Neural quantum states for hypernuclear systems with contact theories.

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- **Equation of State** (EoS) → barion stars' internal structure (BS) → prediction of the maximum stellar mass.
- **Hyperons in the core** of the most massive BSs lead to the **hyperon puzzle** → softer EoS (reduce Pauli blocking), reducing the maximum stellar mass.
- Observational data of the most recent compact object's masses have provided stringent constraints on the EoS that are in contrast with its softening.
- The main ingredient that determines the stiffness/softness of the EOS after the introduction of hyperons in the core is the **microscopic interaction** between these particles and the nuclear matter.

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  - → Hypernuclei considered in this work are bound state between an ordinary nucleus with only one hyperon (Λ^0)

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- **Objectives**
  - → **Parametrize for the wavefunction (variational state) in terms of Neural Networks**,
  - → **Fit an Improved LO interaction** potential derived from $\not{\pi}EFT$.
  - → **Compare NNQS results** with exact few-body techniques over fitted observables.
  - → **Predict Λ-separation energies** for high A systems ($^{7}_{\Lambda}$Li, $^{13}_{\Lambda}$C, $^{16}_{\Lambda}$O and ~~$^{40}_{\Lambda}$Ca~~).

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- Through NNQS, we have obtained **promising results** with hypernuclear states.

Microscopic Interaction: $\not\pi$EFT Contact potentials

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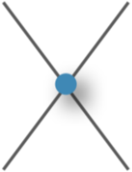
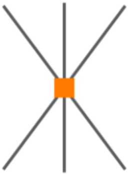
- Unresolved pions leads to a spin-dependent contact potential, which is described by a set of Low Energy Constants (LECs):

Regulator's cutoffs and LECs are both fitted → **SVM (Suzuki - Varga) and Gaussian Processes**.

- NN potential: Fitted to np/nn scattering lengths and effective ranges.
- 3NF are adjusted to reproduce the ^3H and ^4He BEs.



$$V_{NN}(\mathbf{x}_{ij}) = \left(C_0(\lambda)^s P^{2b}_{S_{tot}=0} + C_0(\lambda)^t P^{2b}_{S_{tot}=1}\right)\delta_\lambda(\mathbf{x}_{ij})$$



$$V_{NNN}(\mathbf{x}_{ij}) = \mathcal{D}_0(\lambda) \sum_{i<j<k} \sum_{cyc} \delta_\lambda(\mathbf{x}_{ik})\delta_\lambda(\mathbf{x}_{ij})$$

Extending $\not{\pi}$EFT to Hyperons

- Extending $\not{\pi}$EFT to Hyperons require the introduction of Λ-hyperons ($m_\Lambda = 1116 MeV$) DoF in the Lagrangian density, $\mathcal{L}$

$$\mathcal{L} = N^\dagger\Big(i\partial_0 + \frac{\nabla^2}{2M_N}\Big)N + \Lambda^\dagger\Big(i\partial_0 + \frac{\nabla^2}{2M_\Lambda}\Big)\Lambda + \mathcal{L}_{2b} + \mathcal{L}_{3b} + \dots$$

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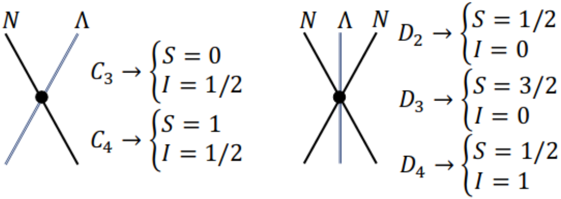
- The interaction potential becomes at LO:

$$V_{\Lambda N} = \sum_{IS} C_\lambda^{IS} \sum_{i<j} \mathcal{P}_{IS}(ij)\delta_\lambda(\vec{r}_{ij})$$

$$V_{\Lambda NN} = \sum_{IS} D_\lambda^{IS} \sum_{i<j} \mathcal{Q}_{IS}(ij\Lambda)\delta_\lambda(\vec{r}_{i\Lambda})\delta_\lambda(\vec{r}_{j\Lambda})$$

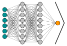


- $\mathcal{P}_{IS}$ ($\mathcal{Q}_{IS}$) are projectors on baryon doublets (triplets) with isospin I and spin S

1. ΛN interaction is fitted to $p\Lambda$ scattering length and effective range.
2. ΛNN interaction is fitted to ${}^3_\Lambda H$, ${}^4_\Lambda H_{S_{tot}=0}$, ${}^4_\Lambda H_{S_{tot}=1}$, and ${}^5_\Lambda He$ binding energies.

The NNQS approach

- The Neural Network Quantum States (Carleo et al. 2017) approach is a form of unsupervised learning.
  - **Any type of Variational State** can be represented via the NNQS.

Universal Approximation Theorem $\rightarrow \Psi_{\mathcal{W}}(\mathbf{R},\mathbf{S}) = \langle \mathrm{R},\mathrm{S} |$  $\rangle$

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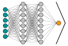
Universal Approximation Theorem $\rightarrow \Psi_{\mathcal{W}}(\mathbf{R}, \mathbf{S}) = \langle \mathrm{R}, \mathrm{S} |$  $\rangle$

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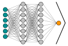
Universal Approximation Theorem → $\Psi_{\mathcal{W}}(\mathbf{R},\mathbf{S}) = \left\langle \mathrm{R},\mathrm{S} \right|$  $\left.\right\rangle$

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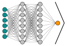

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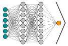

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- Disadvantages:
  1. EFT contact potentials $\propto \delta_{\lambda}(\mathbf{x}_{ij})$ introduces **irreducible error at large cut-offs** in Monte Carlo integration due to small statistics in the interaction range →Is better to keep the cutoff small!!.

Description of the NNQS

NNQS is a Variational Approach:

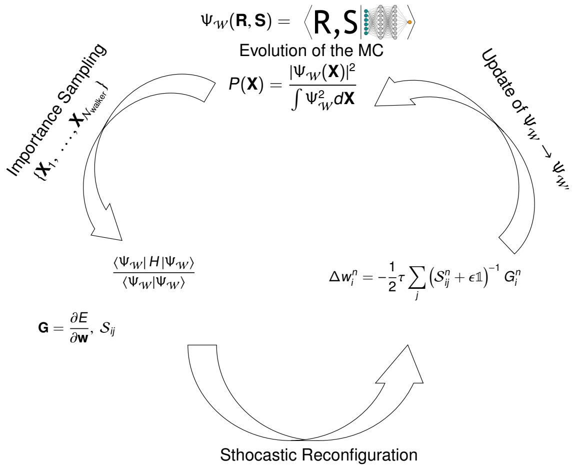
1. Apply the V.P.

$$E_V = \frac{\langle \Psi_{\mathcal{W}} | H | \Psi_{\mathcal{W}} \rangle}{\langle \Psi_{\mathcal{W}} | \Psi_{\mathcal{W}} \rangle} \geq E_0$$

2. Iterative optimization till

$$\frac{\delta E_V(\{\mathcal{W}\})}{\delta \{\mathcal{W}\}} = 0$$

- The determination of $E_V \sim E_0$ and Ψ_0:
  1. Sampling the Wavefunction using $\mathcal{N}$ Markov Chains in parallel.
  2. Evaluating observables and gradients' expectation values with Importance Sampling.
  3. Updating parameters using Stochastic Reconfiguration.



NNQS - Hidden Nucleon Wavefunction

Step 0: modellization of the wavefunction with Hidden Nucleon approach:

Fermionic wave functions from neural-network constrained hidden states - Carleo, Moreno, Georges, Stokes PNAS Vol. 119 | No. 32 (2022)

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→ **We introduce A_h "Hidden" DoFs → not real partices**:

- Represented by the **hidden orbitals** χ_i
- Each virtual particle coordinate $\tilde{x}_j = f(\{X\})$ **is a bosonic function** of all the real particles coordinates

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$$\det \begin{vmatrix} \phi_v(\mathbf{X}) & \phi_v(f(\{\mathbf{X}\})) \\ \chi_h(\mathbf{X}) & \chi_h(f(\{\mathbf{X}\})) \end{vmatrix} = \det \begin{bmatrix} \phi_1(x_1) & \phi_1(x_2) & \phi_1(f(\{X\})) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(f(\{X\})) \\ \chi_3(x_1) & \chi_3(x_2) & \chi_3(f(\{X\})) \end{bmatrix}$$

Visible orbitals on visible coordinates | Visible orbitals on hidden coordinates

Hidden orbitals on visible coordinates | Hidden orbitals on hidden coordinates

What about statistical correlations?

NNQS - Hidden Nucleon Wavefunction

$$\phi_1(f(x)) \cdot \left(\phi_2(x_1)\chi_3(x_2) - \chi_3(x_1)\phi_2(x_2)\right)$$
$$- \phi_2(f(x)) \cdot \left(\phi_1(x_1)\chi_3(x_2) - \chi_3(x_1)\phi_1(x_2)\right)$$
$$+ \chi_3(f(x)) \cdot \left(\phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)\right)$$

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$$
\begin{aligned}
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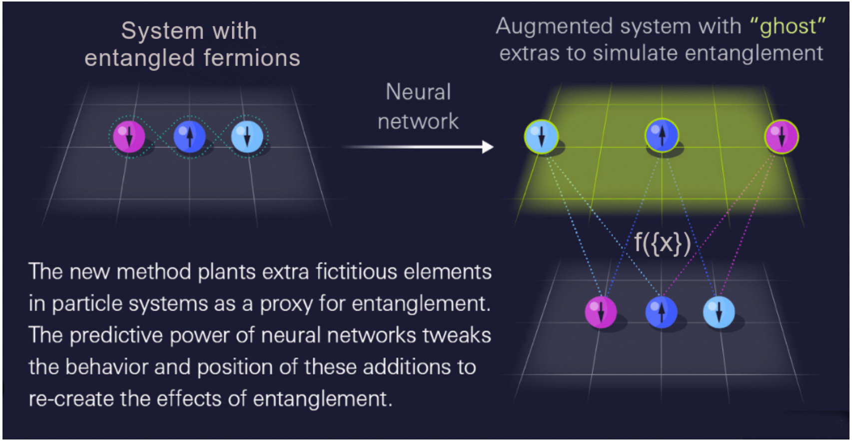
\end{aligned}
$$

it is an equivalent form of the C.I. expansion with only one excited states. (but it's more than this!)

$$
|\Phi\rangle = C_0|\Psi_0\rangle + \sum_{ra} C_a^r |\Psi_a^r\rangle + \sum_{\substack{a<b \\ r<s}} C_{ab}^{rs} |\Psi_{ab}^{rs}\rangle + \sum_{\substack{a<b<c \\ r<s<t}} C_{abc}^{rst} |\Psi_{abc}^{rst}\rangle + \dots \tag{1}
$$

NNQS - Hidden Nucleon Wavefunction

- Introduce dynamical correlations between particles by means of functions of bosonic nature $f(\{\mathbf{x}\})$ which accounts for Jastrow correlators for all the particles in the system:



HN wavefunction in the Visible coordinate sector

- The hidden coordinate sector is represented through a phase - amplitude modulation of the wave function

$$\det\left[\begin{array}{cc|c} \phi_1(x_1) & \phi_1(x_2) & \phi_1(f(\{X\})) \\ \phi_2(x_1) & \phi_2(x_2) & \phi_2(f(\{X\})) \\ \hline \chi_3(x_1) & \chi_3(x_2) & \chi_3(f(\{X\})) \end{array}\right]$$

$$\phi_\alpha(x_i) = e^{u^\alpha_\phi(x_i)} \tanh[v^\alpha_\phi(x_i)] \sim e^{u^\alpha_\phi(x_i) + j \cdot v^\alpha_\phi(x_i)}$$

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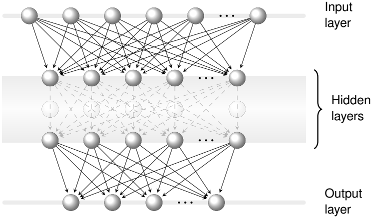
- u and v are both FF Neural Networks with only one hidden layer (Let's call this a "standard network" for this work.).



A standard Single Particle FFNN has

- Input Nodes = 5 $\rightarrow [\mathbb{R}^3, s_z, t_z]$
- Output Nodes = 1 $\rightarrow \phi(x_i)$

NNQS Hidden coordinate sector - Deep Sets Architecture

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- **Deep Sets architecture:** any permutation invariant neural network ($\mathcal{U}$ and $\mathcal{V}$) can be sum-decomposed in the following way:

$$\mathcal{F}(\{\mathbf{X}\}) = \rho_{\mathcal{F}}\Big[\sum_{i\neq j}\phi_{\mathcal{F}}([\mathbf{x}_i,\mathbf{x}_j])\Big] \qquad \mathcal{F} = \mathcal{U},\mathcal{V}$$

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- ϕ and ρ are both Neural Network, the sum operation destroy the order dependence of the network's inputs.
- This decomposition is called **Sum-Pooling**, since the aggregation function is $g(\cdot) = \sum_{x\in\mathfrak{X}}$.

Application of NNQS to hypernuclear variational states

- Variational state of a hypernucleus (only one Λ):

$$\Psi_{HN} = \phi_\Lambda(\mathbf{x}_\Lambda, g(\{\mathbf{x}_1, \ldots, \mathbf{x}_{A-1}, \mathbf{x}_\Lambda\})) \cdot \det_{A-1_Z} \begin{vmatrix} \phi_v(\mathbf{X}) & \phi_v(f(\{\mathbf{X}\})) \\ \chi_h(\mathbf{X}) & \chi_h(f(\{\mathbf{X}\})) \end{vmatrix}$$

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- In order to represent ΛN correlations related with the ${}^3_\Lambda H$ mixed asymmetry spin state, the aggregator function for non-identical particles has to be modified

$$g(\mathcal{S}[\mathbf{x}_1, \dots, \mathbf{x}_{A-1}], \mathbf{x}_\Lambda) = \left[\mathbf{x}_\Lambda, \sum_{i=1}^{A-1} \phi(\mathbf{r}_i, \mathbf{s}_i)\right]$$

The coordinate of the Lambda are concatenated with the sum pooling → the ΛN permutation invariance is not introduced

Application of NNQS to hypernuclear variational states

- Variational state of a hypernucleus (only one Λ):

$$\Psi_{HN} = \phi_\Lambda(\mathbf{x}_\Lambda, g(\{\mathbf{x}_1, \dots, \mathbf{x}_{A-1}, \mathbf{x}_\Lambda\})) \cdot \det_{A-1Z} \begin{vmatrix} \phi_v(\mathbf{X}) & \phi_v(f(\{\mathbf{X}\})) \\ \chi_h(\mathbf{X}) & \chi_h(f(\{\mathbf{X}\})) \end{vmatrix}$$

- In order to represent ΛN correlations related with the ${}^3_\Lambda H$ mixed asymmetry spin state, the aggregator function for non-identical particles has to be modified

$$g(\mathcal{S}[\mathbf{x}_1, \dots, \mathbf{x}_{A-1}], \mathbf{x}_\Lambda) = \left[\mathbf{x}_\Lambda, \sum_{i=1}^{A-1} \phi(\mathbf{r}_i, \mathbf{s}_i)\right]$$

The coordinate of the Lambda are concatenated with the sum pooling → the ΛN permutation invariance is not introduced

- ϕ_Λ has already mentioned phase-amplitude modulation

$$\phi_\Lambda\Big(g(\mathcal{S}(\{\mathbf{x}_i\}), \mathbf{x}_\Lambda)\Big) = \tanh\left[\rho_p\Big(g(\mathcal{S}(\{\mathbf{x}_i\}), \mathbf{x}_\Lambda)\Big)\right] \cdot \exp\left[\rho_a\Big(g(\mathcal{S}(\{\mathbf{x}_i\}), \mathbf{x}_\Lambda)\Big)\right]$$

Pre-processing (backflow) of coordinates via MPNN

What if we want to use one only one hidden state state?

- We can introduce the following backflow transformation for the single particle's coordinates:

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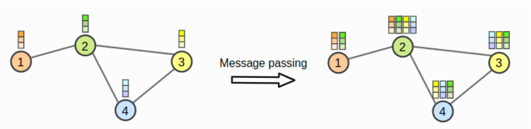


In the NN language it consist in the application of a minimal MPNN:
an all-toall connected graph, encoding effective particle positions (x_i-nodes) and their interactions (m_{ij}-edges)

Backflow Λ-coordinate

$$m_{Lj} = \phi([x_{\text{lam}}, x_j])$$
$$m_L = \frac{1}{N_{\text{part}}} \sum_{j=1}^{N_{\text{part}}} m_{Lj}$$
$$\mathbf{X}_L = [x_{lam}, m_L]$$

Backflow Ns coordinates

$$m_{ij} = \chi([x_i, x_j])$$
$$m_i = \frac{1}{N_{\text{part}}} \sum_{j=1}^{N_{\text{part}}} m_{ij}$$
$$\mathbf{X}_i = [x_i, m_i]$$

→ MPNN NQS for the Homogeneous Electron Gas - Lovato, Carleo, Kim, Pescia, Nys (2023) arXiv:2305.07240v3

Hidden Nucleon generalization for $n - \Lambda$-hypernuclear states

Is possible to include more than one Λs?

Hidden Nucleon generalization for $n - \Lambda$-hypernuclear states

Is possible to include more than one Λs?
Putting all the previous ideas together...

$$\Psi_{HN} = \det_{\Lambda} \begin{vmatrix} \phi_{\text{v}}(x_{lam}) & \phi_{\text{v}}(f(\{\mathbf{X}_L\})) \\ \chi_{\text{h}}(x_{lam}) & \chi_{\text{h}}(f(\{\mathbf{X}_L\})) \end{vmatrix} \cdot \det_{^{A-1}Z} \begin{vmatrix} \phi_{\text{v}}(\mathbf{X}_i) & \phi_{\text{v}}(f(\{\mathbf{X}_i\})) \\ \chi_{\text{h}}(\mathbf{X}_i) & \chi_{\text{h}}(f(\{\mathbf{X}_i\})) \end{vmatrix}$$

Observables evaluation

Step 1: Importance Sampling and Metropolis

- Expectation values are computed through **importance sampling**. By rewriting the multidimensional integral for a generic observable $\mathcal{O}$:

$$\mathcal{O}_V = \frac{\langle\Psi|\mathcal{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\int d\mathbf{R}\,\langle\Psi|\mathbf{R},\mathbf{S}\rangle\langle\mathbf{R},\mathbf{S}|\mathcal{O}|\Psi\rangle\frac{\langle\mathbf{R},\mathbf{S}|\Psi\rangle}{\langle\mathbf{R},\mathbf{S}|\Psi\rangle}}{\int d\mathbf{R}\,\langle\Psi|\mathbf{R},\mathbf{S}\rangle\langle\mathbf{R},\mathbf{S}|\Psi\rangle} =$$

$$\overset{\mathbf{X}=\{\mathbf{R},\mathbf{S}\}}{=} \frac{\int d\mathbf{R}|\Psi(\mathbf{X})|^2\mathcal{O}_L(\mathbf{X})}{\int d\mathbf{R}|\Psi(\mathbf{X})|^2} = \int d\mathbf{R}\,P(\mathbf{X})\mathcal{O}_L(\mathbf{X})$$

with $\mathcal{O}_L(\mathcal{O}) = \frac{\mathcal{O}\Psi(\mathbf{X})}{\Psi(\mathbf{X})}$ and $P(\mathbf{X}) = \frac{|\Psi(\mathbf{X})|^2}{\int d\mathbf{R}|\Psi(\mathbf{X})|^2} \rightarrow \{\mathbf{X}_1,\ldots,\mathbf{X}_{\mathcal{N}_{\text{walker}}}\}$

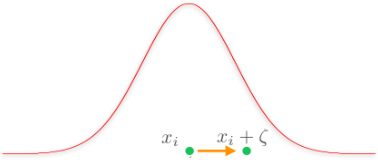
$$\mathcal{O}_V = \frac{1}{\mathcal{N}_{\text{walker}}}\sum_{s=1}^{\mathcal{N}_{\text{walker}}}\mathcal{O}_L(\mathbf{X}_s) \qquad \sigma_{\mathcal{O}_V} = \sqrt{\frac{1}{\mathcal{N}_{\text{walker}}-1}\sum_{s=1}^{\mathcal{N}_{\text{walker}}}\left(\mathcal{O}_L(\mathbf{X}_s)-\mathcal{O}_V\right)^2}$$

Metropolis Hastings Algorithm

Step 2: MH Our goal is to sample the probability distribution described by $P(\mathbf{X}) = \frac{|\Psi_T(\mathbf{X})|^2}{\int d\mathbf{R}|\Psi(\mathbf{X})|^2}$.
The $M(RT)^2$ algorithm is based on the idea of random walk: **a Markov Chain with transition matrix Π.**

$$\mathcal{P}(X_{i+1} = x_{i+1}|X_0 = x_0, \cdots, X_i = x_i) = \Pi(x_i, x_{i+1}) = q(x_{i+1}|x_i)r(x_{i+1}|x_i)$$

- $x_{i+1} = x_i + \zeta_{N(\mu=0,\sigma=1)}$
- $r(x_{i+1}|x_i) = \min\left(1, \frac{P(x_{i+1})\cancel{q(x_i|x_{i+1})}}{P(x_i)\cancel{q(x_{i+1}|x_i)}}\right)$



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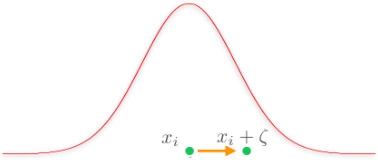
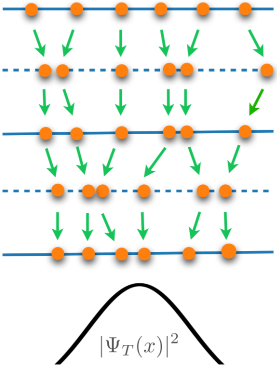
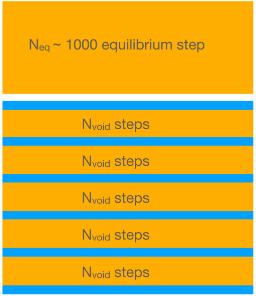




1. Wait for thermalization
2. Evaluate $\mathcal{N}_{avg}$ spaced by $\mathcal{N}_{void}$ step.



The Stochastic Reconfiguration algorithm

Step 3: Optimization of the Parameters:

- Stochastic-Reconfiguration (S. Sorella 2005), in the context of VMC, is equivalent to performing **imaginary-time evolution in the parameters space**, and it is related to the Natural Gradient descent method (Amari et al.).

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Step 3: Optimization of the Parameters:

- Stochastic-Reconfiguration (S. Sorella 2005), in the context of VMC, is equivalent to performing **imaginary-time evolution in the parameters space**, and it is related to the Natural Gradient descent method (Amari et al.).
- Imaginary-time evolution $e^{iH(i\tau)} \approx (1 - H\tau)$ in the parameter space reads

$$(1 - H\tau)\left|\Psi_T(\mathcal{W})\right\rangle = \left|\Psi_T(\mathcal{W} + \Delta\mathcal{W})\right\rangle = \Delta\mathcal{W}_0\left|\Psi_T(\mathcal{W})\right\rangle + \sum_j \Delta\mathcal{W}_j\mathcal{O}^j\left|\Psi_T(\mathcal{W})\right\rangle$$

where $\mathcal{O}^i\left|\Psi_T(\mathcal{W})\right\rangle = \left|\frac{\partial}{\partial \mathcal{W}_i}\Psi(\mathcal{W})\right\rangle$. Multiplying from left by

$$\frac{\left\langle\Psi(\mathcal{W})\right|}{\left\langle\Psi_T(\mathcal{W})\middle|\Psi_T(\mathcal{W})\right\rangle} \quad \text{and} \quad \frac{\left\langle\Psi(\mathcal{W})\right|\mathcal{O}^i}{\left\langle\Psi_T(\mathcal{W})\middle|\Psi_T(\mathcal{W})\right\rangle}$$

gives the two following equations

$$\begin{cases}\langle(1 - H\tau)\rangle = \Delta\mathcal{W}_0 + \sum_i \Delta\mathcal{W}_i\langle\mathcal{O}^i\rangle \\ \langle\mathcal{O}^i(1 - H\tau)\rangle = \Delta\mathcal{W}_0\langle\mathcal{O}^i\rangle + \sum_j \Delta\mathcal{W}_j\langle\mathcal{O}^i\mathcal{O}^j\rangle\end{cases}$$

The Stochastic Reconfiguration Algorithm

- solving the first for $\Delta\mathcal{W}_0$ and exploiting it in the second gives

$$\underbrace{\Big(\langle H\rangle\langle O^i\rangle - \langle HO^i\rangle\Big)}_{-\frac{1}{2}G_i}\tau = \sum_j \Delta\mathcal{W}_j \underbrace{\Big(\langle O^i O^j\rangle - \langle O^i\rangle\langle O^j\rangle\Big)}_{\mathcal{S}_{ij}}$$

It naturally leads to the updating rule

$$\mathcal{W}_i^{n+1} = \mathcal{W}_i^n + \Delta\mathcal{W}_i^n = \mathcal{W}_i^n - \frac{1}{2}\tau\sum_j\Big(\underbrace{\mathcal{S}_{ij}^n + \epsilon\mathbb{1}_{ij}}_{\text{avoid saddle points}}\Big)^{-1} G_j^n$$

where the quantities of interests are all evaluated through importance sampling

$$G_i = \frac{\partial E(\mathcal{W})}{\partial \mathcal{W}_i} = 2\Big(\langle O_i H\rangle - E_V\langle O_i\rangle\Big) \qquad \mathcal{S}_{ij} = \langle O_i O_j\rangle - \langle O_i\rangle\langle O_j\rangle$$

The QGT looks like a variance..

In classical Information Theory the Riemannian structure of the parameter space $\mathcal{P}$ of a statistical model $P(\mathbf{x}|\mathbf{w})$, which depends on some parameters $\mathbf{w}$, is defined by the **Fisher information**:

$$g_{ij}(\mathbf{w}) = \mathbb{E}_{p(\mathbf{x}|\mathbf{w})}\left[\frac{\partial \log(p(\mathbf{x}|\mathbf{w}))}{\partial w_i}\frac{\partial \log(p(\mathbf{x}|\mathbf{w}))}{\partial w_j}\bigg|\mathbf{w}\right] = -\mathbb{E}_{p(\mathbf{x}|\mathbf{w})}\left[\frac{\partial^2}{\partial w_i \partial w_j}\log\left(p(\mathbf{x}|\mathbf{w})\right)\bigg|\mathbf{w}\right]$$

Fisher Information is:

1. **The Variance of the derivative of the log-likelihood (Score Function)**
2. **The curvature of the log-likelihood**

Peaked Loglikelihood $= \partial^2_{\mathbf{w_i}}$ high curvature $=$ sample brings high information about $\mathbf{w}_i$

we suppress the variation of such a parameter $G_i^n \to \sum_j (\mathcal{S}_{ij}^n)^{-1} G_j^n$

In Quantum Information Theory:

$$d_{FS}(\Psi,\Phi) = \arccos\left(|\langle \Psi_{\text{norm}}, \Phi_{\text{norm}}\rangle|^{\frac{1}{2}}\right) \to d_{FS}[\Psi_V(\mathbf{X}|\mathbf{w}), \Psi_V(\mathbf{X}|\mathbf{w}+d\mathbf{w})]^2 = \sum_{ij} \mathcal{S}_{ij}(\mathbf{w}) dw_i dw_j$$

If Ψ is defined over a basis $|\psi(\mathbf{X}|\mathbf{w})\rangle \approx \sum_{\mathbf{X}\in\{\mathbf{X}\}} \sqrt{p(\mathbf{X}|\mathbf{w})}\,|\mathbf{X}\rangle$ can be shown that $\mathcal{S}_{ij}(\mathbf{w}) = \frac{1}{4} g_{ij}(\mathbf{w})$.

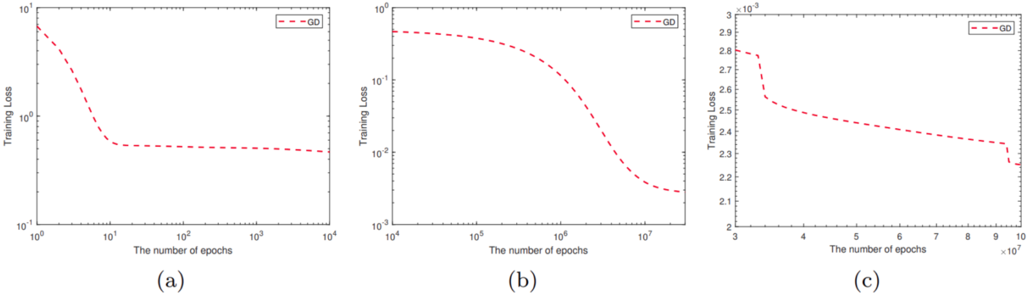
Quantum Natural Gradient - Carleo et al. (Quantum May 2020), page 10.

The Natural Gradient Descent

Amari (S. I. Amari, Neural Computation 10, 251 (1998).) → steepest descent direction of a cost function $L(w)$ in a Riemannian space is given by the **Natural Gradient**.

$$-\tilde{\nabla} L(\mathbf{w}) = -g^{-1}(\mathbf{w})\nabla L(\mathbf{w})$$

- The NG flatten the metric of the parameter space!
- Using the Natural Gradient the plateau phenomenon might disappear.



SR with RMSProp

- In the RMSProp the gradient express the **acceleration** in the parameter space. The $\mathcal{S}$ matrix is regularized with the running averages of the squared gradients.

$$\mathbf{m}^{n+1} = \beta \mathbf{m}^{n} + (1-\beta)\mathbf{G}^{n} \odot \mathbf{G}^{n}$$

$$\mathcal{S}_{ij}^{n} + \epsilon \cdot \text{diag}(1) \rightarrow \mathcal{S}_{ij}^{n} + \epsilon \cdot \text{diag}(\sqrt{\mathbf{m}^{n}} + 10^{-8})$$

- The ϵ hyperparameter add an L^2 penality term to the solution of the system from which $\Delta\mathcal{W}$ are determined $\rightarrow ||\Delta\mathcal{W}\mathcal{S} - \mathbf{G}|| = ||\epsilon\Delta\mathcal{W}||$

Now let's see some results..

Interaction Potential:

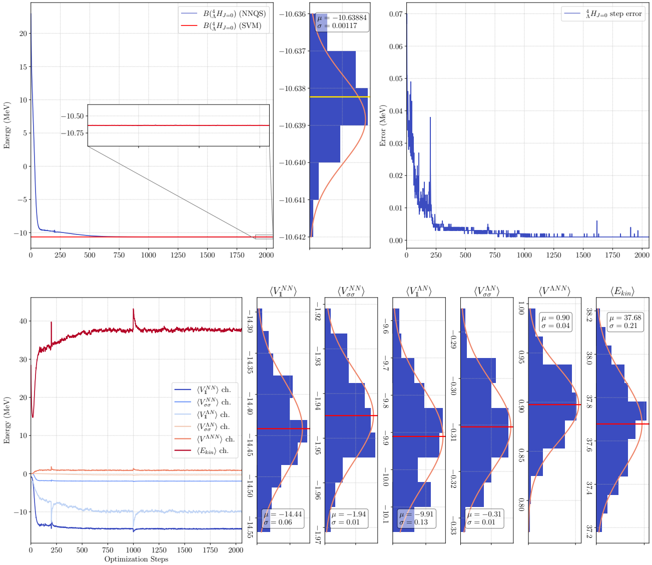
Idea of the improved LO interaction → Two- and three-nucleon contact interactions and ground-state energies of light- and medium-mass nuclei, Phys. Rev. C 103, 054003 2021, Schiavilla et al. - model "o"

- Coulomb interaction derived from the same paper.

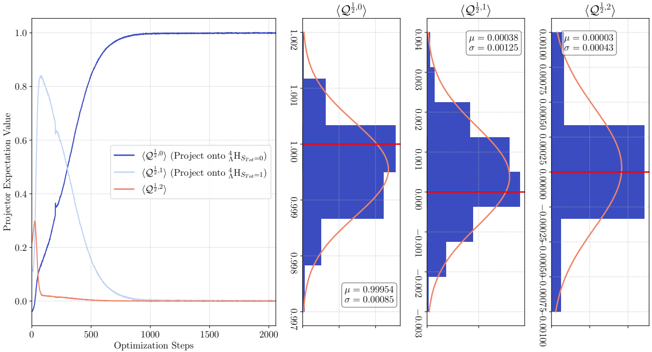
Gaussian regulators: $\delta_\lambda(x) = \frac{\Lambda^3}{8\pi^{\frac{3}{2}}} e^{-\frac{\Lambda^2 r^2}{4}}$

- NN and NNN interaction:
  1. NN fitted to pn/nn: $a_0^{s,t}$, and $r_0^{s,t}$ with variable phase method.
  2. NNN fitted to ^{3}H and ^{4}He BE with Gaussian Processes
- ΛN and ΛNN interaction:
  1. ΛN fitted to pΛ $a_0^{s,t}$, and $r_0^{s,t}$.
  2. ΛNN fitted to the $^3_\Lambda$H, $^4_\Lambda$H$_{S_{tot}=0}$, $^4_\Lambda$H$_{S_{tot}=1}$, and $^5_\Lambda$He BE.

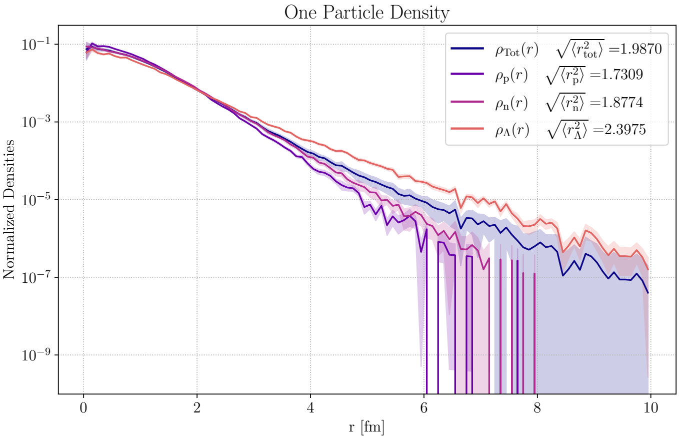
${}^{4}_{\Lambda}H_{S_{tot}=0}$ with Fitted Potential



${}^{4}_{\Lambda}H_{S_{tot}=0}$ Projectors

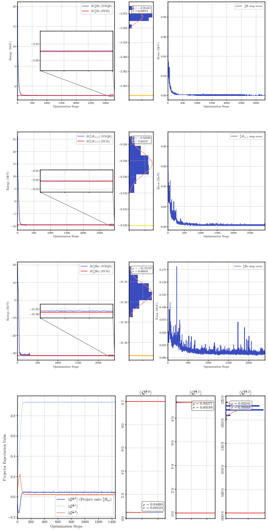


${}^{4}_{\Lambda}H_{S_{tot}=0}$ Density

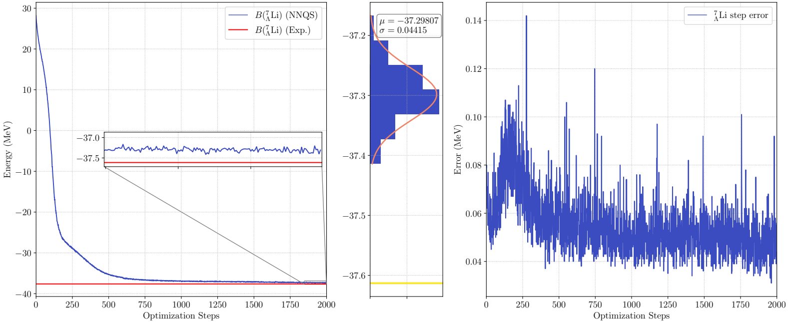


Work in progress:

- In several systems the total spin is not a good quantum number.
- The main effect is a fluctuation of the energy around the convergence region for the target energies of the fit with an average accuracy of $5 \div 60 KeV$.



$^{7}_{\Lambda}Li$ with Fitted Potential



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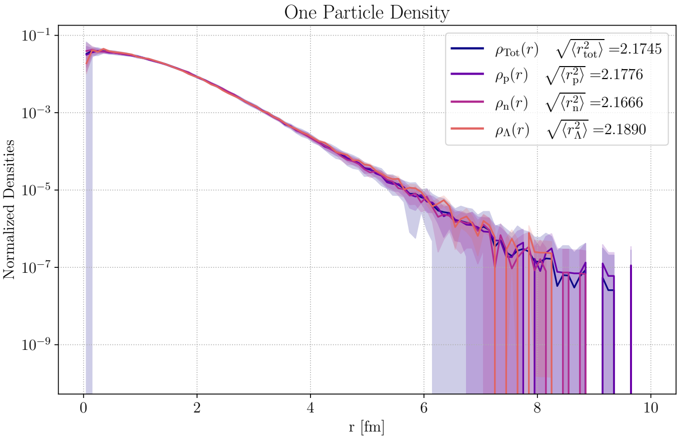
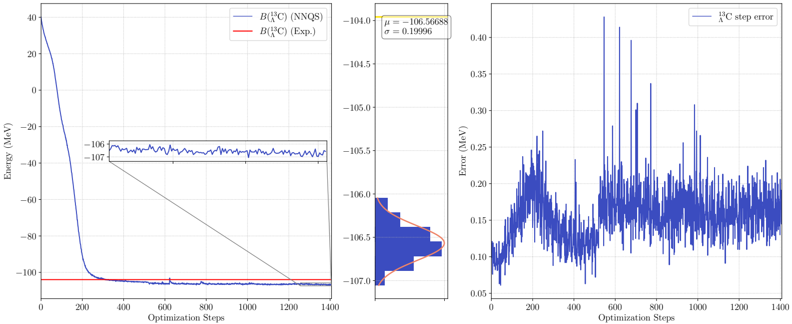


$^{13}_{\Lambda}C$ with Fitted Potential



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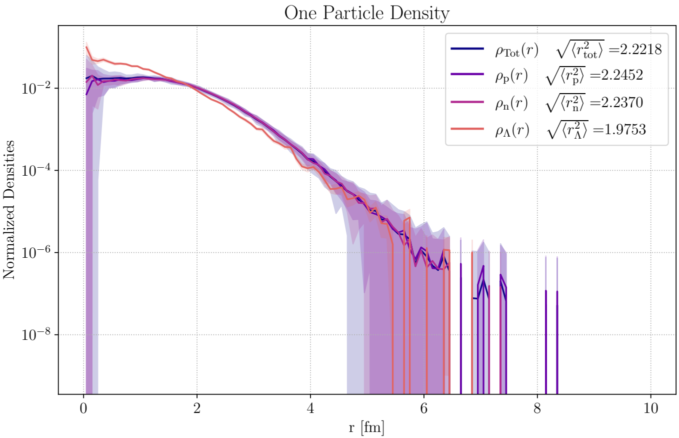
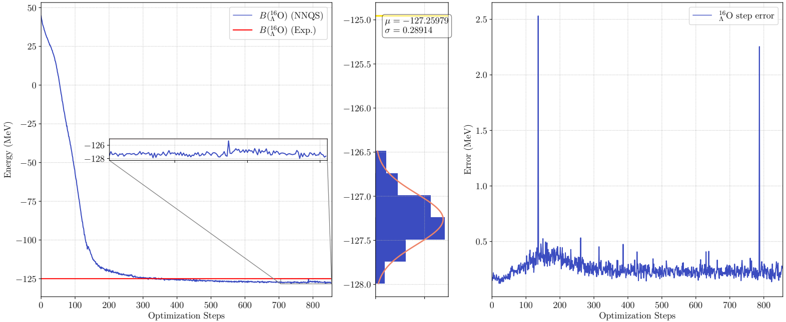
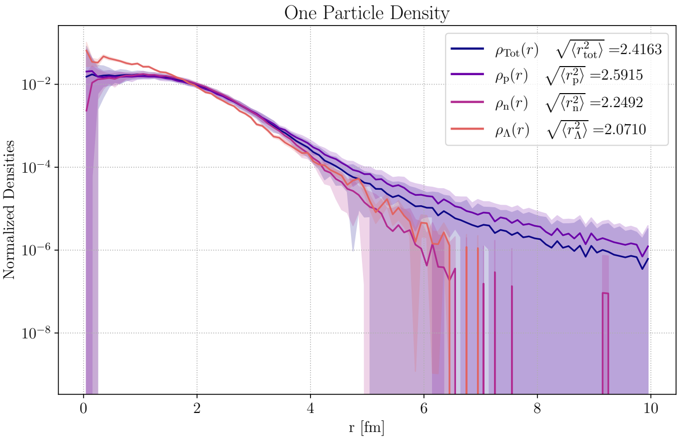
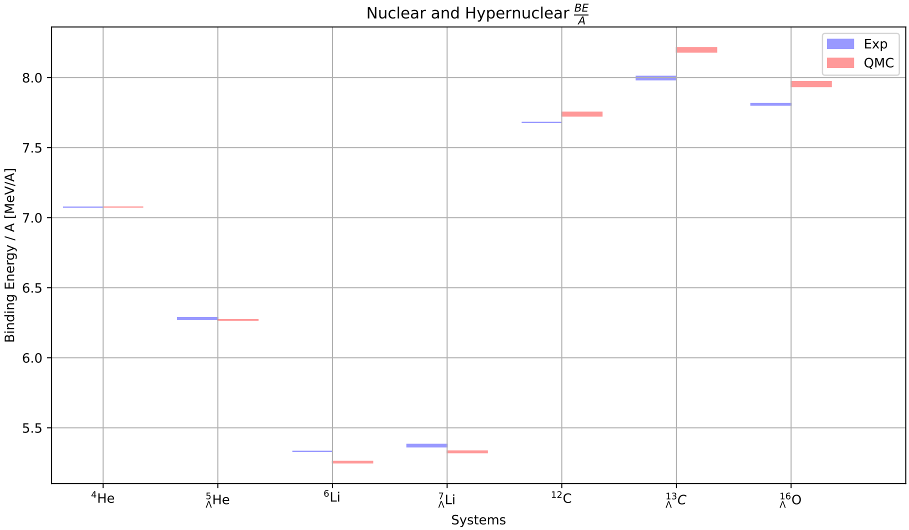


$^{16}_{\Lambda}O$ with Fitted Potential



$^{16}_{\Lambda}O$ with Fitted Potential




Nuclear and Hypernuclear $\frac{BE}{A}$
Exp
QMC
Binding Energy / A [MeV/A]
8.0
7.5
7.0
6.5
6.0
5.5
^{4}He
$^{5}_{\Lambda}$He
^{6}Li
$^{7}_{\Lambda}$Li
^{12}C
$^{13}_{\Lambda}C$
$^{16}_{\Lambda}$O
Systems

Conclusions

- NNQS shows great flexibility in modeling hypernuclear bound states.
  - NQS Variational State → match with accuracy the binding energy of hypernuclear systems.
  - Fitted interaction: Improved LO guarantes the desired accuracy.
  - Still improvements needs to be done: Obtain a wavefunction with good quantum numbers for the total Spin.
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  1. Moving to NLO and restore cutoff dependence.
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  3. Hypernuclear matter → EoS

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Thank you!

Neural-Network Quantum States

The Neural Network Quantum States (NNQS) approach can be classified as a form of **unsupervised machine learning** but actually occupy a middle ground between supervised and unsupervised learning, as it incorporates elements from both approaches:

Approach	**Input**	**Learning Procedure**	**Output**
Supervised Learning	Labeled input-output pairs	Minimize the cost function through gradient-descent → *Backpropagation*	Model that map inputs to corresponding output labels
NNQS	Quantum system coordinates Unlabeled $(\mathbf{x}, \mathbf{s}, \mathbf{t})$	Variational optimization (Energy-gradient informed cost function → Backprop.)	Amplitude of the ground state wavefunction
Unsupervised Learning	Unlabeled data	Training with unlabeled data (Clustering- Dimensionality red. ...)	Model that represent patterns or structure in the data

Similarly to Supervised Learning (GD, SGD, RMSProp, Momentum, AdaGrad...) in NNQS we use first- and second-order derivatives information (gradient, hessian) to improve convergence and performance.

The Quantum Geometric Tensor

The Riemannian structure of the parameter space $\mathcal{P}$ of a statistical model $p(\mathbf{x}|\mathbf{w})$, which depends on some parameters $\mathbf{w}$ is defined by the Fisher information:

$$g_{ij}(\mathbf{w}) = \mathbb{E}_{p(\mathbf{x}|\mathbf{w})}\left[\frac{\partial \log(p(\mathbf{x}|\mathbf{w}))}{\partial w_i}\frac{\partial \log(p(\mathbf{x}|\mathbf{w}))}{\partial w_j}\bigg|\mathbf{w}\right] = -\mathbb{E}_{p(\mathbf{x}|\mathbf{w})}\left[\frac{\partial^2}{\partial w_i \partial w_j}\log\left(p(\mathbf{x}|\mathbf{w})\right)\bigg|\mathbf{w}\right]$$

An intuition about this property of the Fisher information in clarified by noting that the Kullback-Liebler divergence

$$D_{KL}(p(\mathbf{x},\mathbf{w}), p(\mathbf{x},\mathbf{w}')) = \int d\mathbf{x} p(\mathbf{x},\mathbf{w}) \log\left(\frac{p(\mathbf{x},\mathbf{w})}{p(\mathbf{x},\mathbf{w}')}\right)$$

evaluated between $p(\mathbf{w})$ and $p(\mathbf{w}')$, with $\mathbf{w}' \to \mathbf{w}$, is Taylor expanded to

$$\begin{aligned} D_{KL}\big(p(\mathbf{x}|\mathbf{w}), p(\mathbf{x}|\mathbf{w}')\big) &\approx \frac{1}{2}\sum_{i,j}\left(\frac{\partial^2}{\partial w'_i \partial w'_j} D_{KL}\big(p(\mathbf{x}|\mathbf{w}), p(\mathbf{x}|\mathbf{w}')\big)\right) dw_i dw_j \\ &= -\frac{1}{2}\sum_{i,j}\int d\mathbf{x} p(\mathbf{x}|\mathbf{w})\left[\frac{\partial^2}{\partial w'_i \partial w'_j}\log\left(p(\mathbf{x}|\mathbf{w}')\right)\right]_{\mathbf{w}'=\mathbf{w}} dw_i dw_j \\ &= \frac{1}{2}\sum_{i,j} g_{ij}(\mathbf{w}) dw_i dw_j \end{aligned}$$

The Quantum Geometric Tensor

We can observe the relation between the Quantum Geometric Tensor $\mathcal{S}_{ij}$ and the fisher information by means of the Fubini-Study metric, which is the natural metric for the two-level pure quantum-machanical system defined by the Block Sphere

$$d_{FS}(\Psi, \Phi) = \arccos\left(|\langle \Psi_{\text{norm}}, \Phi_{\text{norm}} \rangle|^{\frac{1}{2}}\right)$$

and considering its infinitesimal form, which correspond to the Quantum Geometric Tensor

$$d_{FS}[\Psi_V(\mathbf{X}|\mathbf{w}), \Psi_V(\mathbf{X}|\mathbf{w} + d\mathbf{w})]^2 = \sum_{ij} \mathcal{S}_{ij}(\mathbf{w}) dw_i dw_j$$

defined over a basis $|\psi(\mathbf{X}|\mathbf{w})\rangle \approx \sum_{\mathbf{X}\in\{\mathbf{X}\}} \sqrt{p(\mathbf{X}|\mathbf{w})}\,|\mathbf{X}\rangle$ can be easily shown that $\mathcal{S}_{ij}$ is proportional to the Fisher Information $\mathcal{S}_{ij}(\mathbf{w}) = \frac{1}{4} g_{ij}(\mathbf{w})$.

When the Fisher information (The variance of the gradient of the log-likelyhood) is high, it implies that the variance of the score function is also high, meaning small changes in the parameter $\mathcal{W}$ lead to large changes in the log-likelihood.

Quantum Natural Gradient - Carleo et al. (Quantum May 2020), page 10.

Metropolis Algorithm

Our goal is to sample the probability distribution described by $P(\mathbf{X}) = \frac{|\Psi(\mathbf{X})|^2}{\int d\mathbf{R}|\Psi(\mathbf{X})|^2}$. The $M(RT)^2$ algorithm is based on the idea of random walk, namely a Markov Chain with transition matrix Π.

$$\mathcal{P}(X_{i+1} = x_{i+1}|X_0 = x_0, \cdots, X_i = x_i) = \Pi(x_i, x_{i+1})$$

We can split $\Pi(x_i, x_{i+1})$ in two terms:

$$\Pi(x_{i+1}|x_i) = q(x_{i+1}|x_i)r(x_{i+1}|x_i)$$

This means that if you move to x_{i+1} from x_i

1. x_{i+1} is proposed it with probability $q(x_{i+1}|x_i)$
2. x_{i+1} is accepted with probability $r(x_{i+1}|x_i)$ otherwise x_i is kept.
   The acceptance probability is given by

$$r(x_{i+1}|x_i) = \min\left(1, \frac{P(x_{i+1})\cancel{q(x_i|x_{i+1})}}{P(x_i)\cancel{q(x_{i+1}|x_i)}}\right) \quad \rightarrow \text{Works for non-normalized P(x)}$$

This ensures that the fraction of time spent in each state is proportional to $P(x_i)$.

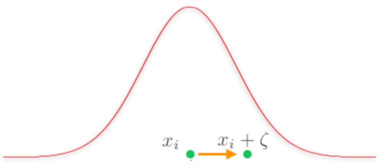
- If $r(x_{i+1}|x_i) = 0.9$ we draw a point z from $U(0,1)$
- if $z_U < 0.9$ we accept the new point, otherwise we reject x_{i+1} and keep x_i.

Metropolis Algorithm

If the proposal is a Normal distribution at each step of the propagation the walkers are moved as follows:

$$q(x_{i+1}|x_i) = N(x_{i+1}|x_i, \mu = 0, \sigma = 1)$$

$$x_{i+1} = x_i + \zeta_{N(\mu=0,\sigma=1)}$$



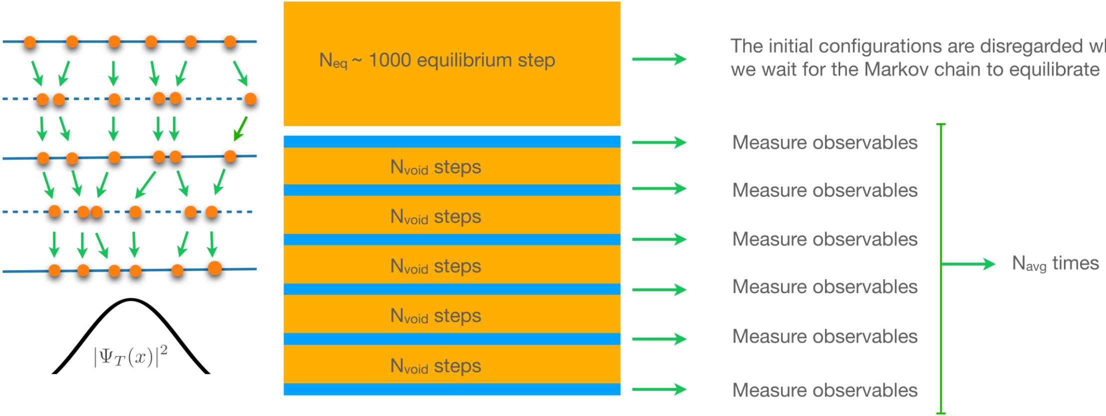
$\mathcal{N}$ MC in parallel

The transfer matrix Π of the MH algorithm ensure that the detailed balance principle is valid and consequently that the Markov chain will converge to the desired target density P after thermalization

$$P(x_i)\Pi(x_{i+1}|x_i) = P(x_{i+1})\Pi(x_i|x_{i+1})$$

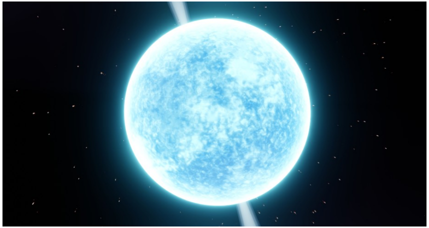
This says that the flow from i to $i+1$ must equal the flow from $i+1$ to i.

Metropolis Algorithm



EoS of Nucleon Stars and the Hyperon puzzle

- One of the most relevant solutions to the Hyperon puzzle relies on the determination of the EoS through **microscopic approaches** which applies a three-body *YNN* interaction potential to compensate the attractive *YN* interaction.



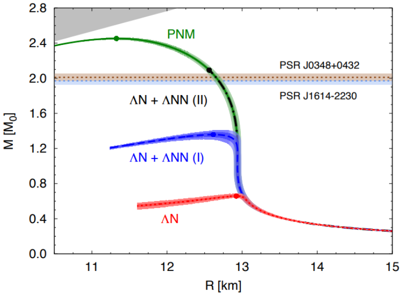
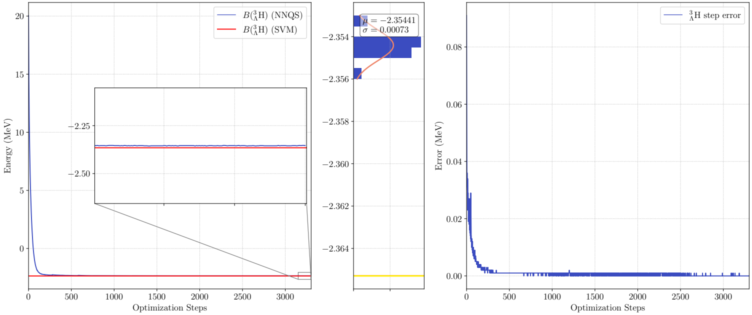
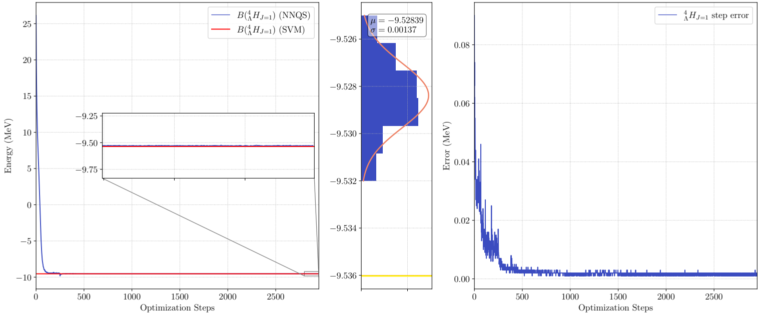
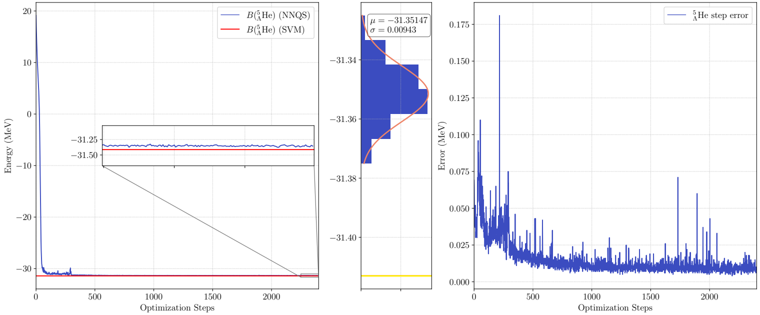


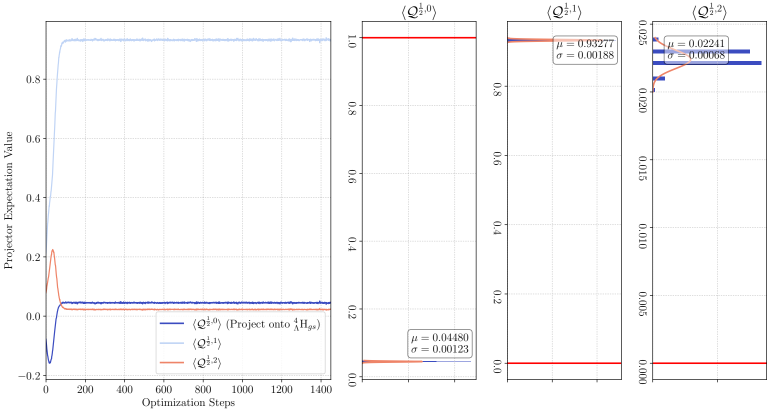
Figure: D. Lonardoni et al., PRL 114 (2015)


$B(^3_\Lambda H)$ (NNQS)
$B(^3_\Lambda H)$ (SVM)
Energy (MeV)
Optimization Steps
$\mu = -2.35441$
$\sigma = 0.00073$
$^3_\Lambda$H step error
Error (MeV)
Optimization Steps


$B(^4_\Lambda H_{J=1})$ (NNQS)
$B(^4_\Lambda H_{J=1})$ (SVM)
Energy (MeV)
Optimization Steps
$\mu = -9.52839$
$\sigma = 0.00137$
$^4_\Lambda H_{J=1}$ step error
Error (MeV)
Optimization Steps



$B(^5_\Lambda\text{He})$ (NNQS)
$B(^5_\Lambda\text{He})$ (SVM)
Energy (MeV)
Optimization Steps
$\mu = -31.35147$
$\sigma = 0.00943$
$^5_\Lambda$He step error
Error (MeV)
Optimization Steps


Projector Expectation Value
Optimization Steps
$\langle \mathcal{Q}^{\frac{1}{2},0} \rangle$ (Project onto ${}^4_\Lambda H_{gs}$)
$\langle \mathcal{Q}^{\frac{1}{2},1} \rangle$
$\langle \mathcal{Q}^{\frac{1}{2},2} \rangle$
$\mu = 0.04480$
$\sigma = 0.00123$
$\mu = 0.93277$
$\sigma = 0.00188$
$\mu = 0.02241$
$\sigma = 0.00068$