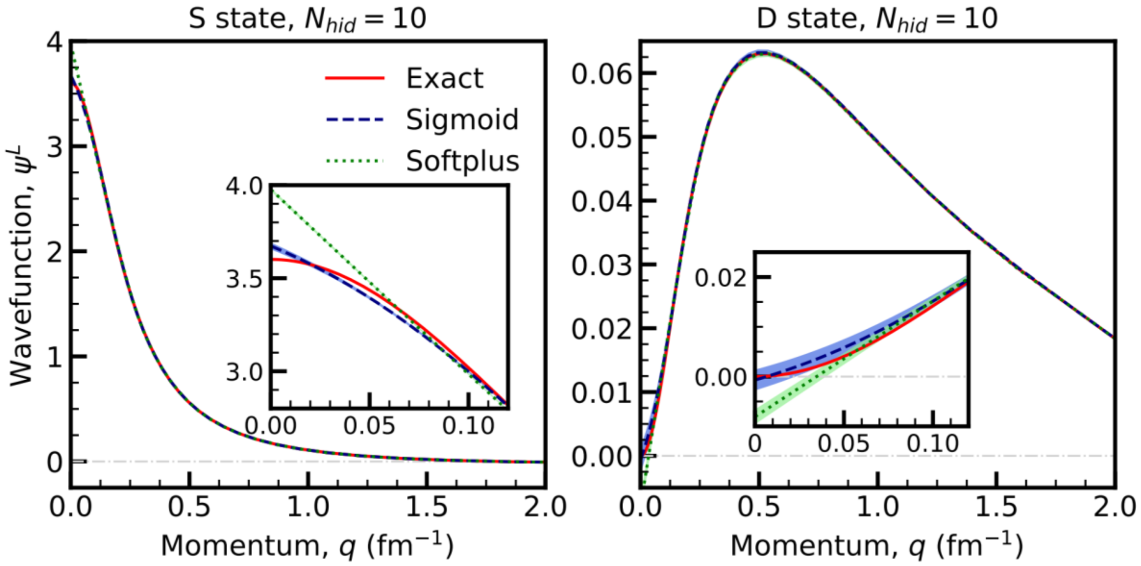


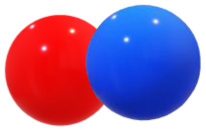


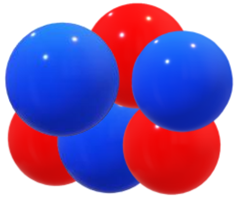
J. Keeble & A. Rios, Phys. Lett. B **809** (2020)

NQS for Nuclei

2020 → …







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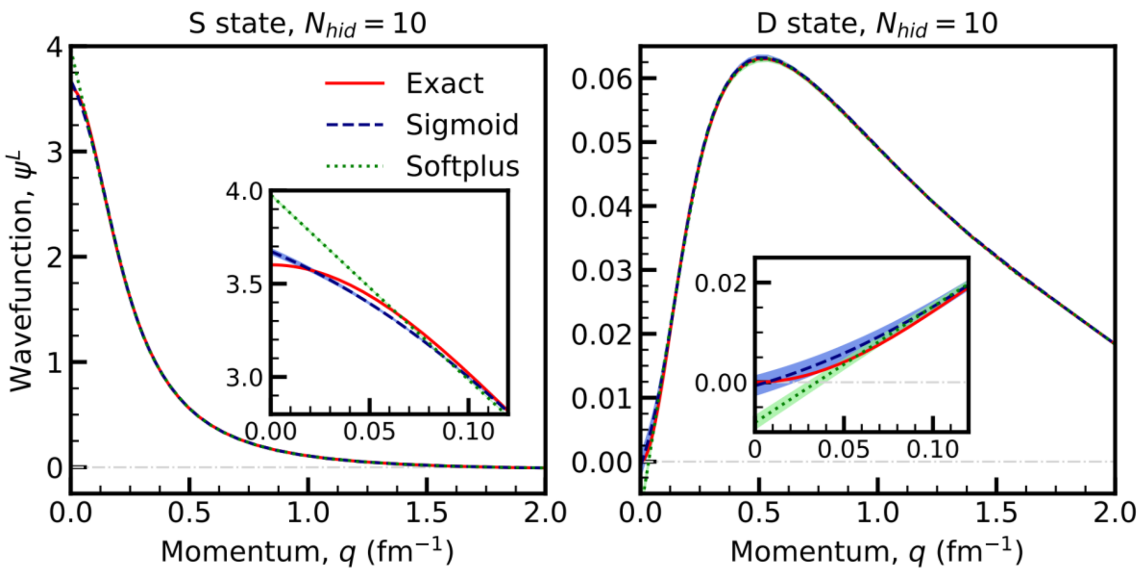
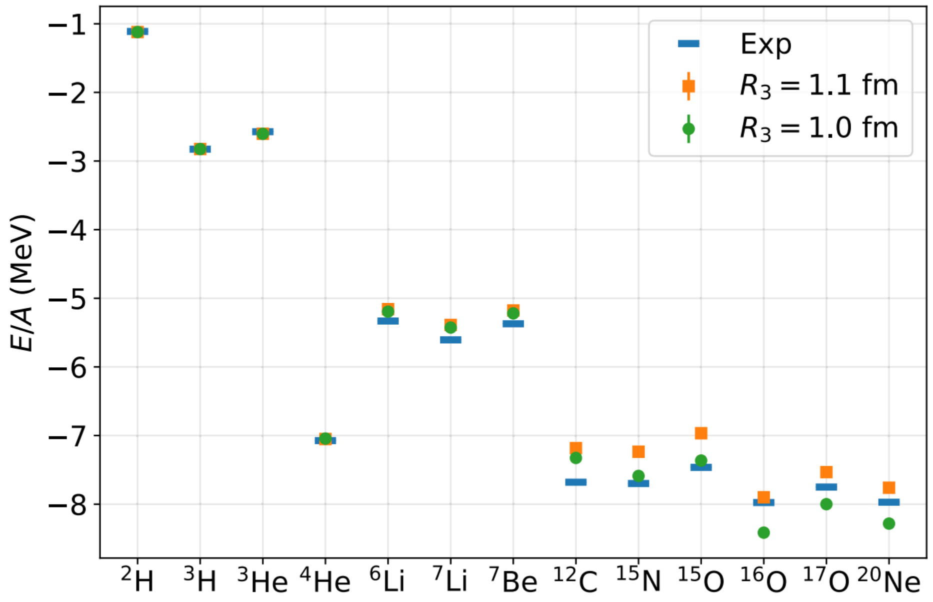
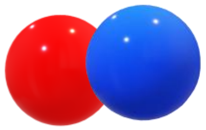
A. Gnech et al, Few-Body Syst. **63** (2022)

NQS for Nuclei

2020 → … → **2024**







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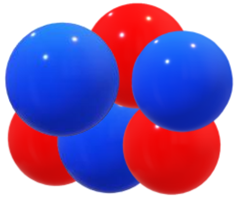

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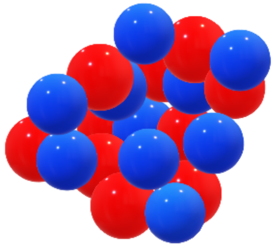

A. Gnech et al, PRL **133** (2024)

Optimisation:
A Big Challenge in NQS

The Optimisation Step

$$\theta_{n+1} = \theta_n - \alpha \nabla E(\theta_n)$$

- **Learning rate:** How big the steps are
- **Gradient:** In which direction we move

The Optimisation Step

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- **Metric tensor:** What is the geometry of the energy landscape?

The Optimisation Step

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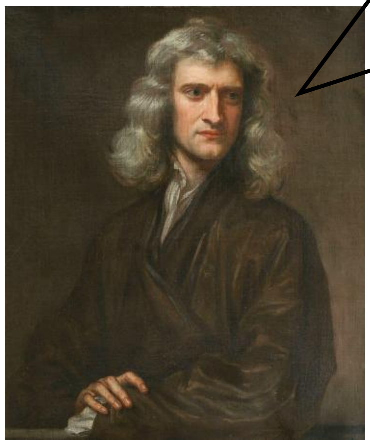
$\alpha?$ $G?$

The Metric Tensor

The Metric Tensor

$$\theta_{n+1} = \theta_n - \alpha G^{-1} \nabla E(\theta_n)$$

$$G(\theta_n) = H(\theta_n)$$



$$G(\theta_n) = \mathrm{QGT}(\theta_n)$$

Modern Literature

The Metric Tensor

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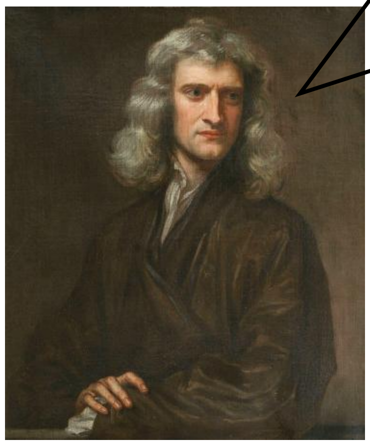

Modern
Literature

- ✓ Very precise
- ✓ $\alpha = 1$
- ✗ Costly to compute

The Metric Tensor

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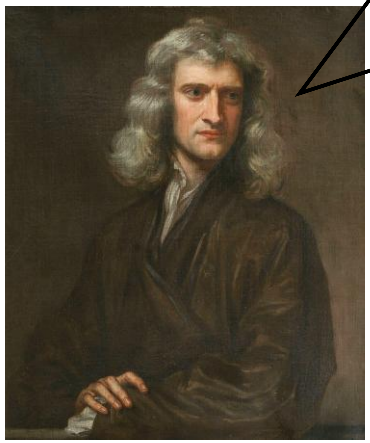

$$G(\theta_n) = \mathrm{QGT}(\theta_n)$$

Modern Literature

- ✓ Very precise
- ✓ $\alpha = 1$
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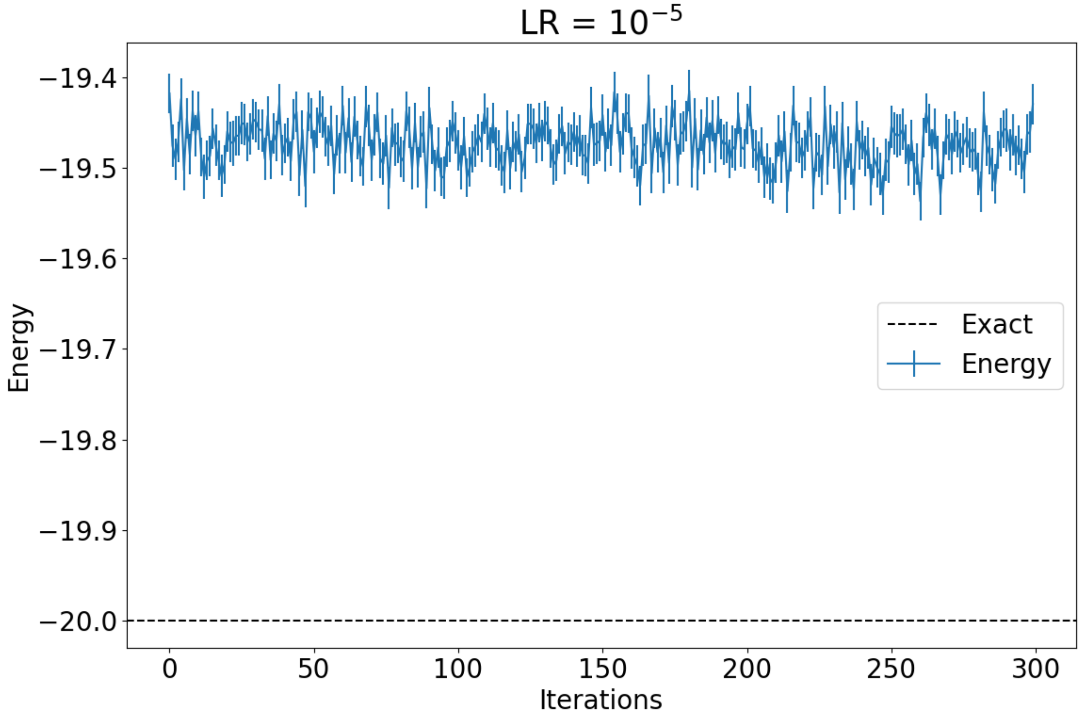
- ✓ Quite good
- ✗ $\alpha \ll 1$
- ✓ Cheap to compute

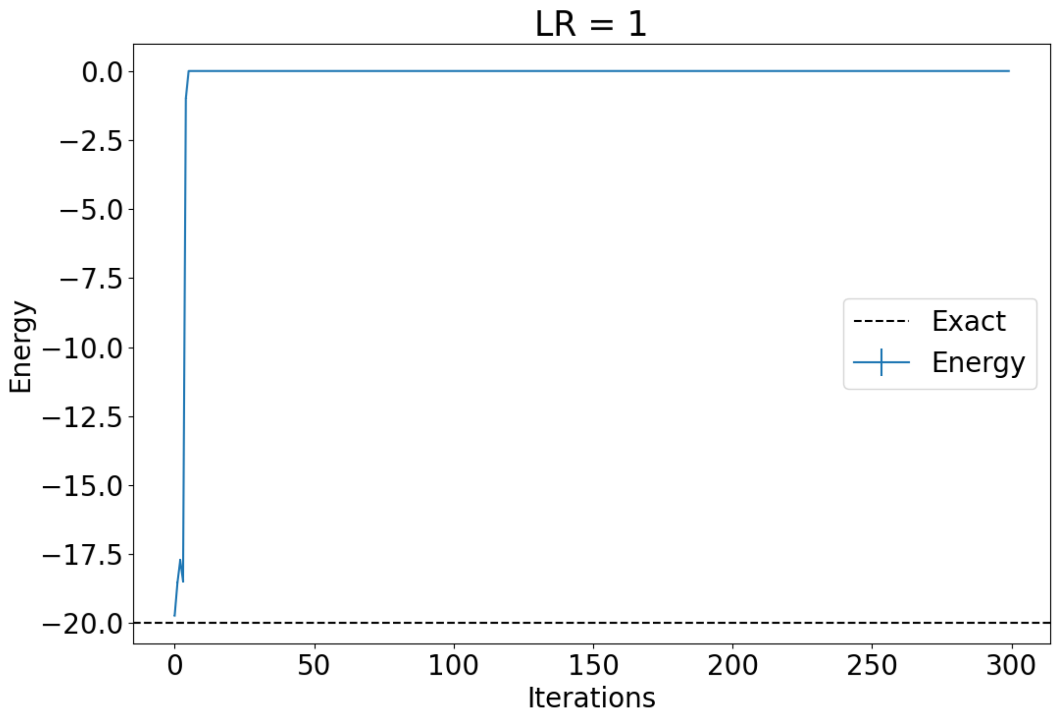
The Learning Rate

A Common Problem...

α is too small



α is too large



$$H = -\sum_{i=1}^{N} \sigma_i^{(z)} \sigma_{i+1}^{(z)} + V \sum_{j=1}^{N} \sigma_j^{(x)}$$

- N=20 particles
- QGT

Can we do better?

Decisional Gradient Descent

A new proposal

- **QGT:** based on the Hilbert distance between states, $< \phi_i | \phi_j >$

$$\mathrm{QGT}(\theta)_{\theta_i\theta_j} = \mathbb{E}_{X\sim p_\theta}\left[\left(\partial_{\theta_\mathrm{i}} \ln \psi_\theta\left(\mathrm{X}\right) - \mathbb{E}_{X\sim p_\theta}[\partial_{\theta_\mathrm{i}} \ln \psi_\theta\left(\mathrm{X}\right)]\right)^* \left(\partial_{\theta_\mathrm{j}} \ln \psi_\theta\left(\mathrm{X}\right) - \mathbb{E}_{X\sim p_\theta}\left[\partial_{\theta_\mathrm{j}} \ln \psi_\theta\left(\mathrm{X}\right)\right]\right)\right]$$

- **DGD:** based on the Hamiltonian distance between states, $< \phi_i | H | \phi_j >$

$$G_{\mathrm{VMC}}(\theta)_{\theta_i\theta_j} \equiv \frac{1}{4}\sum_{k=1}^{A} \mathbb{E}_{X\sim p_\theta}\left[\partial_{\theta_i}\partial_{x_k} \ln p_\theta(X)\ \partial_{\theta_j}\partial_{x_k} \ln p_\theta(X)\right]$$

A new proposal

- **QGT:** based on the Hilbert distance between states, $< \phi_i | \phi_j >$

$$\mathrm{QGT}(\theta)_{\theta_i\theta_j} = \mathbb{E}_{X\sim p_\theta}\left[\left(\partial_{\theta_\mathrm{i}} \ln\psi_\theta\left(\mathrm{X}\right) - \mathbb{E}_{X\sim p_\theta}\left[\partial_{\theta_\mathrm{i}} \ln\psi_\theta\left(\mathrm{X}\right)\right]\right)^*\left(\partial_{\theta_\mathrm{j}} \ln\psi_\theta\left(\mathrm{X}\right) - \mathbb{E}_{X\sim p_\theta}\left[\partial_{\theta_\mathrm{j}} \ln\psi_\theta\left(\mathrm{X}\right)\right]\right)\right]$$

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$\hookrightarrow$ Similar to the Hessian $\longrightarrow$ $\alpha \simeq 1$

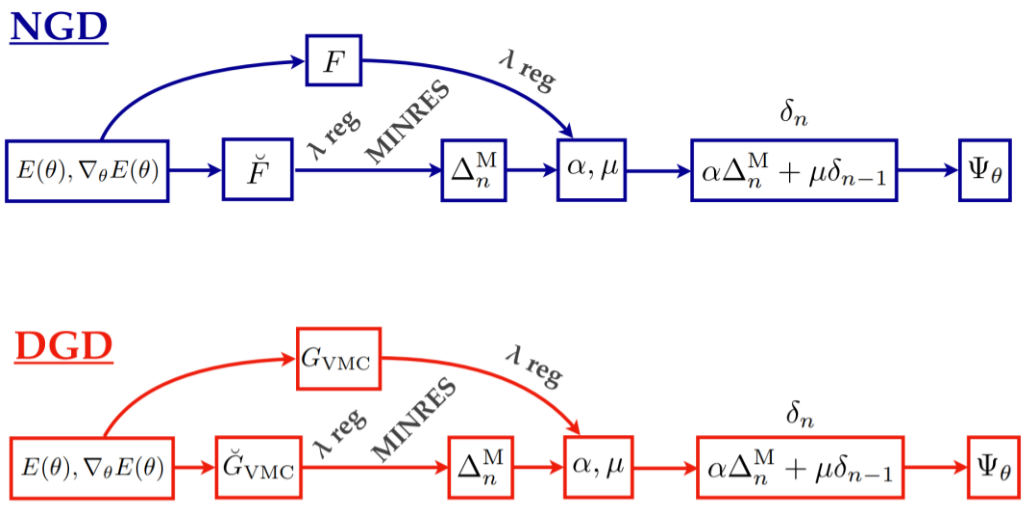
Results: Fermions on the continuum

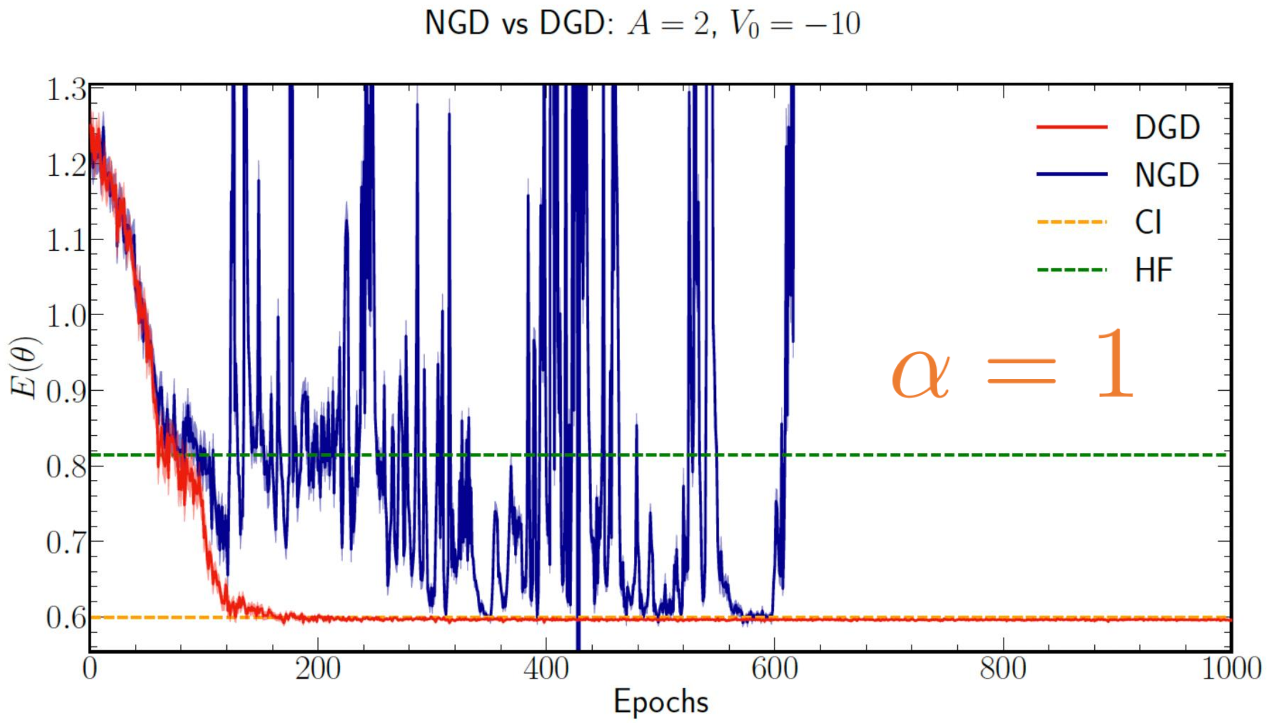
DGD vs. QGT

- **System:** chain of **1D spinless fermions**

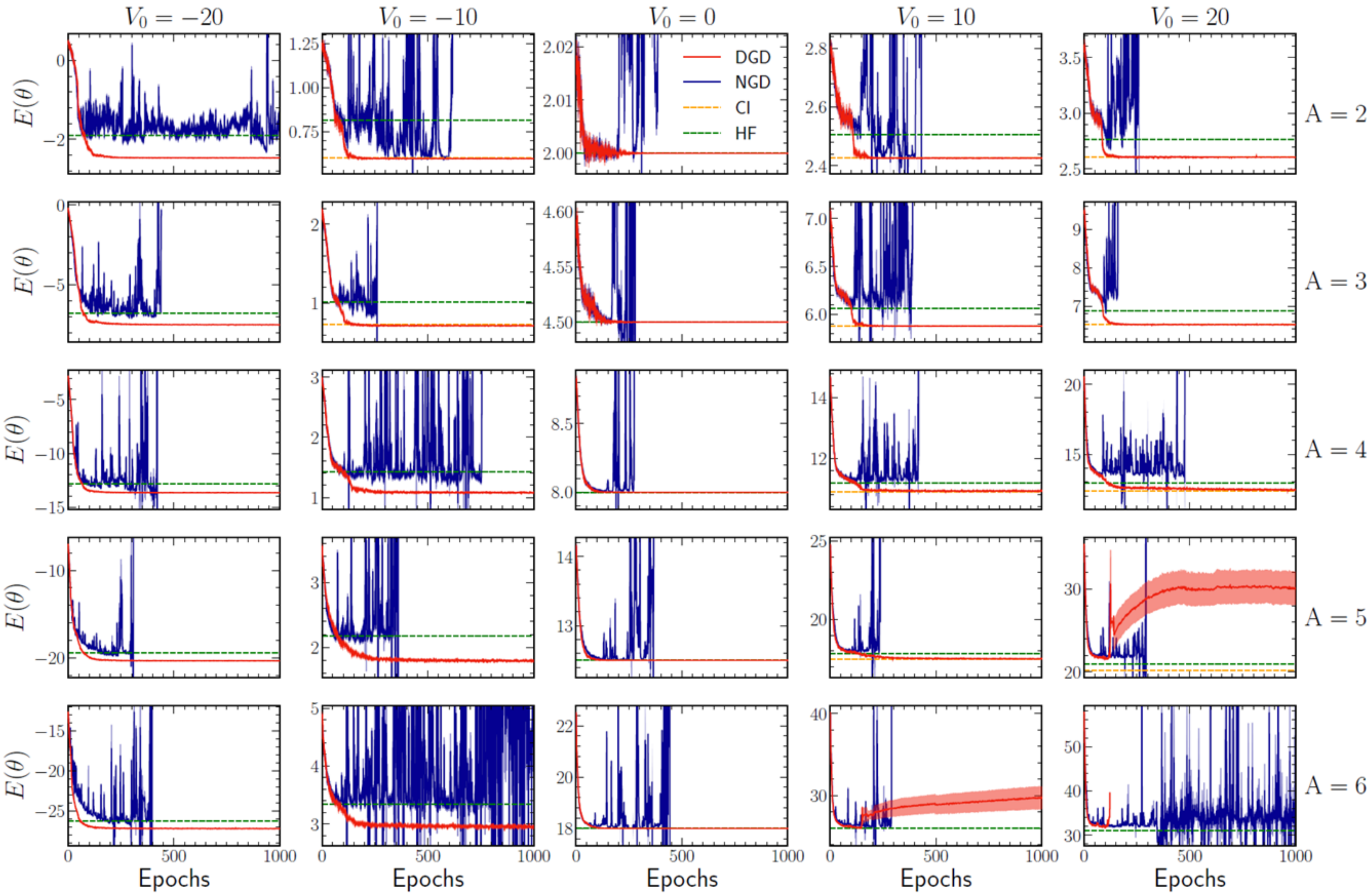
$$H = -\frac{1}{2}\sum_{i=1}^{A}\nabla_i^2 + \frac{1}{2}\sum_{i=1}^{A}x_i^2 + \frac{V_0}{\sqrt{2\pi}\sigma_0}\sum_{i<j} e^{-\frac{(x_i-x_j)^2}{2\sigma_0^2}}$$

- **Comparison:** **Natural Gradient Descent** vs. **Decisional Gradient Descent**





DGD vs. QGT



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Results: Fermions on a lattice

DGD for lattice systems

- **Transverse-Field Ising Model:**

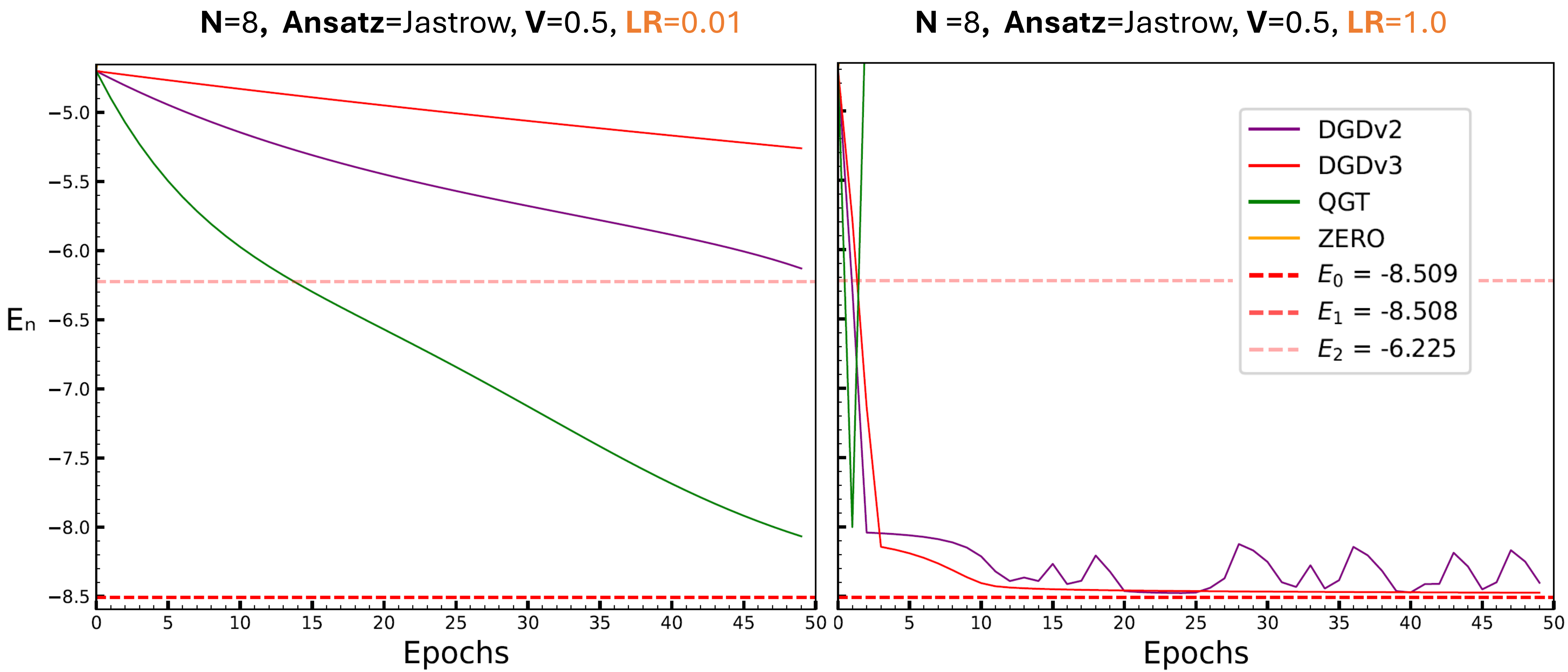
$$G(\theta_n)_{kl} = 4\mathrm{e}^{\beta(c^{\mathrm{MFA}}-\mu)} \prod_{i=1}^{N} \cosh \frac{\beta \mathrm{d}_{\mathrm{i}}^{\mathrm{MFA}}}{2} \times \mathrm{QGT}(\theta_n)_{kl}$$
$$+ \sum_{j=1}^{N} \tanh \frac{-\beta d_j^{MFA}}{2} \times E_{\sigma\sim|\psi_\theta|^2} \left\{ \mathrm{sgn}(\sigma_j) \left| \frac{T_j[\psi_\theta](\sigma)}{\psi_\theta(\sigma)} \right| \left(\partial_k \ln T_j\,[\psi_\theta](\sigma) \right)^* \left(\partial_{\mathrm{l}} \ln T_j\,[\psi_\theta](\sigma) \right) \right\}$$

- **J_1-J_2 Heisenberg:**

$$G(\theta_n)_{kl} = \left(\frac{1}{\beta} - \mu + \mathrm{J}_1 \mathrm{N}_{<\mathrm{i,j}>} + \mathrm{J}_2 \mathrm{N}_{<<\mathrm{i,j}>>} \right) \times 2\mathrm{Re}(\mathrm{QGT}(\theta_n)_{kl}) \; + 2Re \left\{ \mathrm{J}_1 \sum_{<i,j>} \underset{\sigma\sim|\psi_\theta|^2}{E} \left[(\mathrm{sgn}(\sigma_i)\mathrm{sgn}(\sigma_j) \right] \right\}$$
$$\times \left(\partial_k \ln \psi_\theta\,(\sigma) - \frac{\psi_\theta\left(f_{ij}(\sigma)\right)}{\psi_\theta(\sigma)} \partial_k \ln \psi \left(f_{ij}(\sigma) \right) - \left(1 - \frac{\psi_\theta\left(f_{ij}(\sigma)\right)}{\psi_\theta(\sigma)} \right) \times E_{\sigma\sim|\psi_\theta|^2}[\partial_k \ln \psi_\theta\,(\sigma)] \right)$$
$$\times \left(\partial_{\mathrm{l}} \ln \psi_\theta\,(\sigma) - \frac{\psi_\theta\left(f_{ij}(\sigma)\right)}{\psi_\theta(\sigma)} \partial_l \ln \psi \left(f_{ij}(\sigma) \right) - \left(1 - \frac{\psi_\theta\left(f_{ij}(\sigma)\right)}{\psi_\theta(\sigma)} \right) \times E_{\sigma\sim|\psi_\theta|^2}[\partial_l \ln \psi_\theta\,(\sigma)] \right)$$

DGD vs. QGT: Ising

$$H = -\sum_{i=1}^{N} \sigma_i^{(z)} \sigma_{i+1}^{(z)} + V \sum_{j=1}^{N} \sigma_j^{(x)}$$

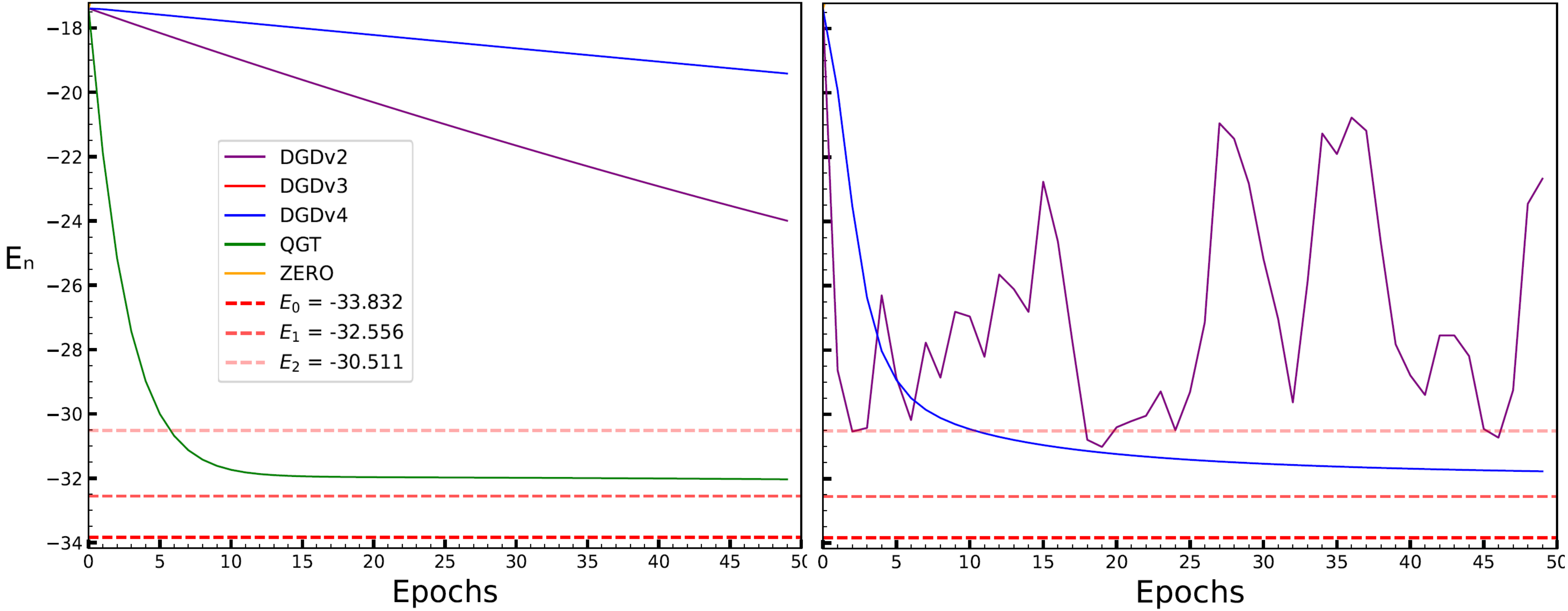


DGD vs. QGT: J_1-J_2

$$H = J_1 \sum_{<i,j>} \vec{S_i} \cdot \vec{S_j} + J_2 \sum_{\ll i,j \gg} \vec{S_i} \cdot \vec{S_j}$$

N=16 (4x4), **Ansatz**=Jastrow, $\mathbf{J_2}$=0.5, **LR**=0.01

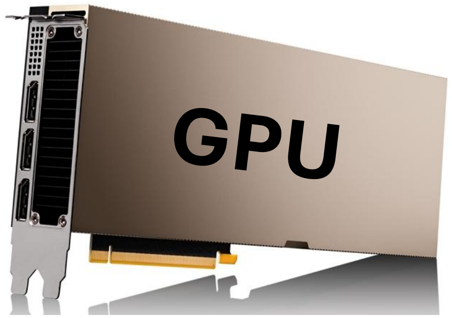
N=16 (4x4), **Ansatz**=Jastrow, $\mathbf{J_2}$=0.5, **LR**=1.0

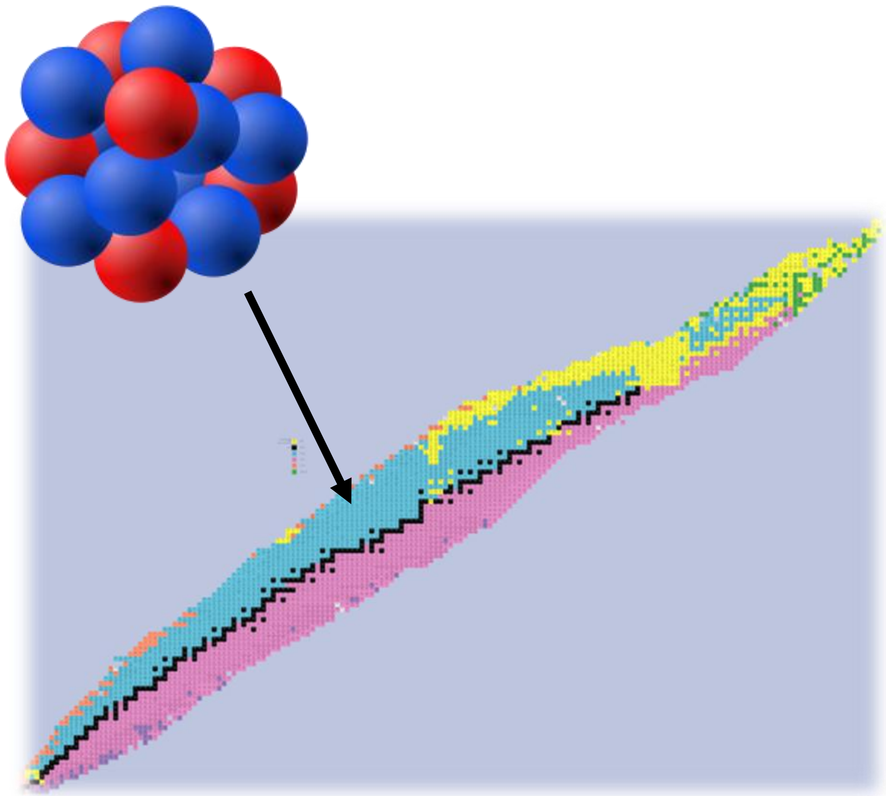


Final Thoughts

Takeaway

$$G(\theta_n) +$$





Thank you

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