ICCUB
Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA

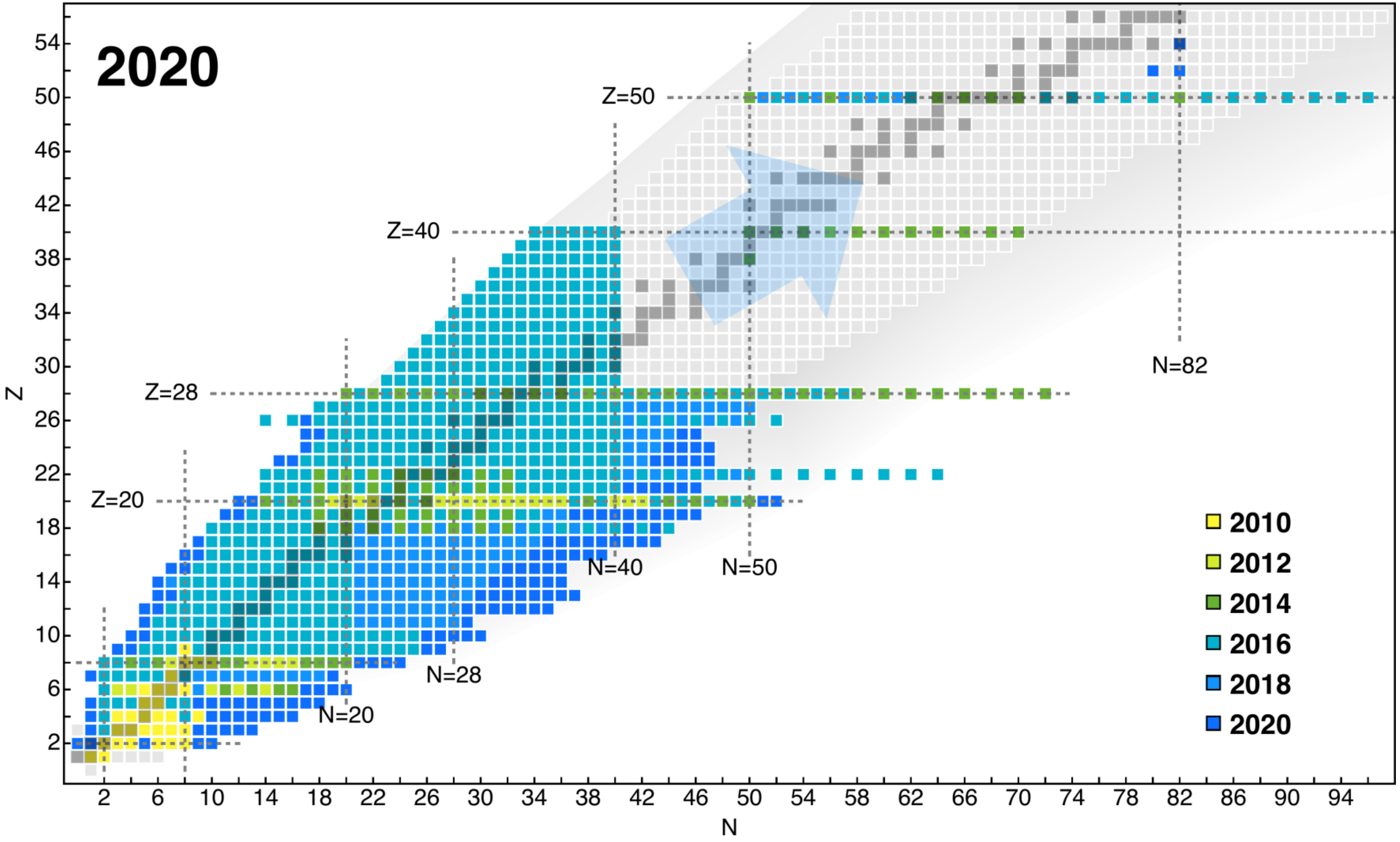
EXCELENCIA MARÍA DE MAEZTU 2020-2023

UNIVERSITAT DE BARCELONA

Ab Initio Nuclear Structure with Machine Learning

Javi Rozalén Sarmiento

Ab Initio Nuclear Structure

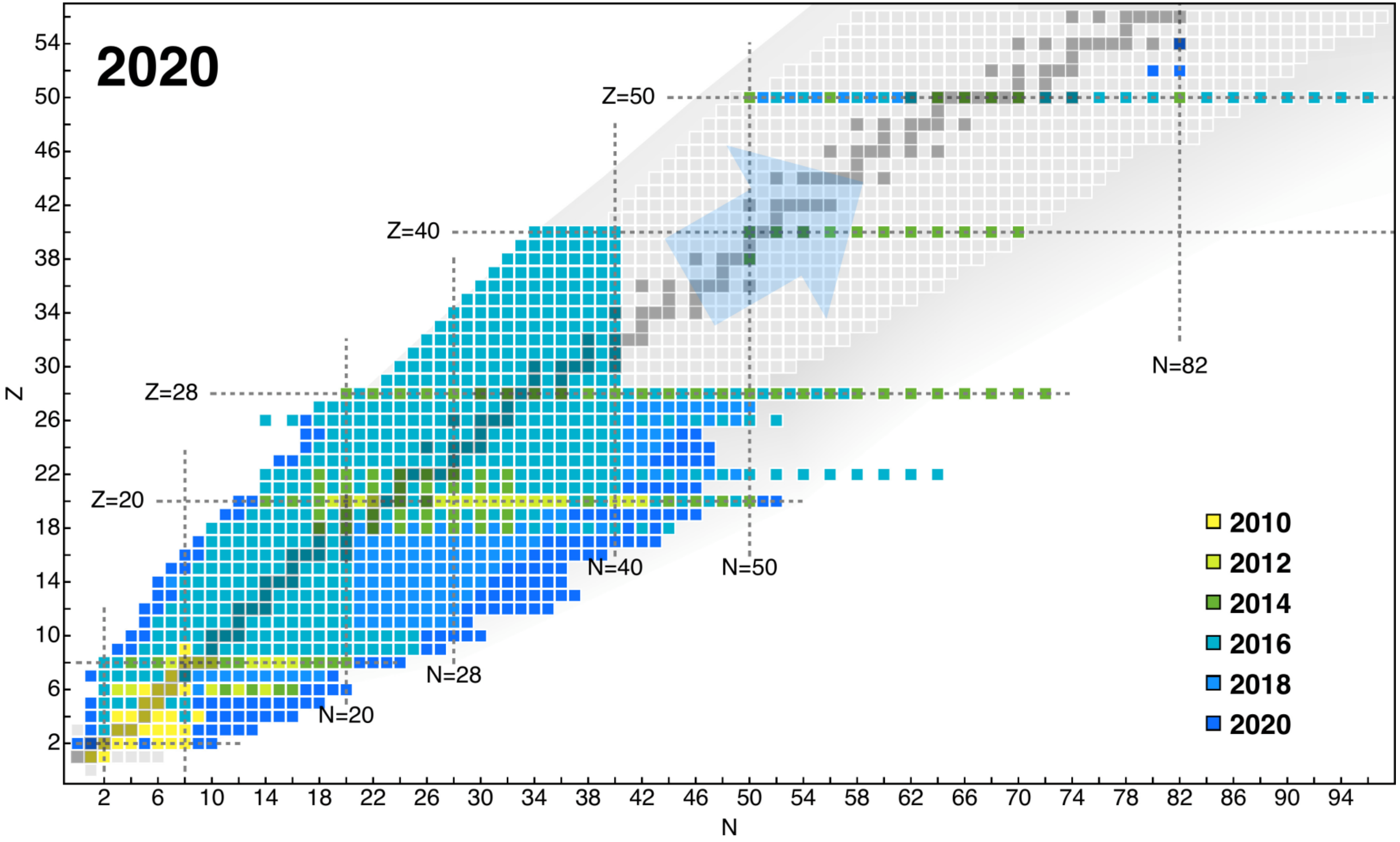


[1]

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

Ab Initio Nuclear Structure

IT-NCSM



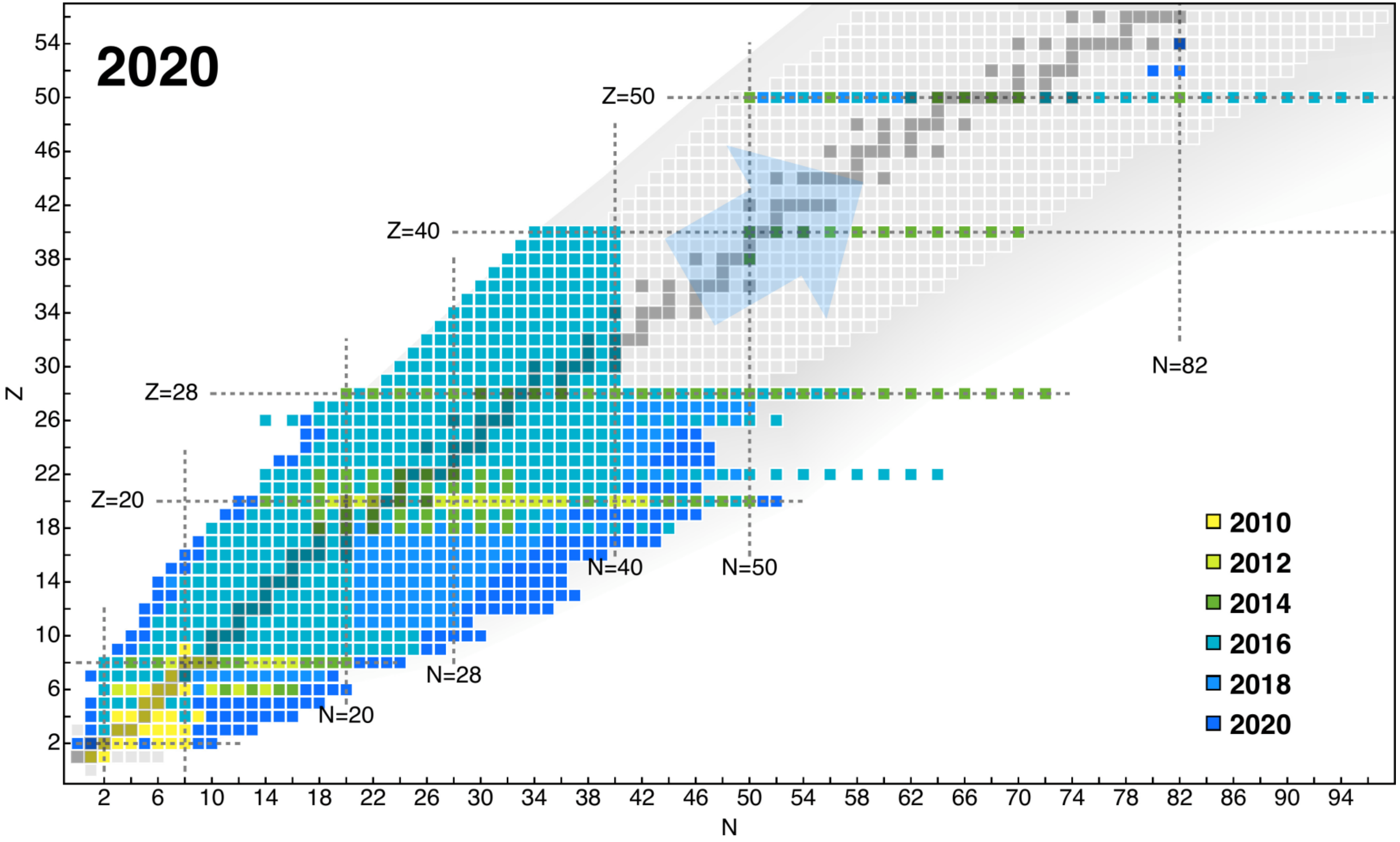
[1]

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

Ab Initio Nuclear Structure

IT-NCSM

MR-IMSRG



[1]

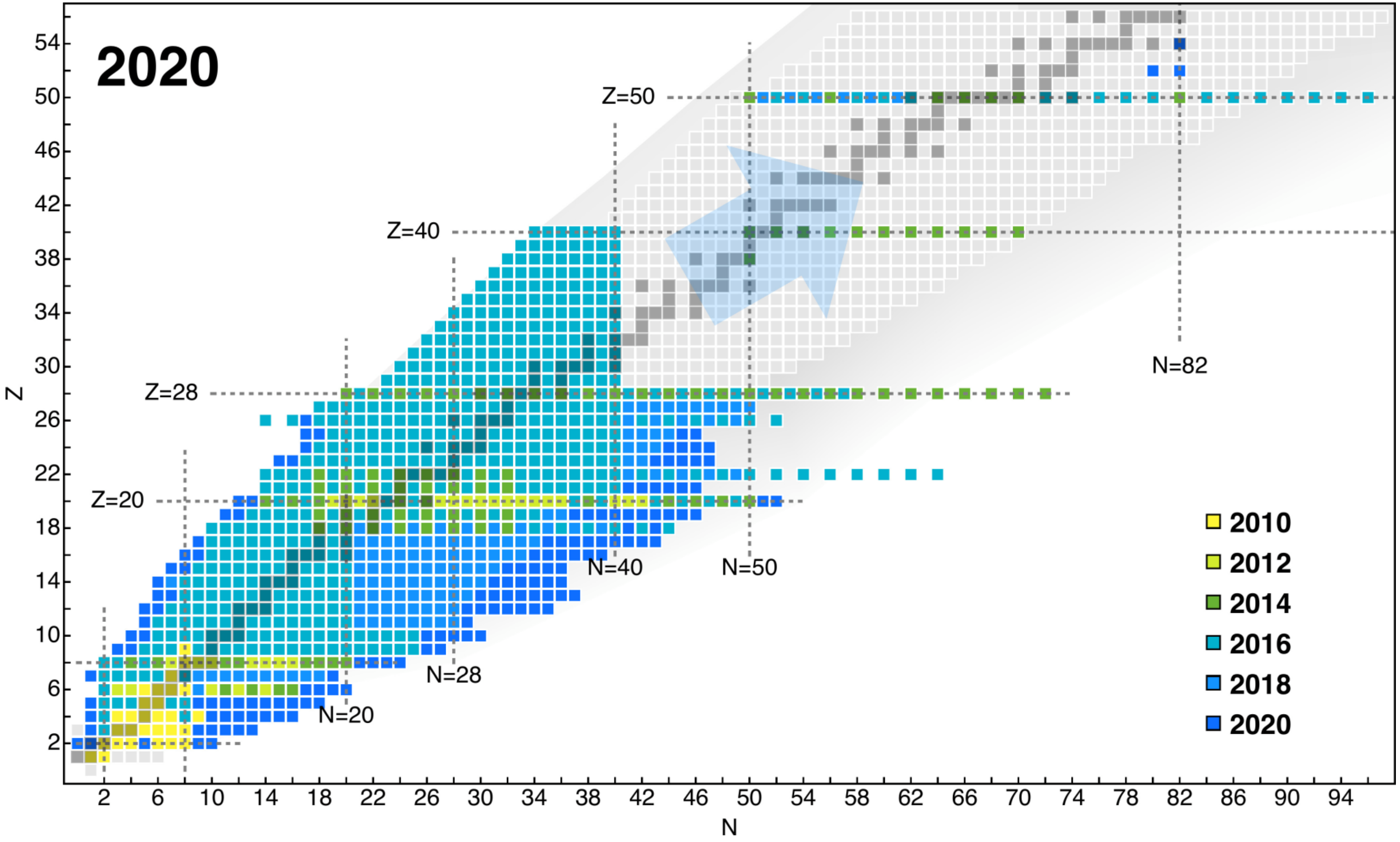
[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

Ab Initio Nuclear Structure

IT-NCSM

MR-IMSRG

VS-IMSRG



[1]

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

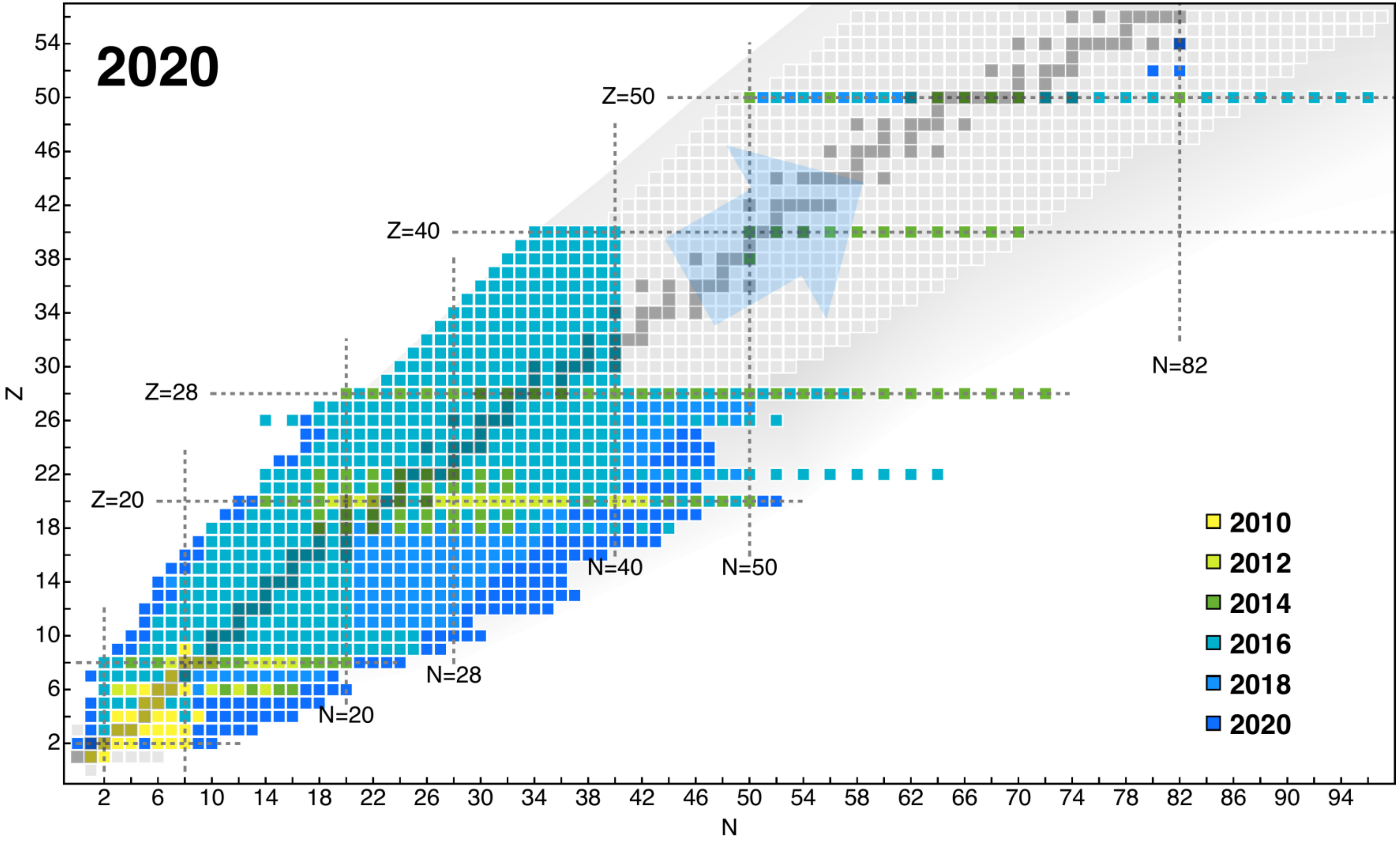
Ab Initio Nuclear Structure

IT-NCSM

MR-IMSRG

VS-IMSRG

ADC



[1]

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

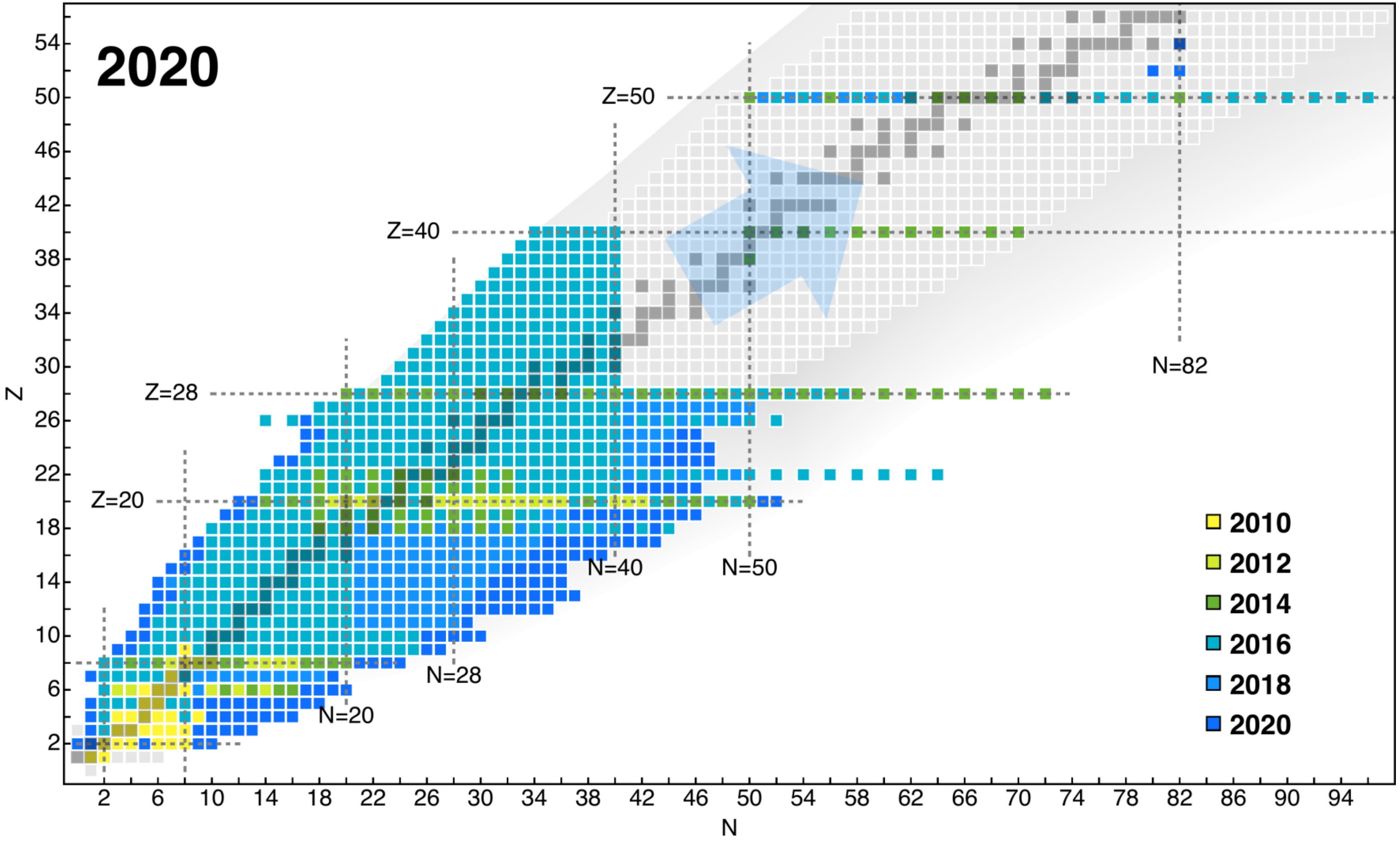
Ab Initio Nuclear Structure

IT-NCSM

MR-IMSRG

VS-IMSRG

ADC



Lattice EFT

[1]

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

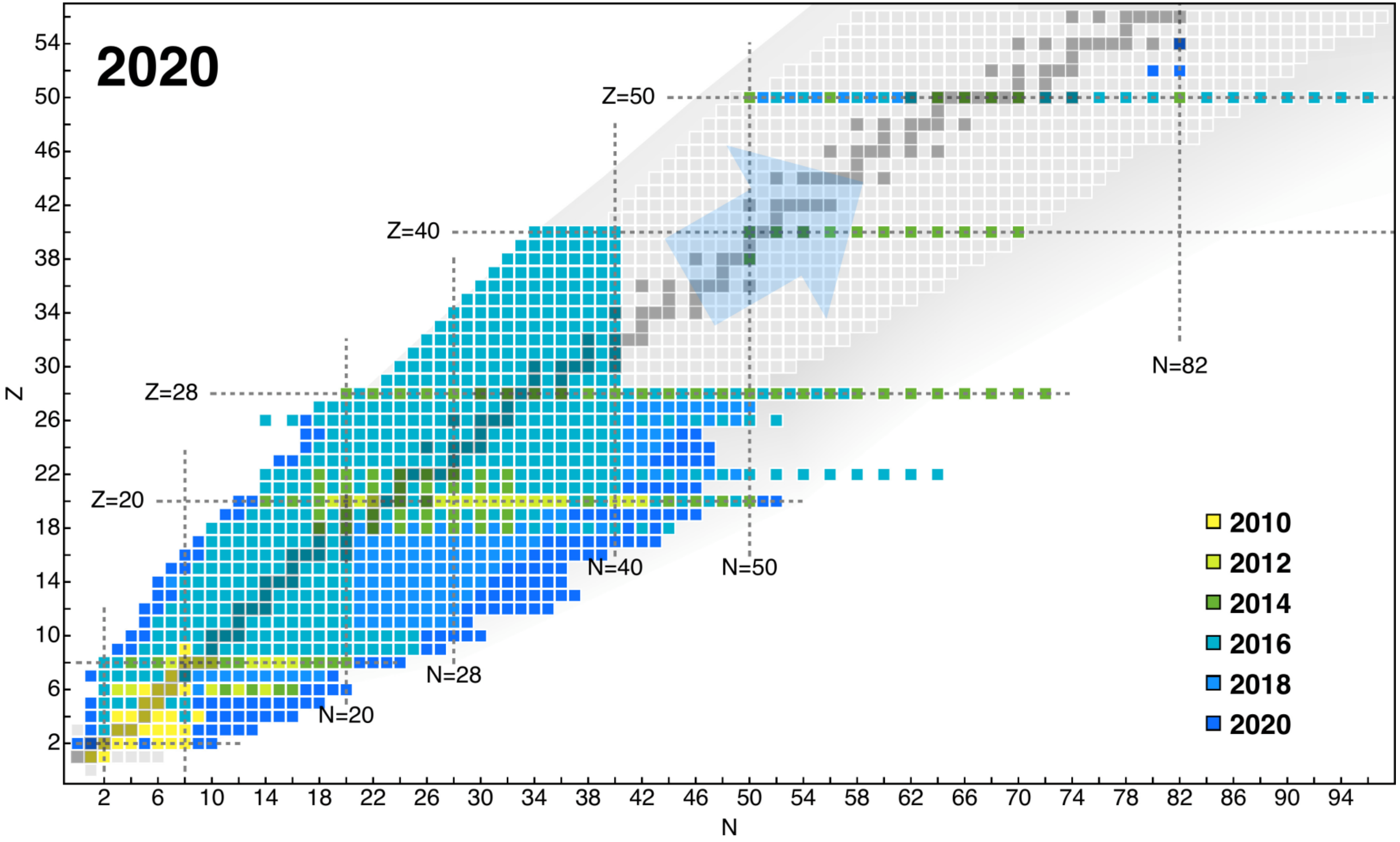
Ab Initio Nuclear Structure

IT-NCSM

MR-IMSRG

VS-IMSRG

ADC



Lattice EFT

CCSD

[1]

---

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory*, 2020

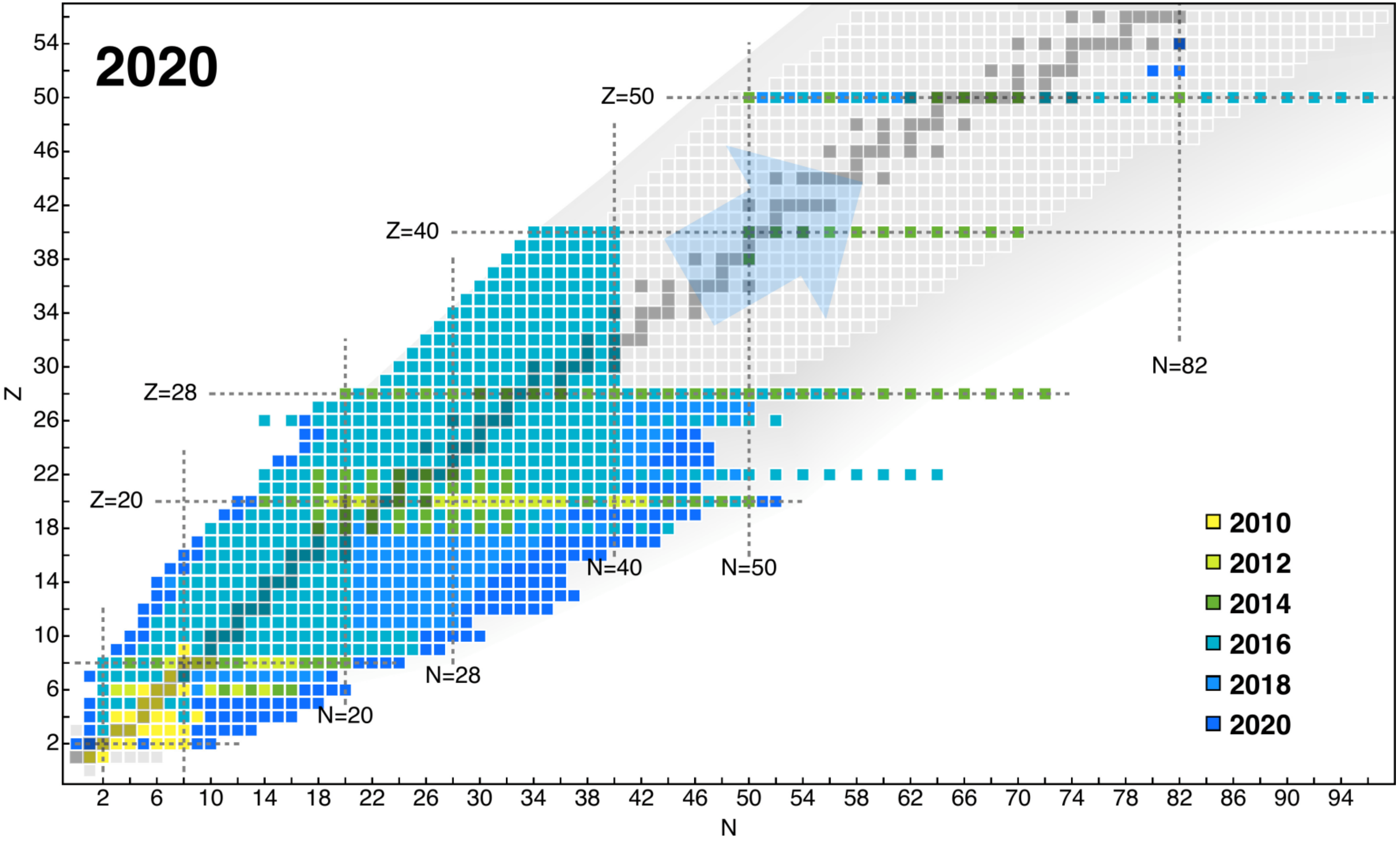
Ab Initio Nuclear Structure

IT-NCSM

MR-IMSRG

VS-IMSRG

ADC



[1]

Lattice EFT

CCSD

Λ-CCSD

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

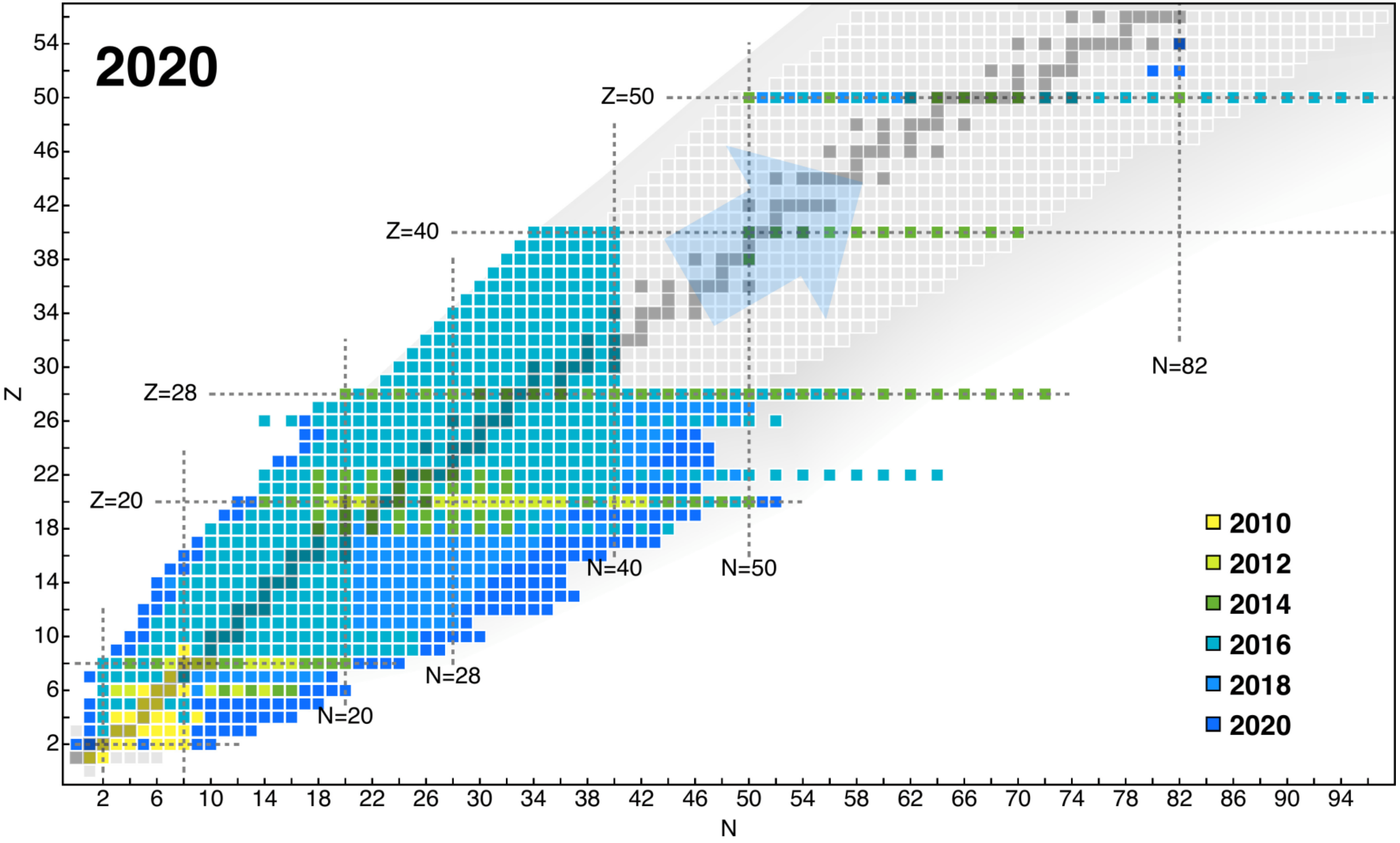
Ab Initio Nuclear Structure

IT-NCSM

MR-IMSRG

VS-IMSRG

ADC



Lattice EFT

CCSD

Λ-CCSD

NQS

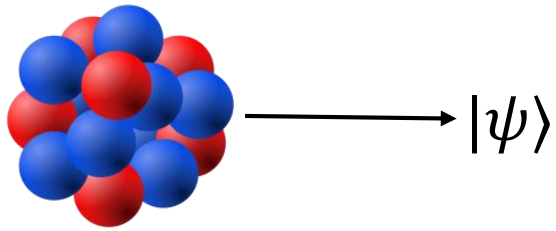
[1]

---

[1] H. Hergert, *A Guided Tour of ab initio Nuclear Many-Body Theory,* 2020

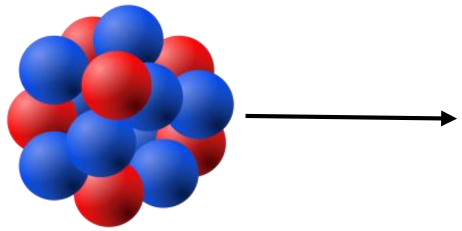
The Quantum Many-Body Problem: NQS

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



The Quantum Many-Body Problem: NQS

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



$|\psi\rangle$

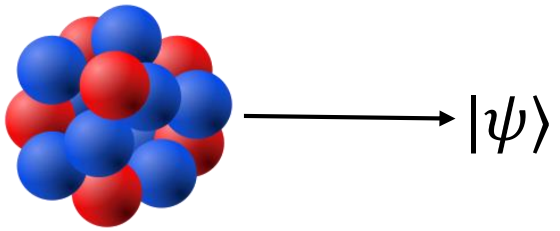
- **How?** Rayleigh-Ritz variational principle

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

$$|\psi_\theta\rangle = \int |p\rangle\, \psi_\theta(\boldsymbol{p}_1, \boldsymbol{p}_2, \ldots, \boldsymbol{p}_N)\mathrm{d}^{3\mathrm{N}}\mathrm{p}$$

The Quantum Many-Body Problem: NQS

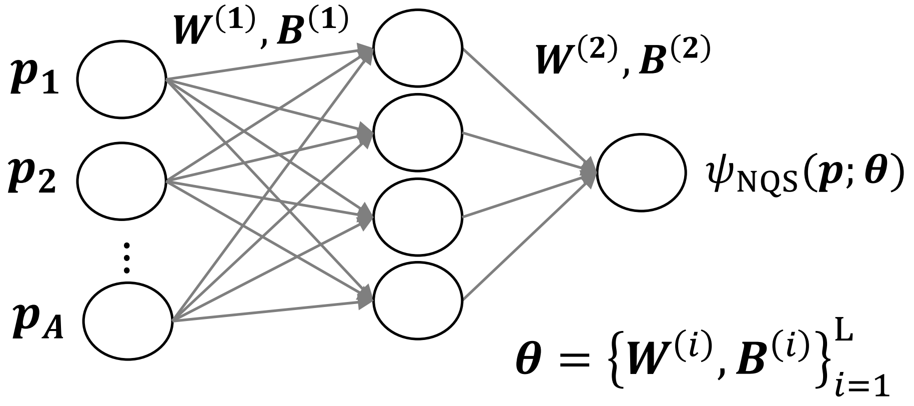
- **Goal**: Solve for the wave function of an atomic nucleus, ψ



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

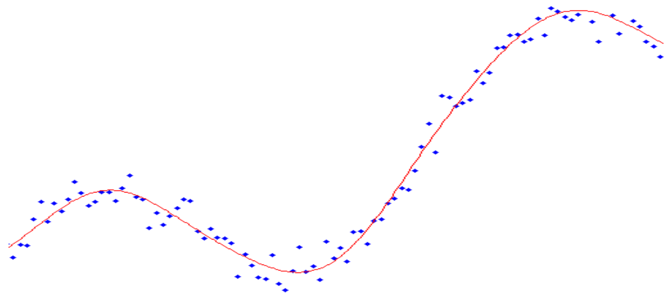
$$\frac{\langle\psi_\theta|\widehat{H}|\psi_\theta\rangle}{\langle\psi_\theta|\psi_\theta\rangle} \geq E_{\mathrm{GS}} \qquad |\psi_\theta\rangle = \int |p\rangle\, \psi_\theta(\boldsymbol{p_1}, \boldsymbol{p_2}, \ldots, \boldsymbol{p_N})\mathrm{d}^{3\mathrm{N}}\mathrm{p}$$

- **NQS Ansatz:** $\psi_{\mathrm{NQS}}(\boldsymbol{p_1}, \boldsymbol{p_2}, \ldots, \boldsymbol{p_A}; \boldsymbol{\theta})$



Why Neural Networks?

- **NNs have "∞ power"**: a neural network can approximate any continuous function [2], [3].

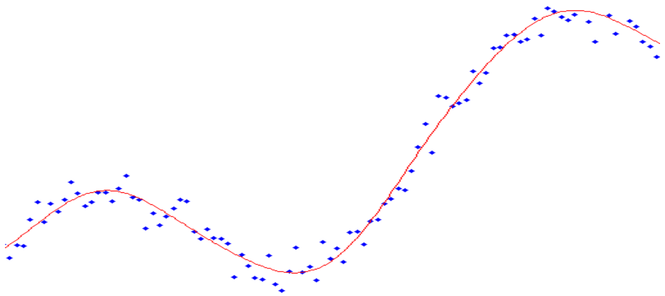


[2] G. Cybenko, *Approximation by superpositions of a sigmoidal function,* 1989

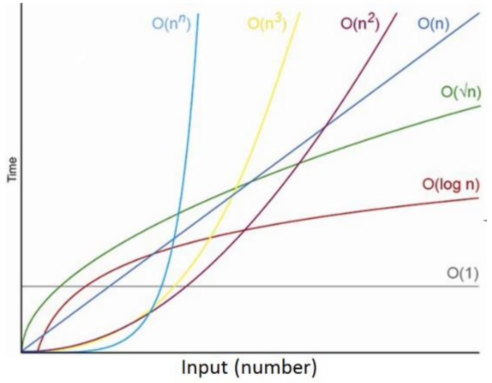
[3] K. Hornik M. Stinchcombe, H. White, *Multilayer feedforward networks are universal approximators,* 1989

Why Neural Networks?

- **NNs have "∞ power"**: a neural network can approximate any continuous function [2], [3].



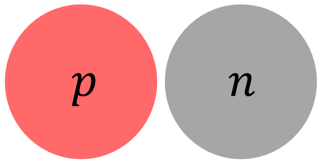
- **Space complexity:** polynomial scaling of memory resources… possibly!



[2] G. Cybenko, *Approximation by superpositions of a sigmoidal function,* 1989

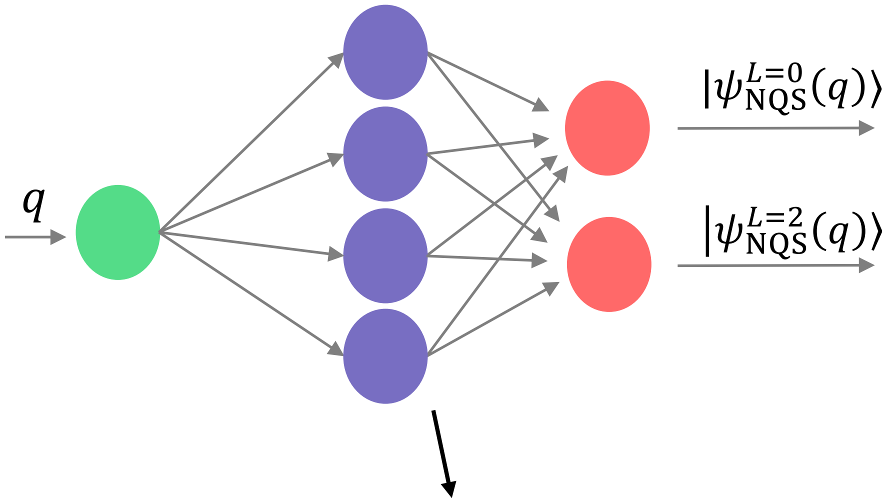
[3] K. Hornik M. Stinchcombe, H. White, *Multilayer feedforward networks are universal approximators,* 1989

Live Neural-Network Training



Deuteron

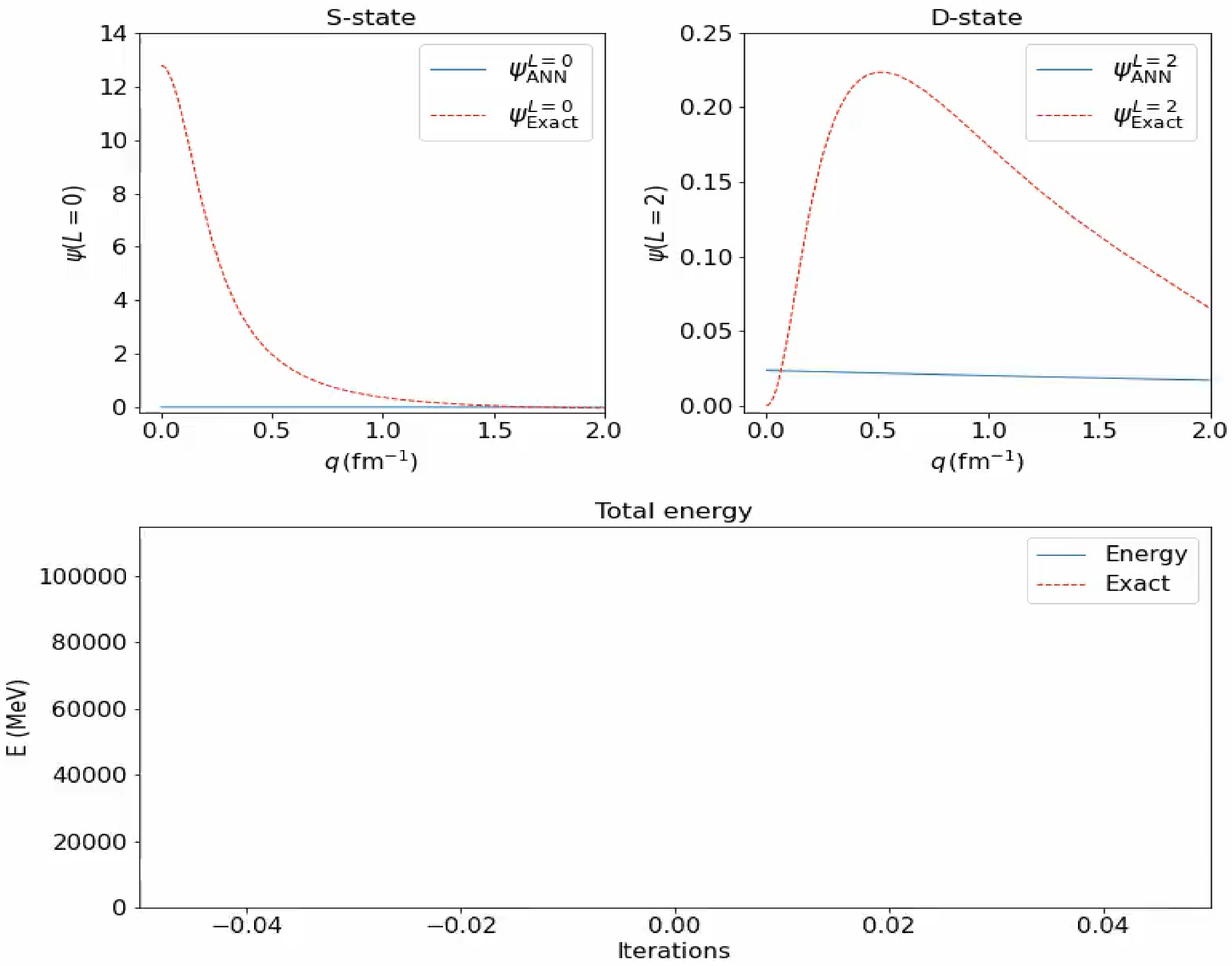
$\mathrm{N}^3\mathrm{LO}$ interaction

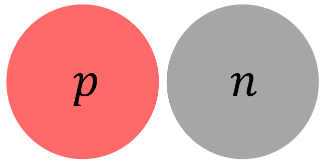


$N_{\mathrm{hid}} = 20$ neurons

J. Keeble & A. Rios, *Machine Learning the Deuteron, 2020*
J. Keeble & A. Rios & J. Rozalén Sarmiento, *2024*

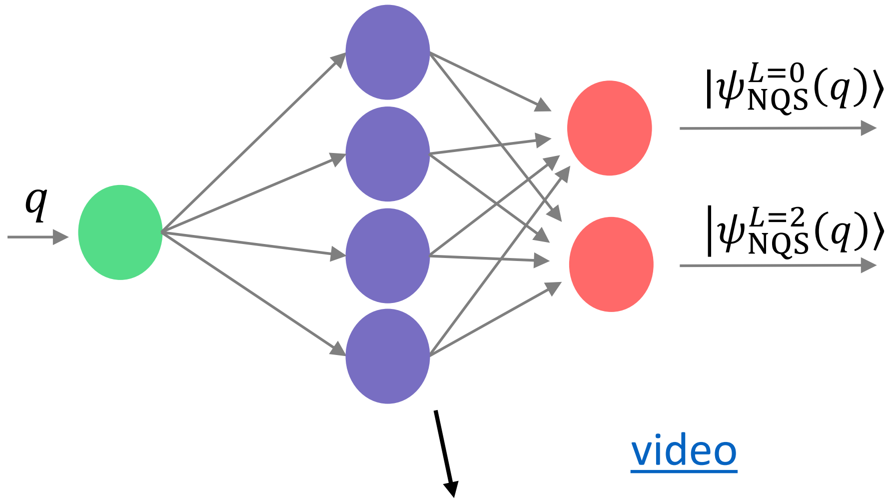
Live Neural-Network Training





Deuteron

$\mathrm{N^3LO}$ interaction

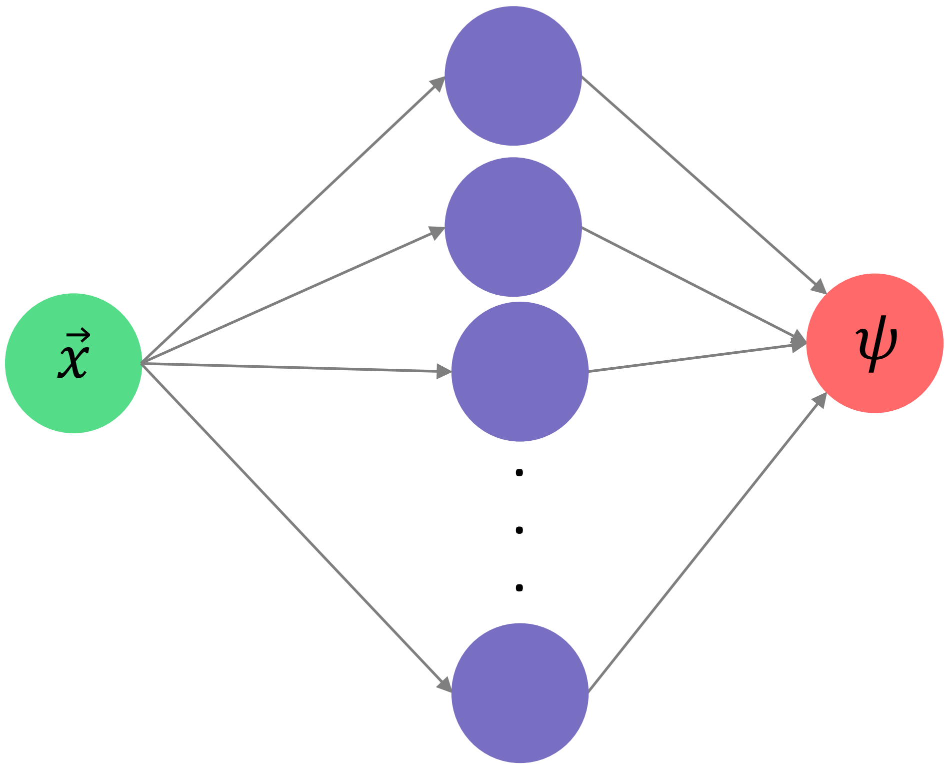


video

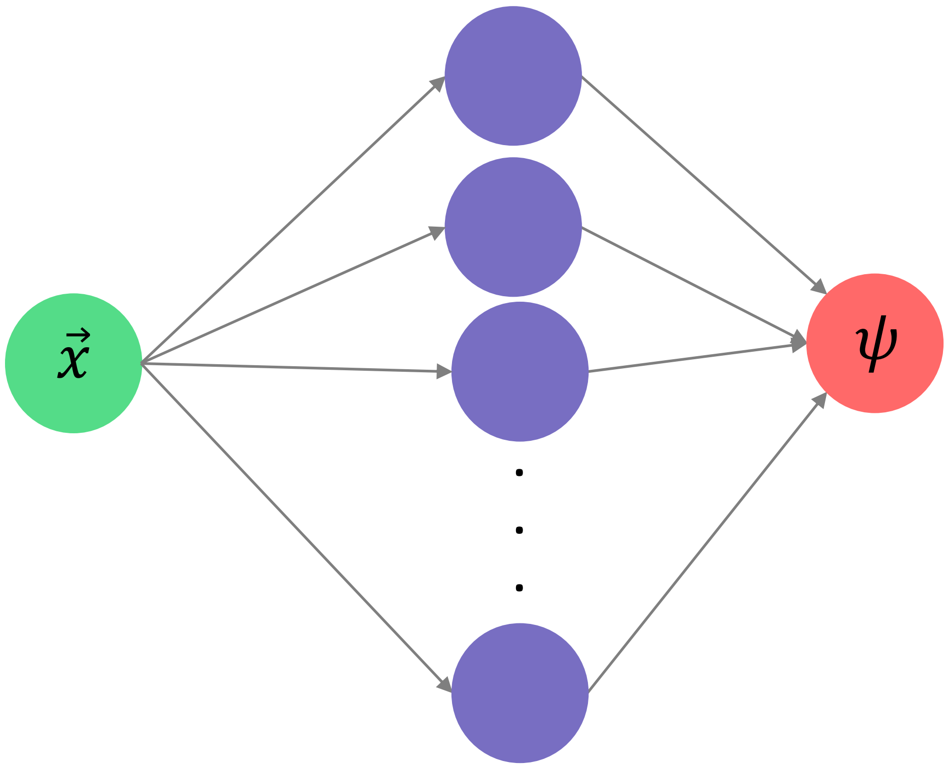
$N_{\rm hid} = 20$ neurons

J. Keeble & A. Rios, *Machine Learning the Deuteron, 2020*
J. Keeble & A. Rios & J. Rozalén Sarmiento, *2024*

Physical properties in NNs



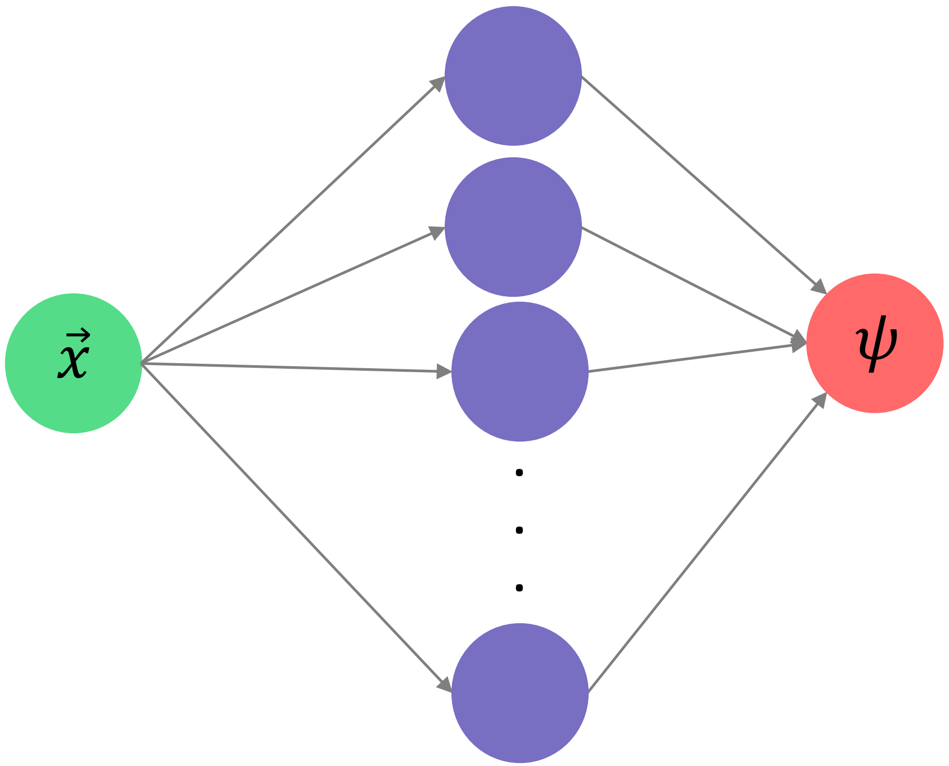
Physical properties in NNs



- **Particle exchange symmetry**

$$\psi(x_1, x_2, \dots, x_N) = \pm\psi(x_2, x_1, \dots, x_N)$$

Physical properties in NNs



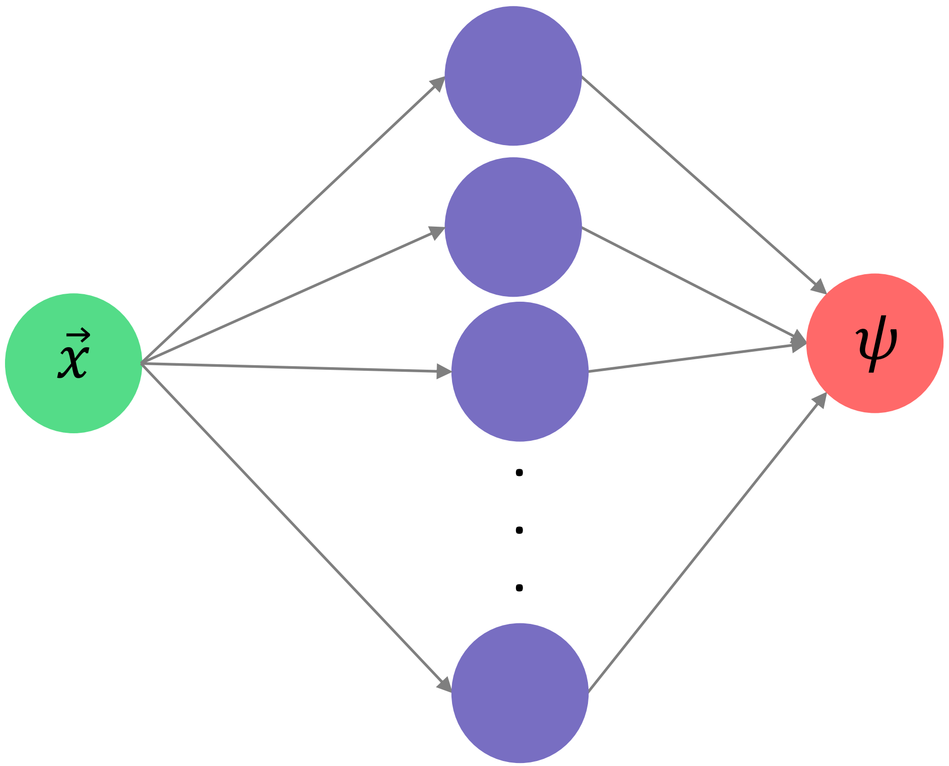
- **Particle exchange symmetry**

$$\psi(x_1, x_2, \dots, x_N) = \pm\psi(x_2, x_1, \dots, x_N)$$

- **Spherical symmetry**

$$\psi(\vec{x}) = \psi(R\vec{x})$$

Physical properties in NNs



- **Particle exchange symmetry**

$$\psi(x_1, x_2, \dots, x_N) = \pm\psi(x_2, x_1, \dots, x_N)$$

- **Spherical symmetry**

$$\psi(\vec{x}) = \psi(R\vec{x})$$

- **Time-reversal symmetry**

$$\psi(\vec{x}, \sigma) = \psi(T(\vec{x}, \sigma))$$

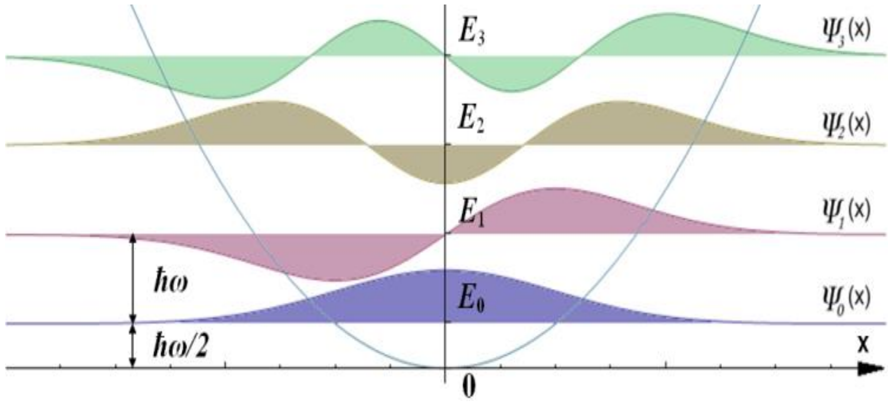
Symmetries in Quantum Mechanics

Symmetries in Quantum Mechanics

- **1D Harmonic Oscillator**

$$\hat{H} = \frac{1}{2}\nabla^2 + \frac{1}{2}mw^2x^2$$

$\Rightarrow [\hat{H}, \hat{P}] = 0$, $\hat{P}$ parity

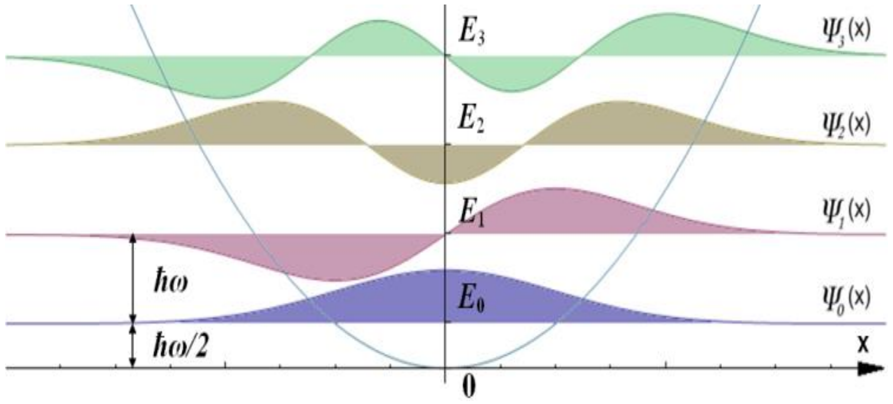


Symmetries in Quantum Mechanics

- **1D Harmonic Oscillator**

$$\hat{H} = \frac{1}{2}\nabla^2 + \frac{1}{2}mw^2x^2$$

$$\Rightarrow [\hat{H}, \hat{P}] = 0,\ \hat{P}\ \text{parity}$$



- **Hydrogen Atom (Coulomb)**

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}$$

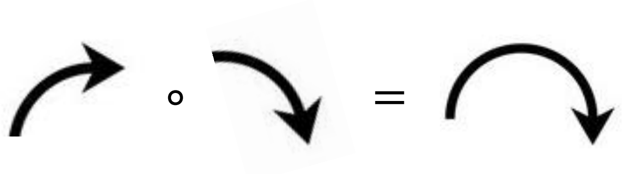
$$\Rightarrow [\hat{H}, \widehat{L^2}] = [\hat{H}, \widehat{L_z}] = 0$$

$$\psi_{nlm} \begin{cases} \psi_{100}(r,\theta,\phi) = \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} 2r\exp(-Zr/a_0) \times \sqrt{\frac{1}{4\pi}} \\ \psi_{110}(r,\theta,\phi) = \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} 2r\exp(-Zr/a_0) \times \sqrt{\frac{3}{4\pi}} \cos\theta \end{cases}$$

Group theory (in a nutshell)

- **Group**

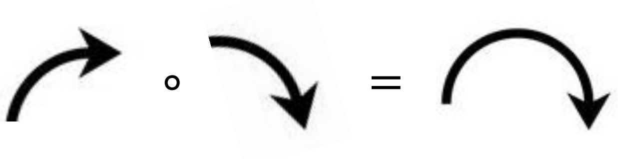
$$G = \{g \mid g_1, g_2 \in G \Rightarrow g_1 \cdot g_2 = g_3 \in G\}$$



Group theory (in a nutshell)

- **Group**

$$G = \{g \mid g_1, g_2 \in G \Rightarrow g_1 \cdot g_2 = g_3 \in G\}$$



- **Linear Representation**

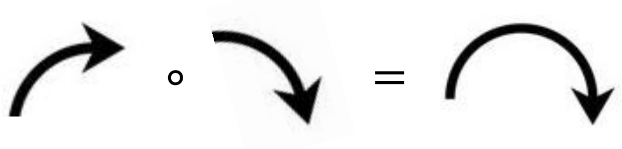
$$r \in \mathrm{SO}(2) \rightarrow D(r_\theta) = \begin{pmatrix} \sin\theta & \cos\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$r_\theta \circ r_\varphi = r_{\theta+\varphi} \Rightarrow D(r_\theta)D(r_\varphi) = D(r_{\theta+\varphi})$$

Group theory (in a nutshell)

- **Group**

$$G = \{g \mid g_1, g_2 \in G \Rightarrow g_1 \cdot g_2 = g_3 \in G\}$$



- **Irreducible Representation (irrep)**

$$D(g) = d_1(g) \oplus d_2(g) \oplus \cdots \oplus d_n(g)$$

$$= \begin{pmatrix} d_1(g) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & d_n(g) \end{pmatrix}$$

$$D(r_\theta) = \begin{pmatrix} \sin\theta & \cos\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \rightarrow \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix}$$

- **Linear Representation**

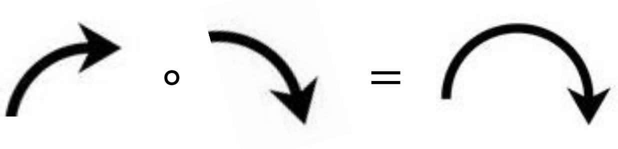
$$r \in \mathrm{SO}(2) \rightarrow D(r_\theta) = \begin{pmatrix} \sin\theta & \cos\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$r_\theta \circ r_\varphi = r_{\theta+\varphi} \Rightarrow D(r_\theta)D(r_\varphi) = D(r_{\theta+\varphi})$$

Group theory (in a nutshell)

- **Group**

$$G = \{g \mid g_1, g_2 \in G \Rightarrow g_1 \cdot g_2 = g_3 \in G\}$$



- **Linear Representation**

$$r \in \mathrm{SO}(2) \rightarrow D(r_\theta) = \begin{pmatrix} \sin\theta & \cos\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$r_\theta \circ r_\varphi = r_{\theta+\varphi} \Rightarrow D(r_\theta)D(r_\varphi) = D(r_{\theta+\varphi})$$

- **Irreducible Representation (irrep)**

$$D(g) = d_1(g) \oplus d_2(g) \oplus \cdots \oplus d_n(g)$$

$$= \begin{pmatrix} d_1(g) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & d_n(g) \end{pmatrix}$$

$$D(r_\theta) = \begin{pmatrix} \sin\theta & \cos\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \rightarrow \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix}$$

- **Schur's Lemma**

$d_1(g)$ irrep, H operator, $\quad d_1(g)H = Hd_1(g)$

$\Rightarrow H = EI, E$ number $\quad H = \begin{pmatrix} E_1 I & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & E_n I \end{pmatrix}$

Convolution is all you need

- **Group Equivariance**

ψ is **equivariant / covariant** under G if:

$$\psi(D(g)x) = D'(g)\psi(x)$$

Convolution is all you need

- **Group Equivariance**

ψ is **equivariant / covariant** under G if:

$$\psi(D(g)x) = D'(g)\psi(x)$$

- **Group convolution**

$$(\psi * \chi)(g) = \sum_{u \in G} \psi(D(u^{-1})g)\chi(u)$$

Convolution is all you need

- **Group Equivariance**

ψ is **equivariant / covariant** under G if:

$$\psi(D(g)x) = D'(g)\psi(x)$$

$\Longleftrightarrow$ [4, 5, 6]

- **Group convolution**

$$(\psi * \chi)(g) = \sum_{u \in G} \psi(D(u^{-1})g)\chi(u)$$

[4] T S Cohen and M Welling, *Group Equivariant Convolutional Networks (2016)*

[5] T S Cohen and M Welling, *Steerable CNNs (2016)*

[6] R Kondor and S Trivedi, *On the Generalization of Equivariance and Convolution in Neural Networks to the Action of Compact Groups (2018)*

Convolution is all you need

- **Group Equivariance**

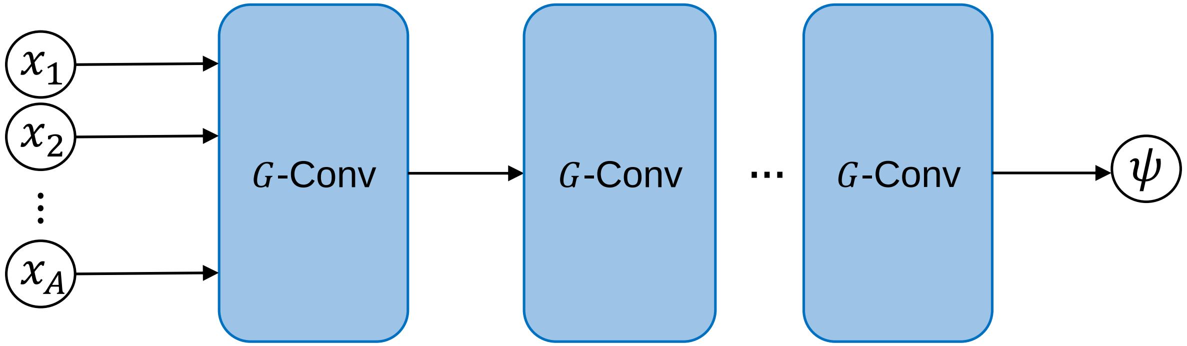
ψ is **equivariant / covariant** under G if:

$$\psi(D(g)x) = D'(g)\psi(x)$$

$\Longleftrightarrow$ [4, 5, 6]

- **Group convolution**

$$(\psi * \chi)(g) = \sum_{u \in G} \psi(D(u^{-1})g)\chi(u)$$



[4] T S Cohen and M Welling, *Group Equivariant Convolutional Networks (2016)*

[5] T S Cohen and M Welling, *Steerable CNNs (2016)*

[6] R Kondor and S Trivedi, *On the Generalization of Equivariance and Convolution in Neural Networks to the Action of Compact Groups (2018)*

Re-thinking previous work...

Parity, $\mathbb{Z}/2\mathbb{Z} = \{e, a\}$

- **Intuition**

$$\psi_{\text{NQS}}(x) \coloneqq \psi_{\text{NN}}(x) \pm \psi_{\text{NN}}(-x)$$

- **Group convolution**

Irreps of $\mathbb{Z}/2\mathbb{Z}$:

$D^t(e) = (1), \quad D^t(a) = (1)$ (Trivial rep)

$D^s(e) = (1), \quad D^s(a) = (-1)$ (Sign rep)

$$\begin{cases} \psi_+(x) \coloneqq \psi(x) + \psi(-x) \\ \psi_-(x) \coloneqq \psi(x) - \psi(-x) \end{cases}$$

Fermionic particle exchange, S_N

- **Intuition**

$$\psi_{\text{NQS}}(x_1, x_2, x_3) = \begin{vmatrix} \psi_1(x_1) & \psi_2(x_1) & \psi_3(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \psi_3(x_2) \\ \psi_1(x_3) & \psi_2(x_3) & \psi_3(x_3) \end{vmatrix}$$

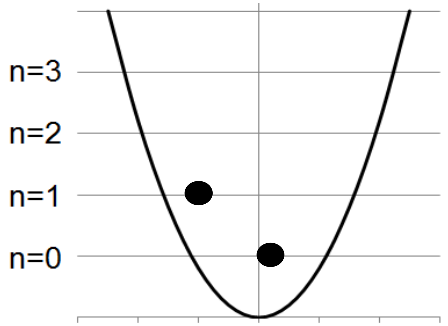
- **Group convolution**

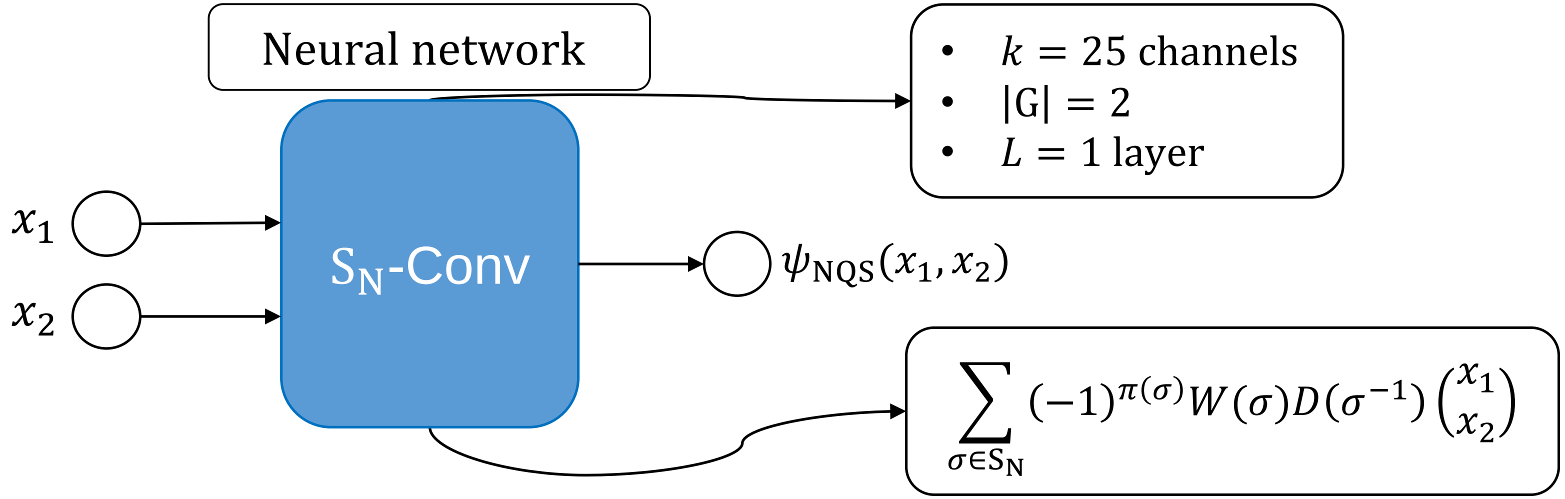
$$\psi_{\text{NQS}}(x_1, x_2, x_3) = \sum_{\sigma \in S_N} (-1)^{\pi(\sigma)} \sigma(\psi_1(x_1)\psi_2(x_2)\psi_3(x_3))$$

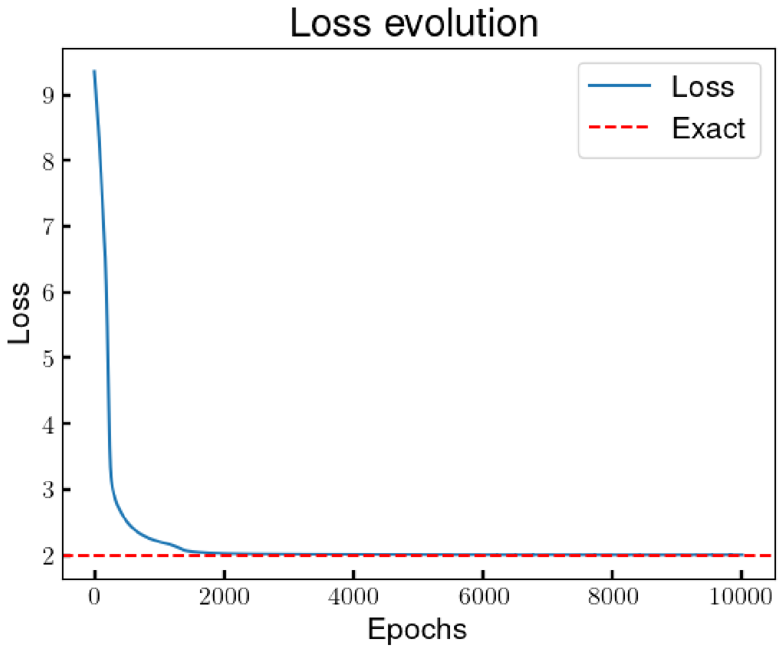
$\sigma \rightarrow$ "Alternating representation of S_N"

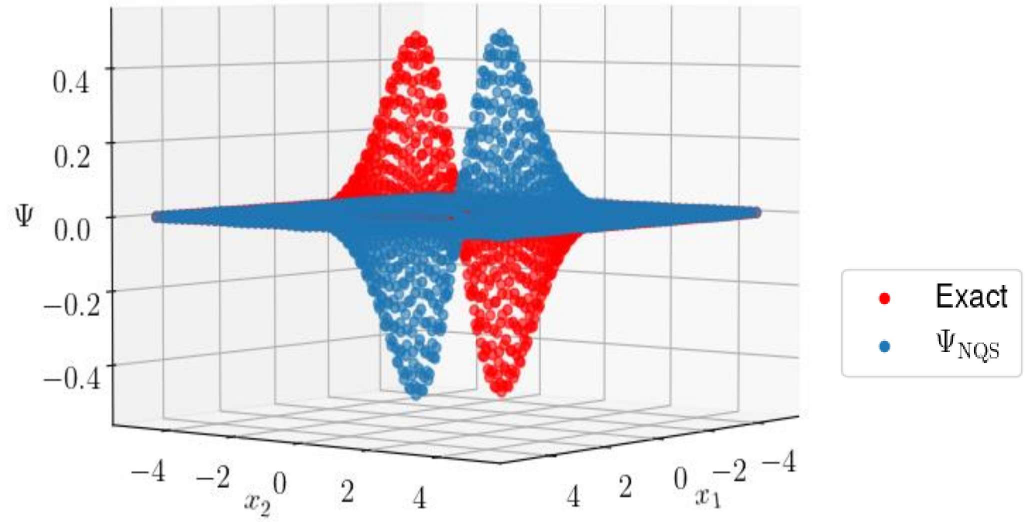
Toy exemple: $G = S_N$

$N = 2$ fermions, 1D HO



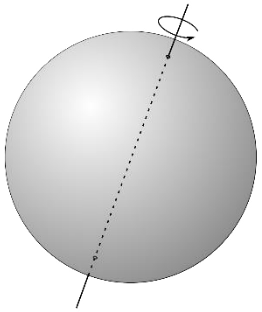




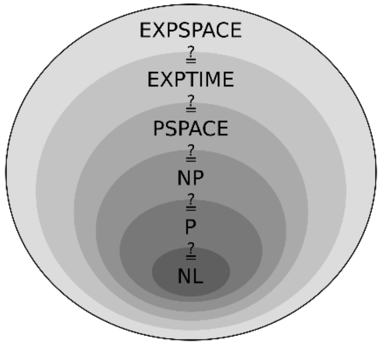


Conclusions and future outlook

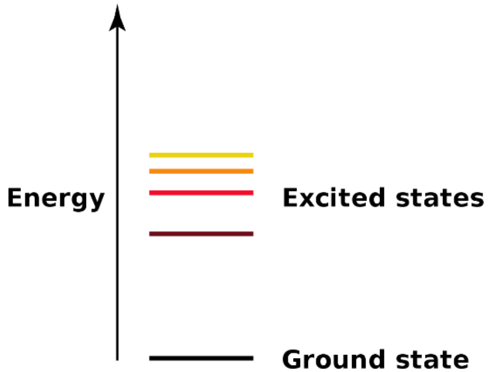
- What about continuous groups ($SU(2)$)?



- What is the computational cost?



- Compute whole nuclear spectrum “at once”



ICCUB Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA
EXCELENCIA MARÍA DE MAEZTU 2020-2023
UNIVERSITAT DE BARCELONA

Thank you