Institut de Ciències del Cosmos
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EXCELENCIA MARÍA DE MAEZTU
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A Variational Approach to Quantum Field Theory

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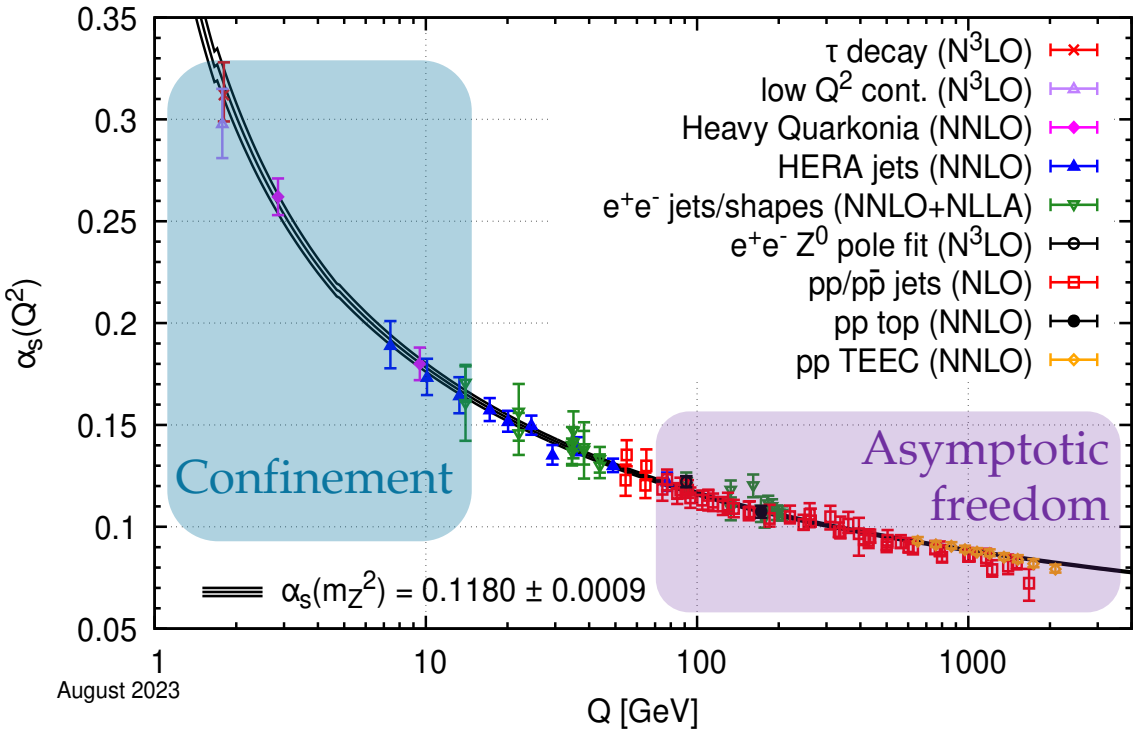
QCD at low energies



S. Navas et al. (Particle Data Group). **Phys. Rev. D, 110(03001)**, 2024.

- Non-perturbative implementation of Field theory:

  Feynmann path integral formalism.

- Expectation values:

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathrm{Z}} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu \hat{\mathcal{O}}[\psi, \bar{\psi}, A] e^{iS_{\mathrm{QCD}}}$$

where

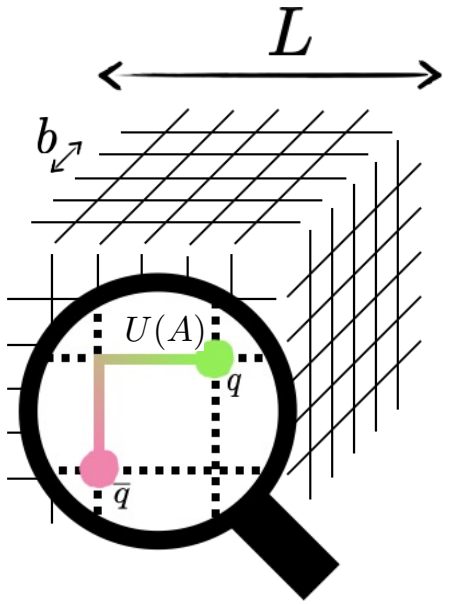
$$\mathrm{Z} = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu e^{iS_{\mathrm{QCD}}}$$

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathrm{Z}} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D} A_\mu \hat{\mathcal{O}}[\psi, \bar{\psi}, A] e^{iS_{\mathrm{QCD}}}$$

Finite volume $L^3 \times T \qquad L \gg m_\pi^{-1}$

Discrete spacetime $b \ll \Lambda_{QCD}^{-1}$

Imaginary time $t \to -\mathrm{i}\tau$



$\times T$

$U_\mu = e^{igbA_\mu(x)}$

©M. Illa

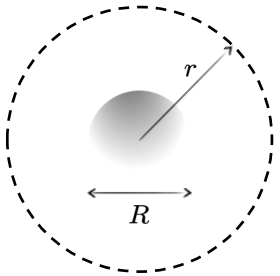
$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathrm{Z}} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D} U_\mu \hat{\mathcal{O}}[\psi, \bar{\psi}, U] e^{-S^E_{\mathrm{QCD}}}$$

$$\langle \hat{\mathcal{O}} \rangle \approx \frac{1}{\mathrm{N_{cf}}} \sum_{i=1}^{\mathrm{N_{cf}}} \hat{\mathcal{O}}(\{U\}_i)$$

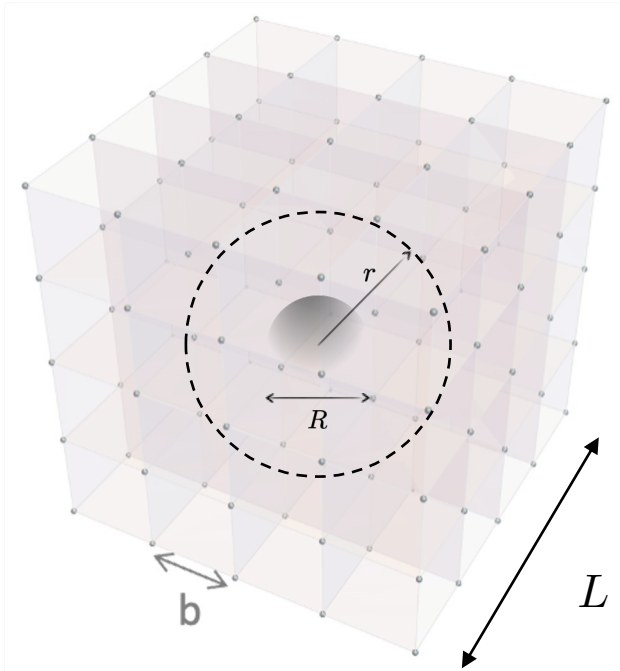
Importance sampling methods

How is scattering approached in LQCD?

infinite volume



finite volume with
cubic boundaries



$$u_l(r;k) = \alpha_l(k)\, j_l(kr) + \beta_l(k)\, n_l(kr)$$

$$e^{2i\delta_l(k)} = \frac{\alpha_l(k) + i\beta_l(k)}{\alpha_l(k) - i\beta_l(k)}$$

generalized $\mathcal{Z}$ function

$$\mathcal{Z}^d_{lm}(s;q^2) = \sum_{\mathbf{r}} \frac{r^l Y_{lm}(\hat{\mathbf{r}})}{\left(|\mathbf{r}|^2 - q^2\right)^s}$$

$L \gg R$

$$\det\left[(\mathcal{M}^\infty)^{-1} + \delta\mathcal{G}^V\right] = 0$$

$\cot\delta(k_n)$ **infinite volume scattering information**

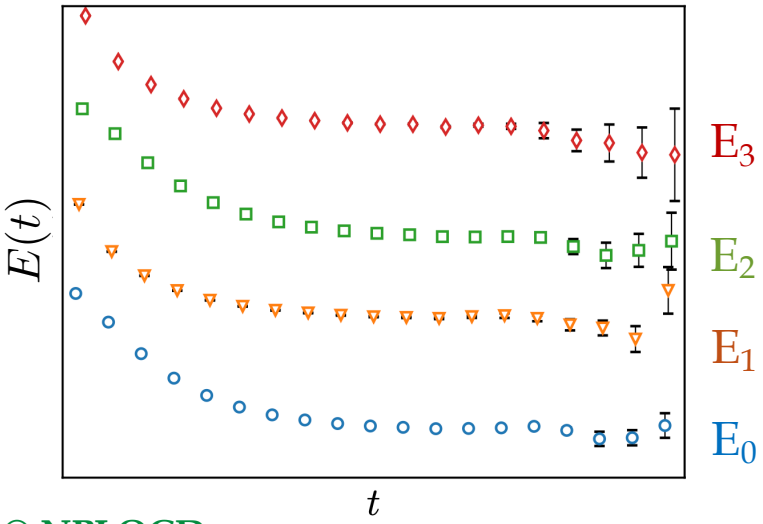
M. Lüscher, Comm. Math. Phys. 105 (1986), **Nuc. Phys. B 354** (1991)

$$C(t) = \langle 0|\phi(t)\,\phi^\dagger(0)|0\rangle \longrightarrow \langle\phi|e^{-Ht}|\phi\rangle = \sum_n \langle\phi|e^{-Ht}|n\rangle\langle n|\phi\rangle = \sum_n \left|\langle\phi|n\rangle\right|^2 e^{-E_n t}$$

$$\phi(t) = e^{Ht}\phi e^{-Ht}$$

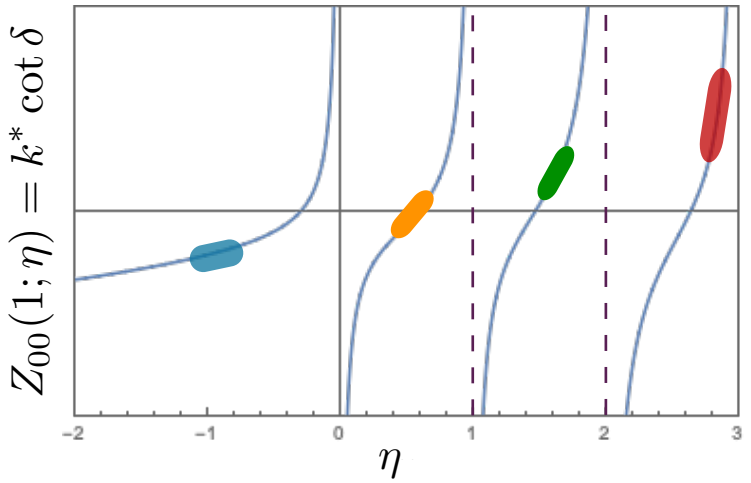
$$= \underbrace{Z_0^{\text{snk}} Z_0^{\dagger\,\text{src}} e^{-E_0 t}}_{\text{LO at large t}} + Z_1^{\text{snk}} Z_1^{\dagger\,\text{src}} e^{-E_1 t} + \ldots$$

i.e. one can obtain the **lowest energy state** provided we see the **large time** exponential fall-off of the correlation function (Euclidean time evolution suppresses excited states)



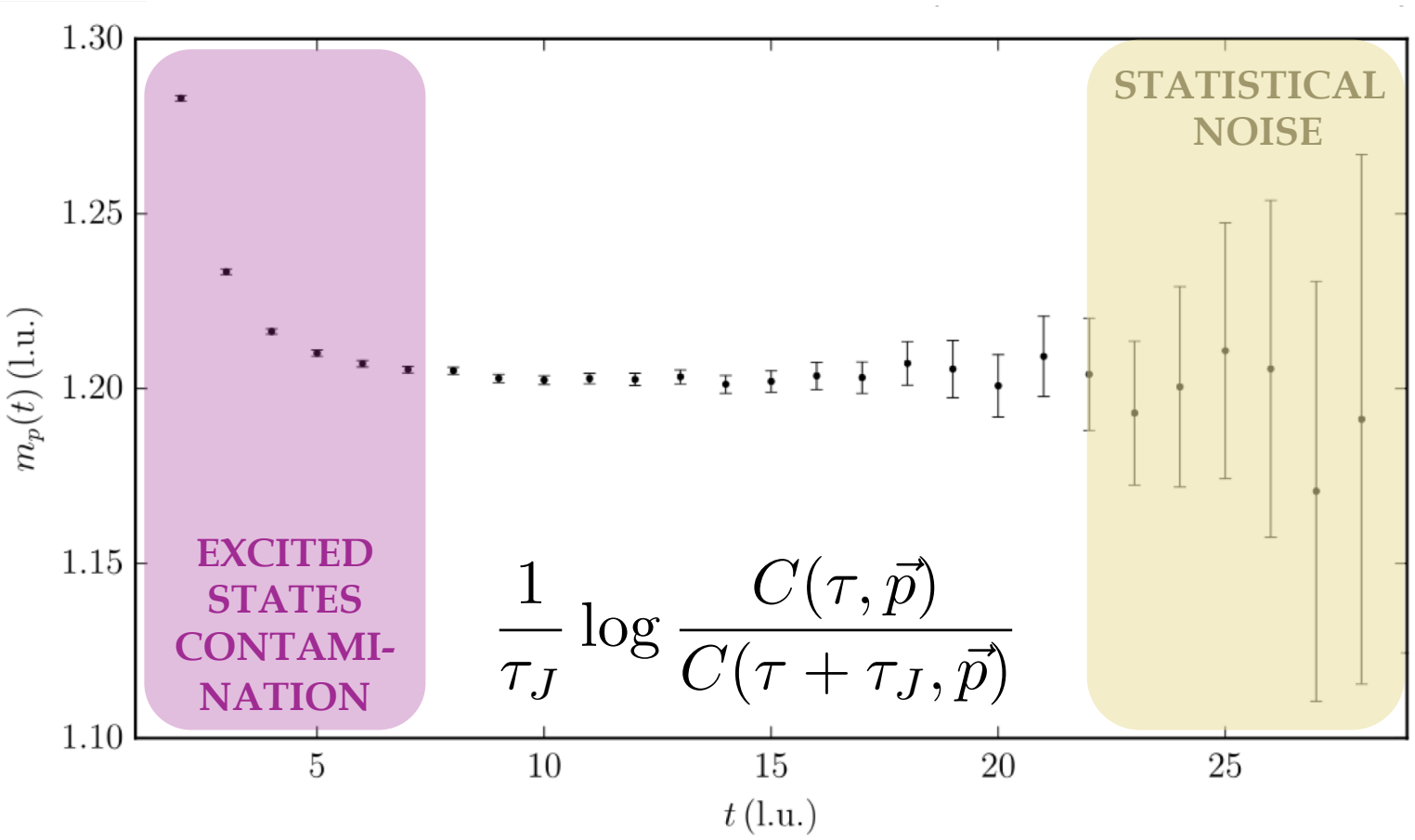
$\Delta E \to k^*$

$$k^* \cot\delta = \frac{2}{\sqrt{\pi}\,L}\,\mathcal{Z}_{00}\left(1;\left(\frac{k^* L}{2\pi}\right)^2\right)$$



Poor signal-to-noise for baryons

Effective mass plot for the proton

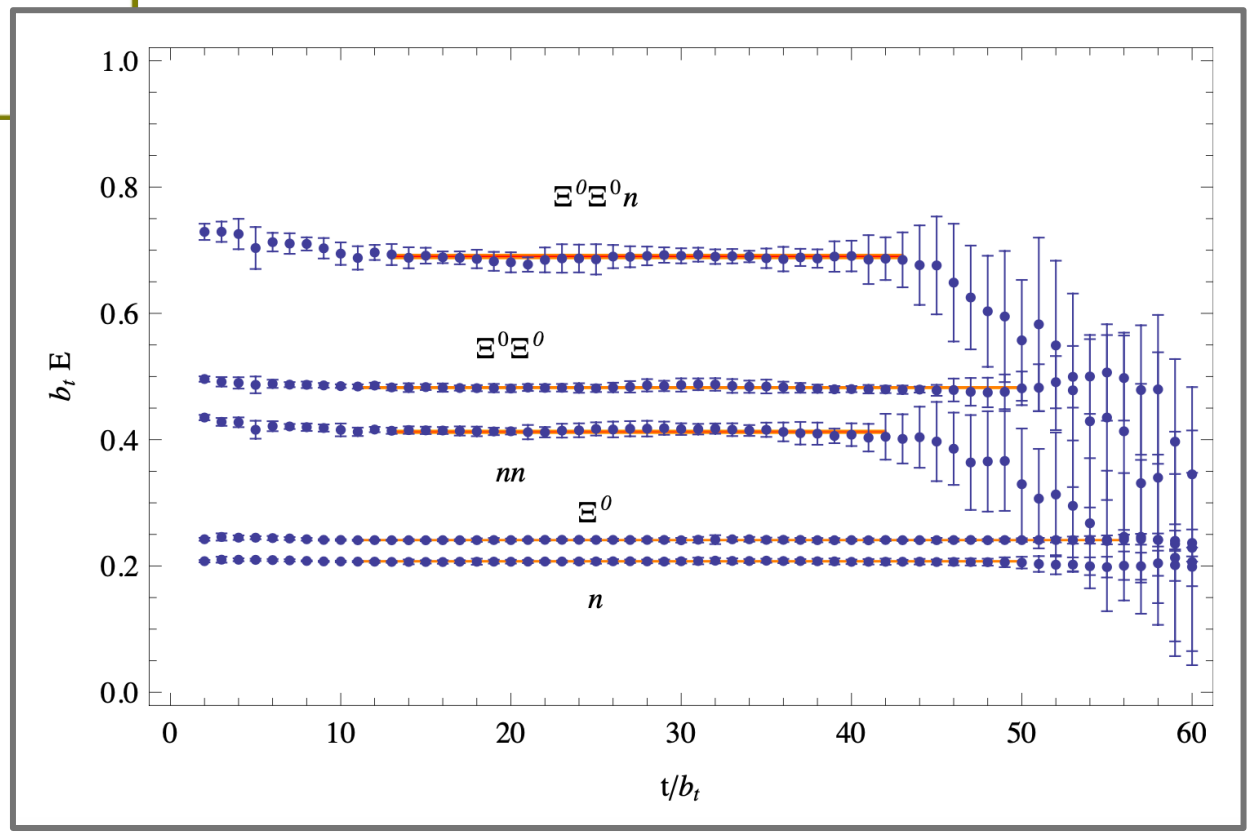


more severe degradation for A nucleons

Expectation is that for A nucleons:

$$\frac{\sigma}{\langle C \rangle} \sim \frac{\exp\left[A\left(M_N - \frac{3m_\pi}{2}\right)t\right]}{\sqrt{N}}$$

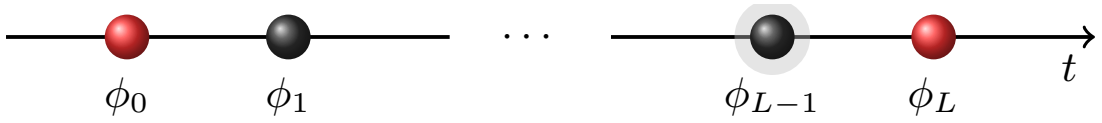
G. Parisi, **Phys. Rept. 103** (1984)
G.P. Lepage, **Boulder TASI** (1989)
M.L. Wagman, M.J. Savage, **Phys. Rev. D 96** (2017)



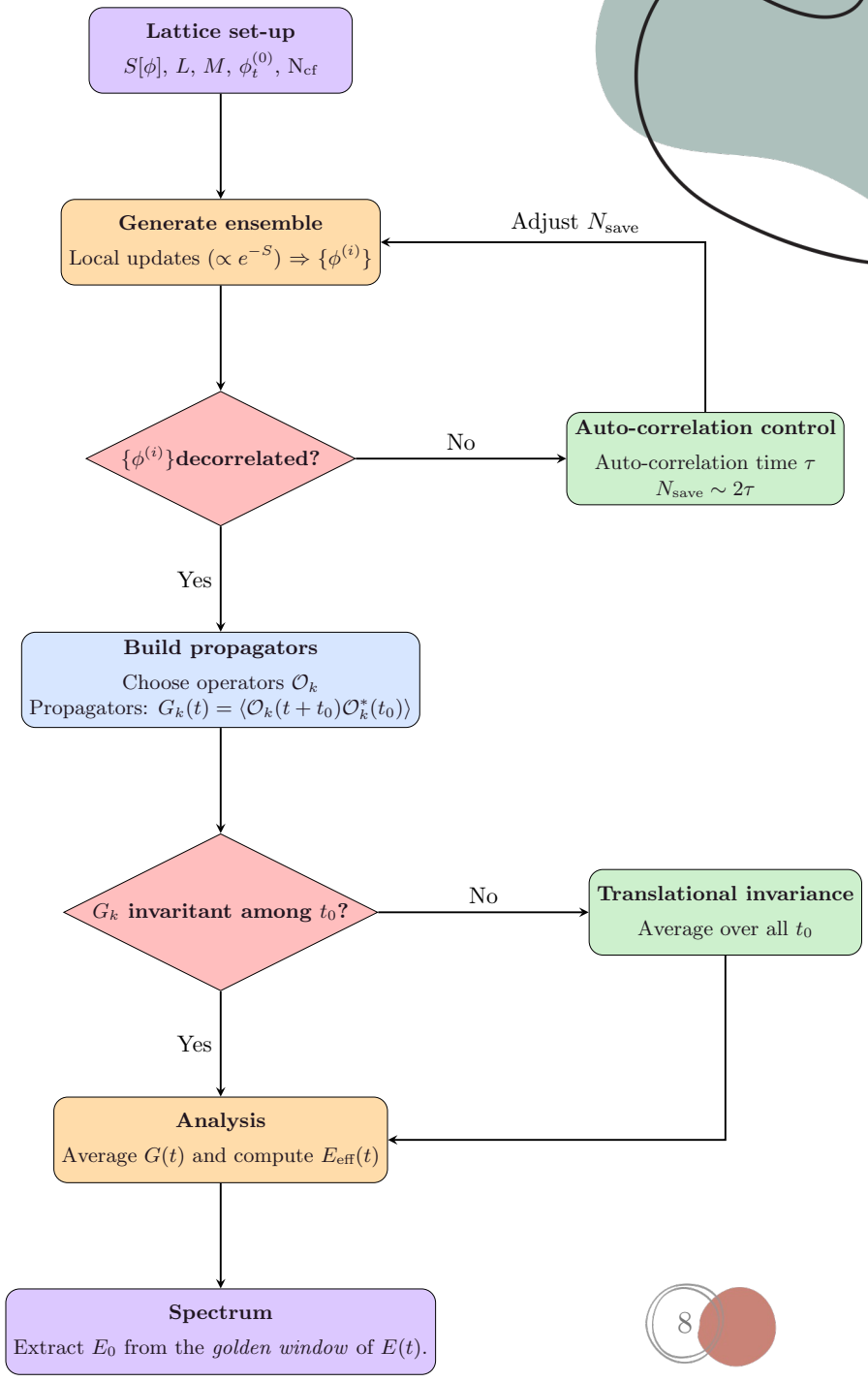
$0 \oplus 1\ \mathbb{C}$ Scalar Field Theory

Path integral formalism

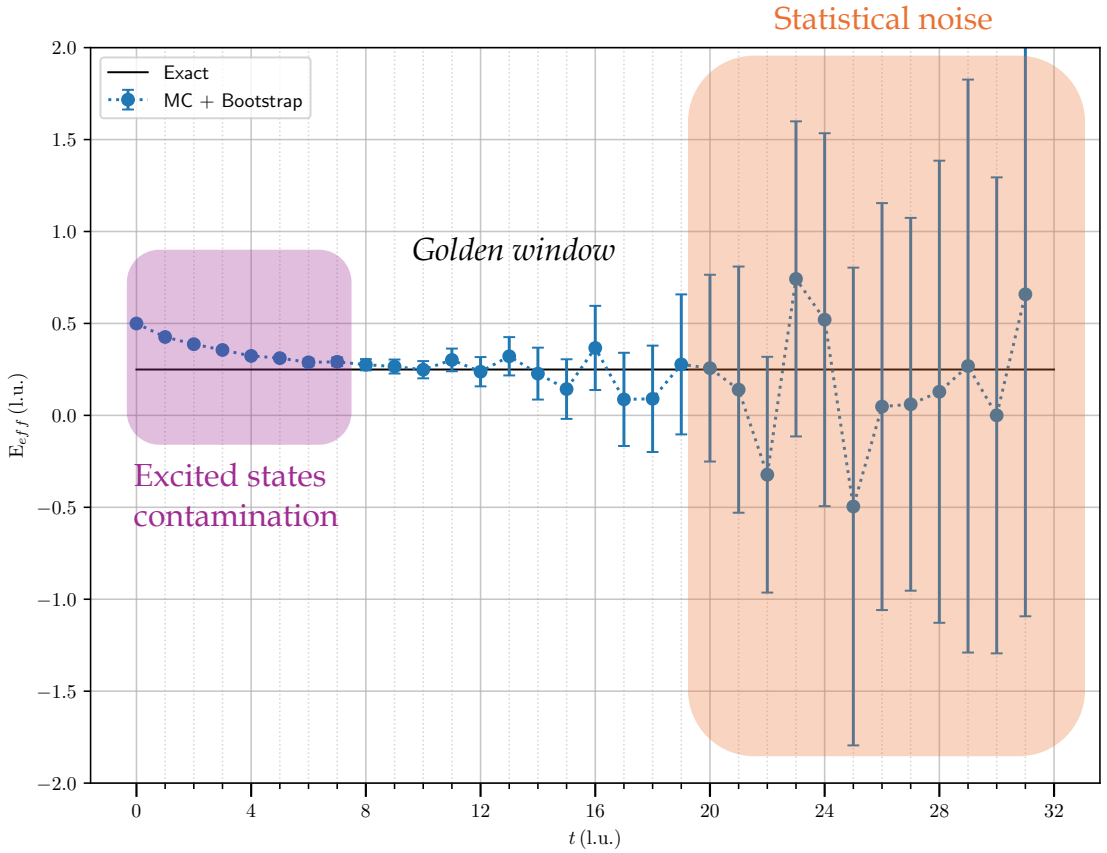
- $S[\phi(t)] = \sum_{t=0}^{L-1} \left\{ \left[\phi^*(t+1) - \phi^*(t)\right]\left[\phi(t+1) - \phi(t)\right] + M^2|\phi(t)|^2 \right\}$
- $G(t,t_0) = \langle \mathcal{O}(t+t_0)\mathcal{O}^*(t_0)\rangle = \frac{1}{Z}\int D\phi\, e^{-S[\phi]}\mathcal{O}(t+t_0)\mathcal{O}^*(t_0)$

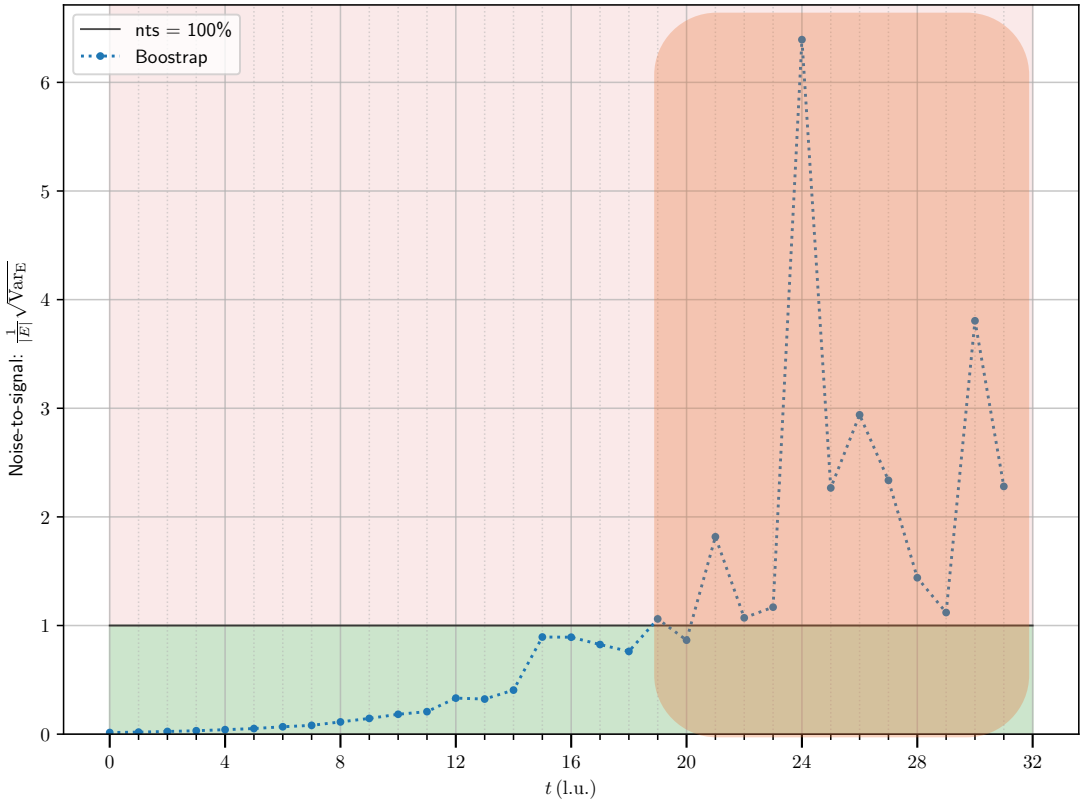


- $S[\phi] = \sum_{t=0}^{L-1} \left[|\phi_{t+1} - \phi_t|^2 + M^2|\phi_t|^2 \right]$
- $G(t,t_0) \simeq \frac{1}{N_{\text{cf}}} \sum_{i=0}^{N_{\text{cf}}-1} \left(\mathcal{O}_{t+t_0}\mathcal{O}^*_{t_0}\right)^{(i)} \qquad \mathcal{O}(t) = e^{\phi(t)} - 1$
- $E(t) = \frac{1}{t_J} \log \frac{G(t)}{G(t+t_J)}$



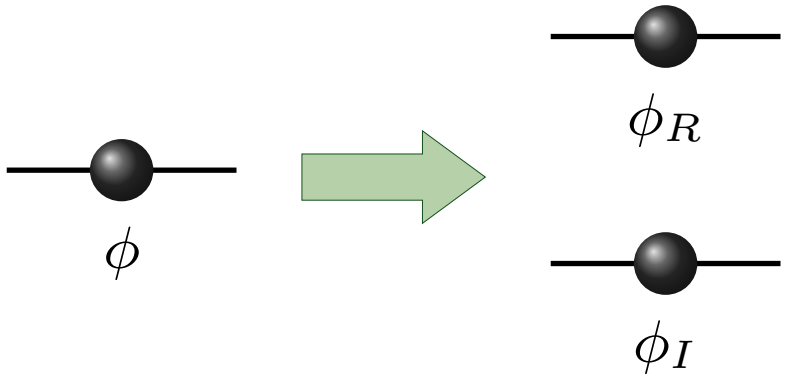
Signal to noise problem





Variational approach

- $\hat{\mathcal{H}} = \pi\pi^\dagger + M^2\phi^\dagger\phi$
- $\mathcal{H}(\phi, \phi^\dagger, \partial\phi, \partial\phi^\dagger) = -\dfrac{\partial^2}{\partial\phi\partial\phi^\dagger} + M^2\phi^\dagger\phi$



- $\mathcal{H}(\phi_R, \phi_I, \partial\phi_R, \partial\phi_I) = \underbrace{-\dfrac{1}{2}\dfrac{\partial^2}{\partial\phi_R^2} + \dfrac{1}{2}M^2\phi_R}_{\mathcal{H}_R} + \underbrace{-\dfrac{1}{2}\dfrac{\partial^2}{\partial\phi_I^2} + \dfrac{1}{2}M^2\phi_I}_{\mathcal{H}_I}$
- $\hat{\mathcal{H}}\psi(\phi_R, \phi_I) = \underbrace{(E_R + E_I)}_{E}\psi(\phi_R, \phi_I)$

Upper bound of the GS energy

- **Variational principle** → $\psi_\theta(\phi_R, \phi_I)$ → $E_\theta = \dfrac{\langle\psi_\theta|\hat{\mathcal{H}}|\psi_\theta\rangle}{\langle\psi_\theta|\psi_\theta\rangle} \geq E_0$

$\langle H^\dagger H\rangle = \langle H^2\rangle$ **no signal to noise problem**

Neural Quantum State as the ansatz

- **Universal approximation theorem**

$$f : \mathbb{R}^n \longrightarrow \mathbb{R} \ ,$$

$$\exists \quad \epsilon > 0, W_{ij}, B_i, h \ , \qquad |f(\boldsymbol{x}) - \mathrm{NN}(\boldsymbol{x})| < \epsilon \ , \quad \forall \boldsymbol{x} \in \mathbb{R}^n$$

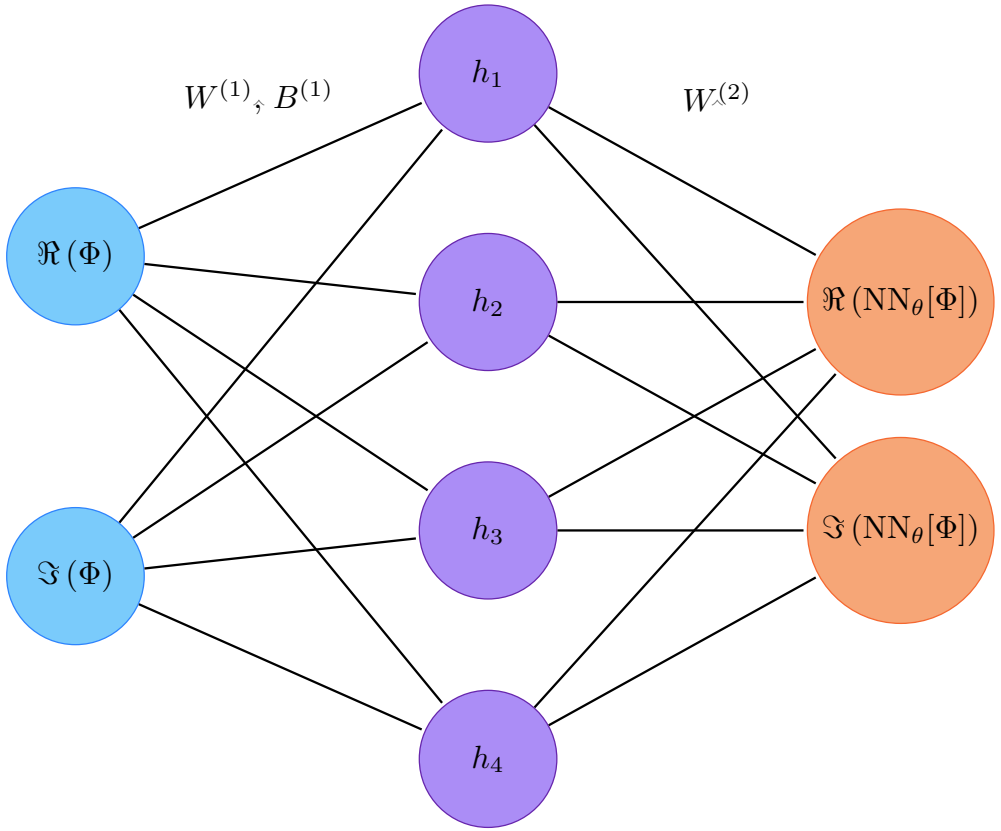
G. Cybenko. **Mathematics of Control, Signals, and Systems, 2(4):303–314**, 1989.

- **NN as the variational ansatz**

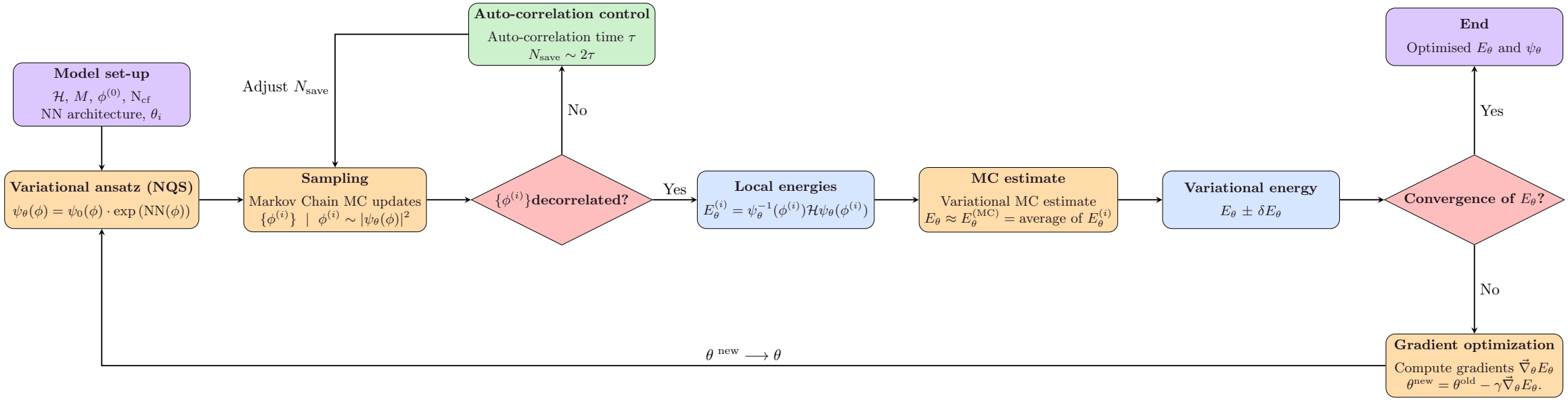
$$\theta = \{W_{ij}^{(1)}, B_i^{(1)}, W_{jk}^{(2)}\}$$

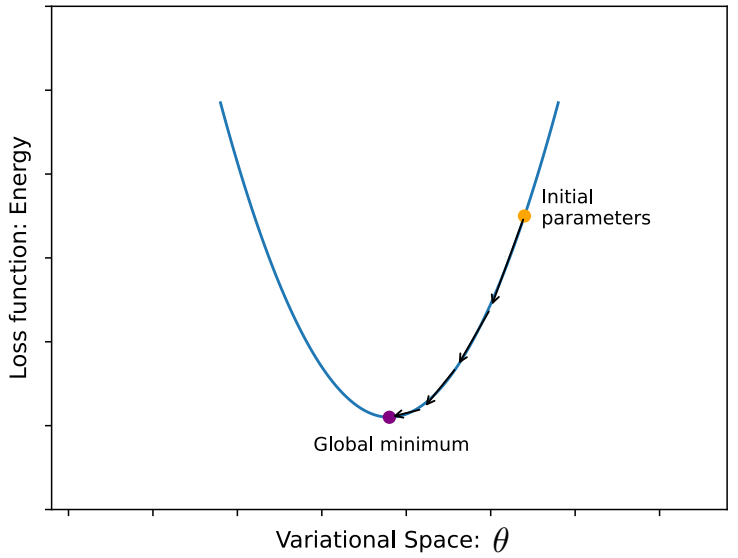
- **NN architecture**

$$h_i = \tanh\left(\sum_j W_{ij}^{(1)} x_j + B_i^{(1)}\right), \qquad y_k = \sum_j W_{jk}^{(2)} h_j$$



Variational Monte Carlo

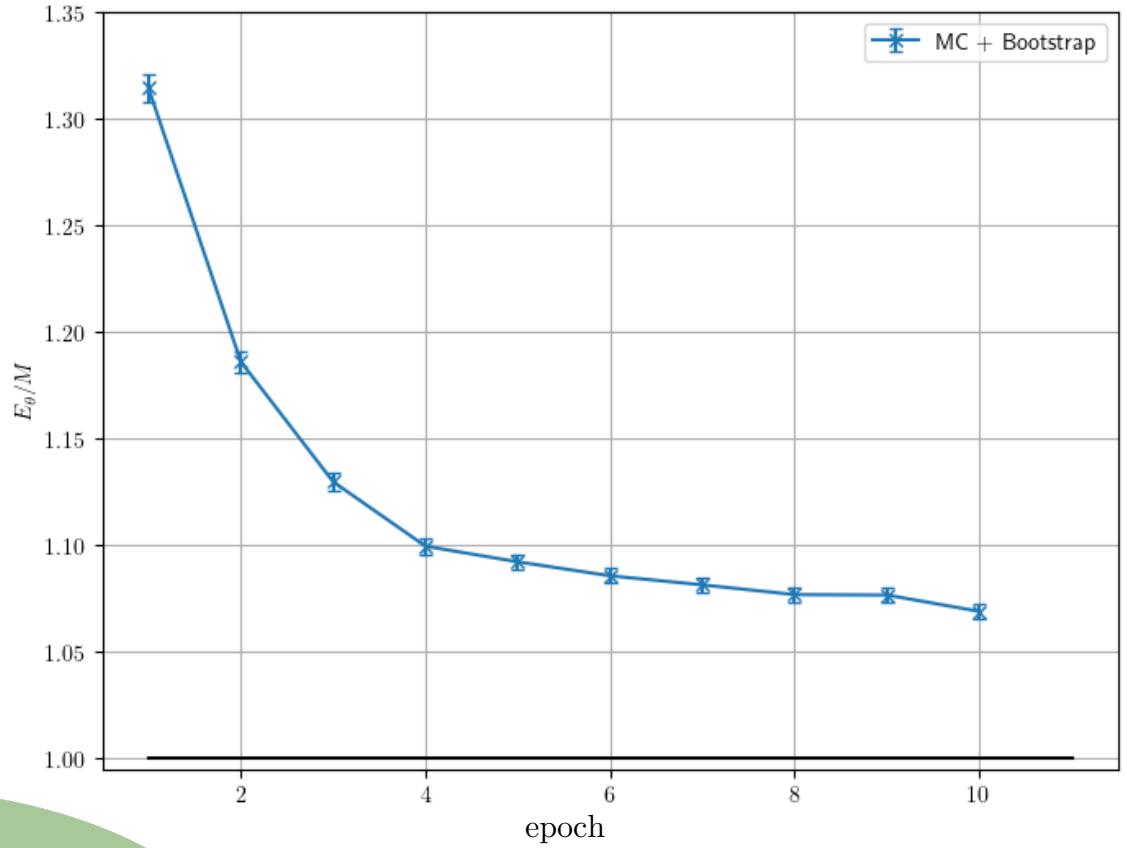


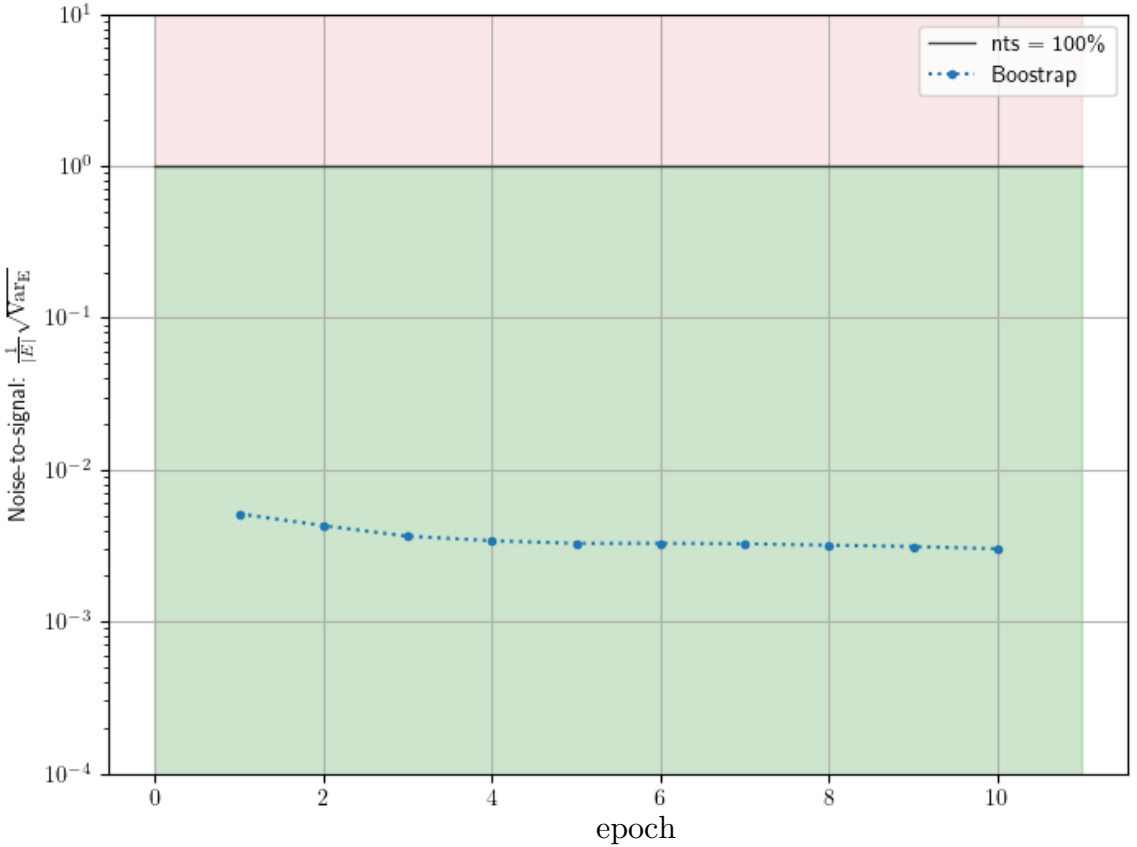


20 dimensional variational space

$$\mathcal{L}_{\mathrm{oss}} = E_\theta - E_0 \sim E_\theta$$

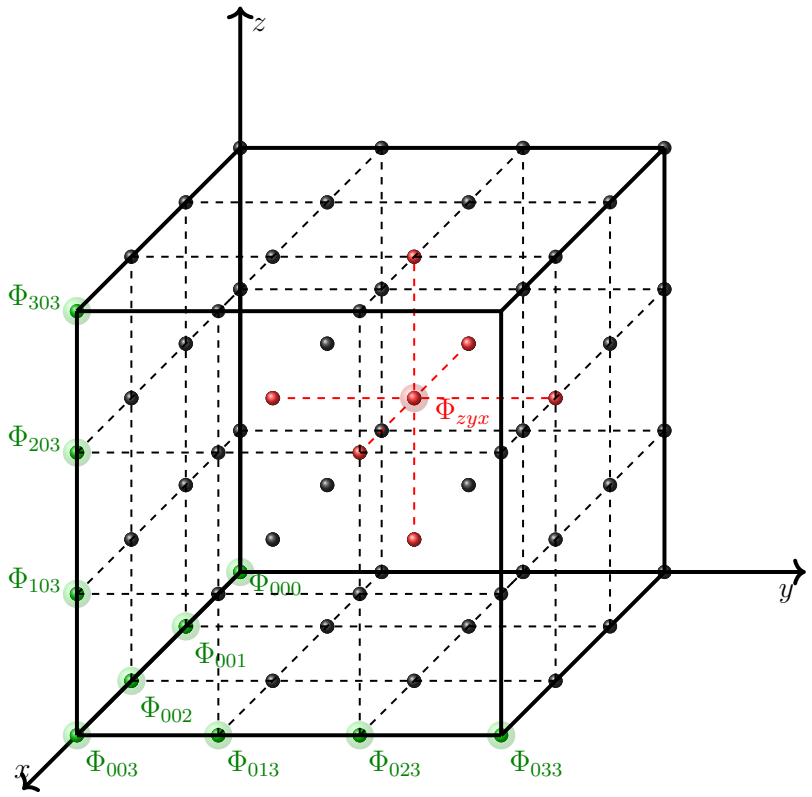
From a signal-to-noise to an *optimization* problem

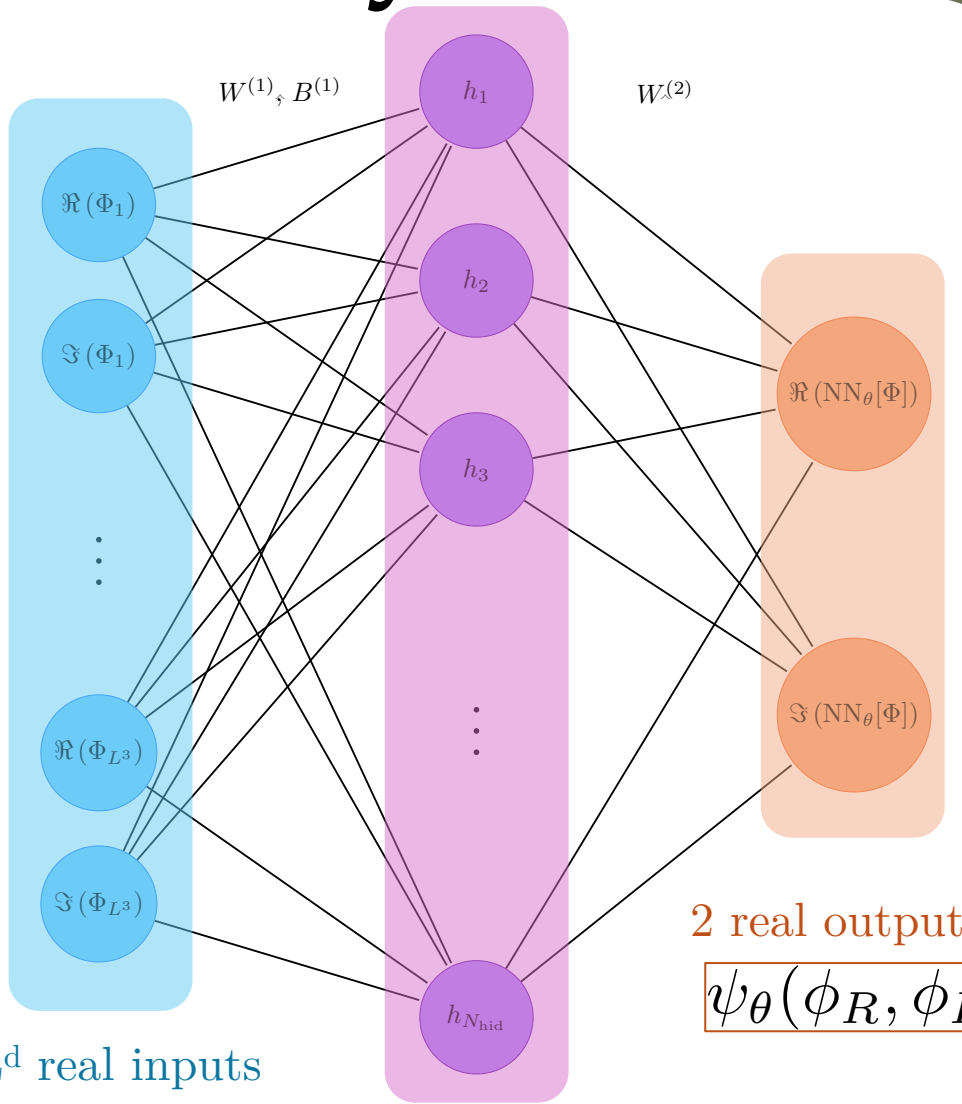




Generalized to any field theory

- QCD is a 3+1 field theory





$2L^d$ real inputs

N_{hid} *hidden* nodes

2 real outputs

$\psi_\theta(\phi_R, \phi_I)$

$$\begin{aligned}\dim &= 2L^d N_{hid} + N_{hid} + 2N_{hid} \\ &= N_{hid}(2L^d + 3)\end{aligned}$$

M. Rovira, R. Perry, A. Parreño. Proceedings of Science
PoS QNP2024 (2025) 036

Summary & future outlook

- VMC approach in the Hamiltonian perspective provides an alternative **without a signal to noise problem**.
- One can study the stationary system and then its evolution (just one point in time).
- The problem is now an **optimization problem**.
- Can we obtain the **low-lying energy spectrum of heavy nuclei?**

  (e.g. lead, uranium) with some systematic errors.

- **Drawbacks**
  - **Generate samples** efficiently.
  - Some ansatz will suffer from strong **autocorrelation**.
  - In high-dimensional theories, **tune the NN ansatz** (N_{hid}) so that it does not scale rapidly with the volume.