Learning the Ground State with Neural Quantum States

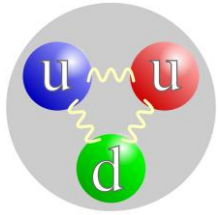
J. Rozalén Sarmiento, A. Rios

HadNucMat Workshop, 2025, Barcelona

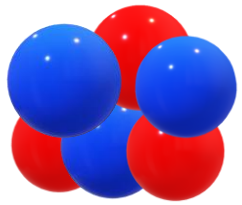
ICCUB | Institut de Ciències del Cosmos UNIVERSITAT DE BARCELONA
EXCELENCIA MARÍA DE MAEZTU 2020–2024
UNIVERSITAT DE BARCELONA

“Ab Initio” Nuclear Structure

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}_i \left(i\gamma^\mu (D_\mu)_{ij} - m\delta_{ij} \right) \psi_j - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a$$



$$\hat{H}_{\mathrm{nuc}} = \hat{T} + \hat{V}_{\mathrm{nuc}}$$



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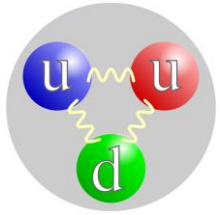

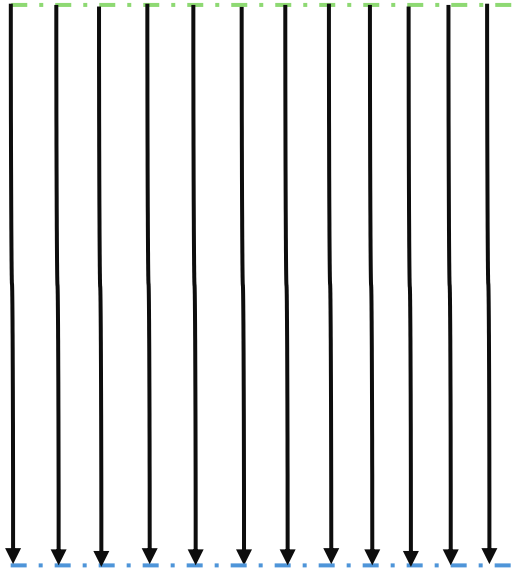

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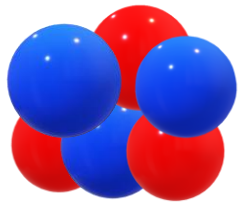

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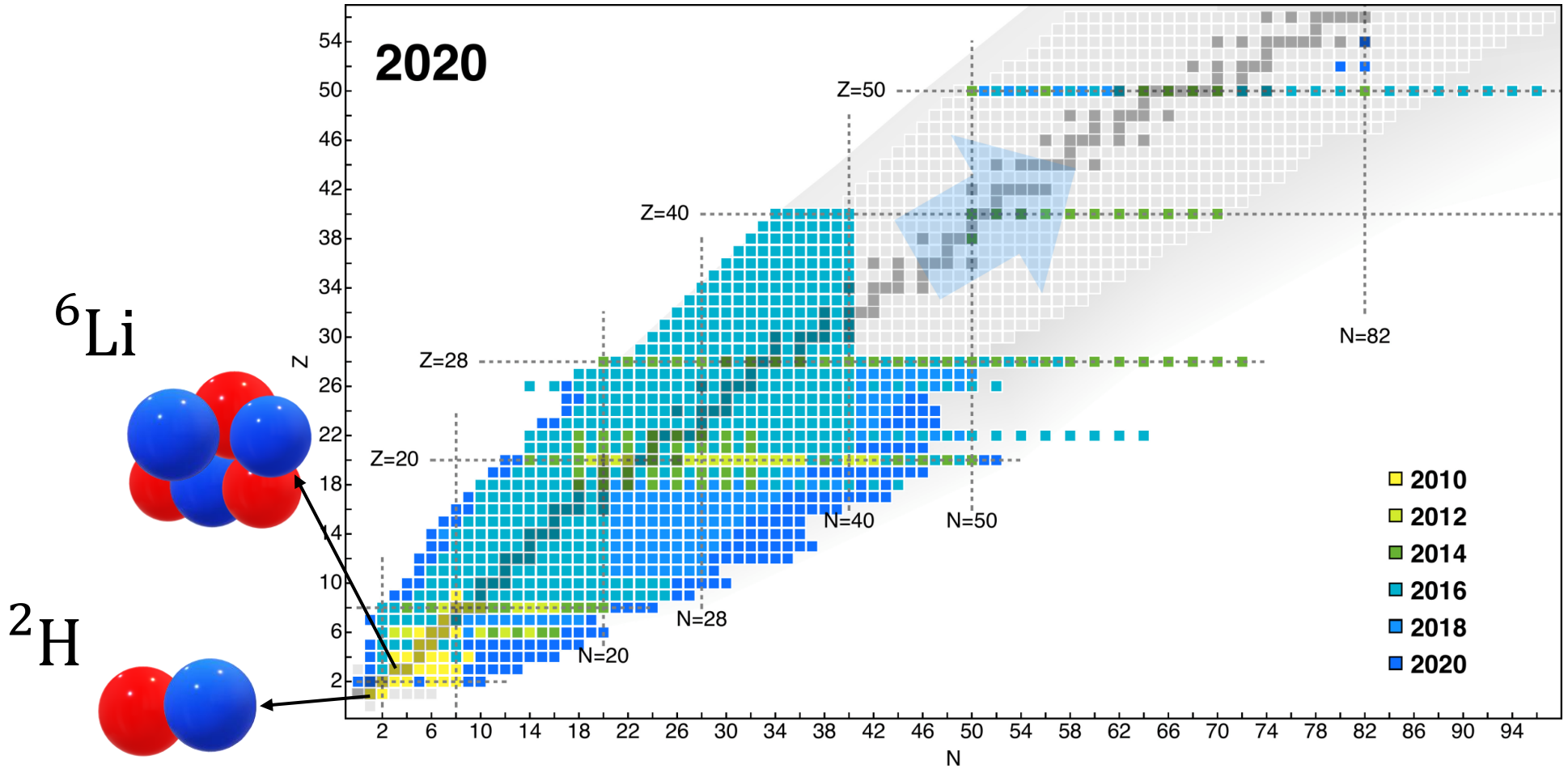
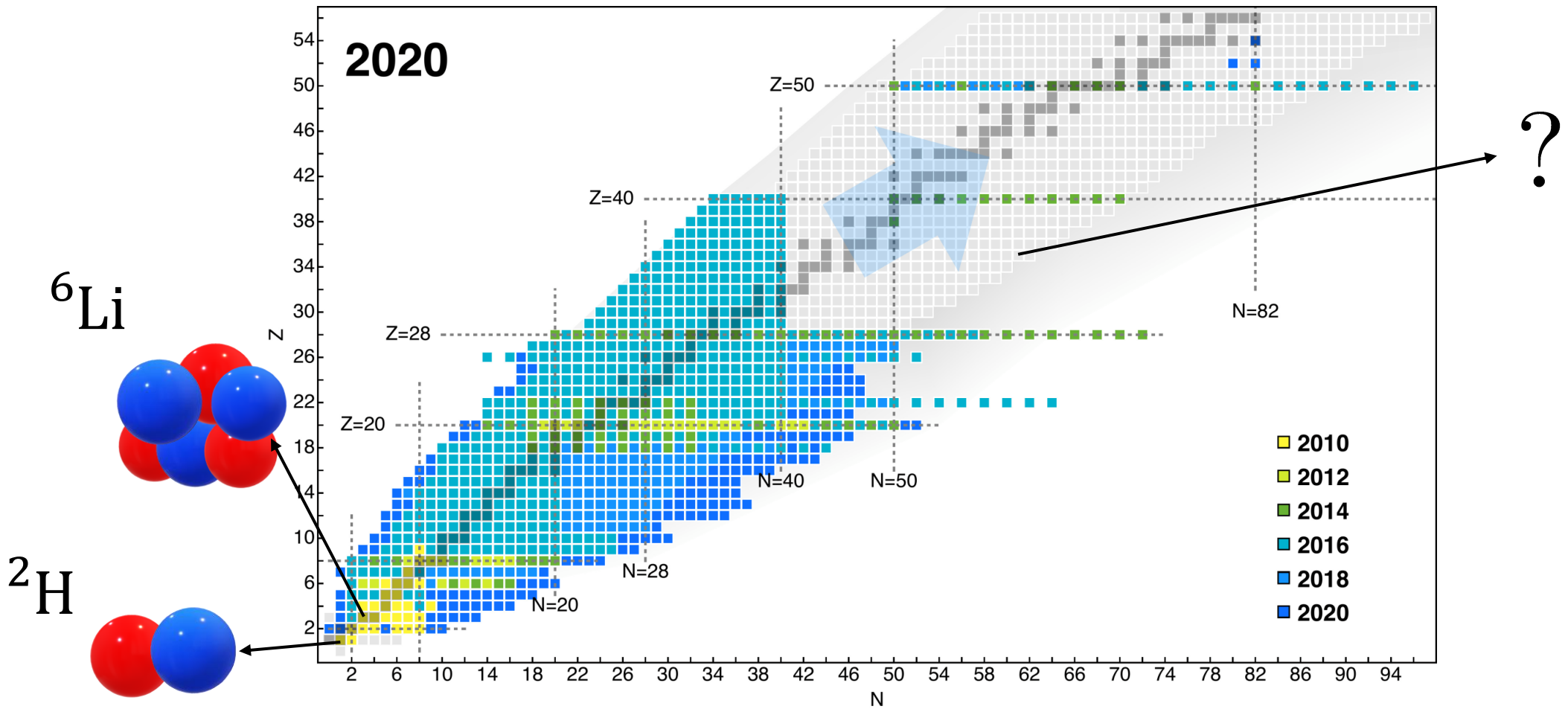


H. Hergert, Front. Phys. **07** (2020)

Ab Initio Nuclear Structure



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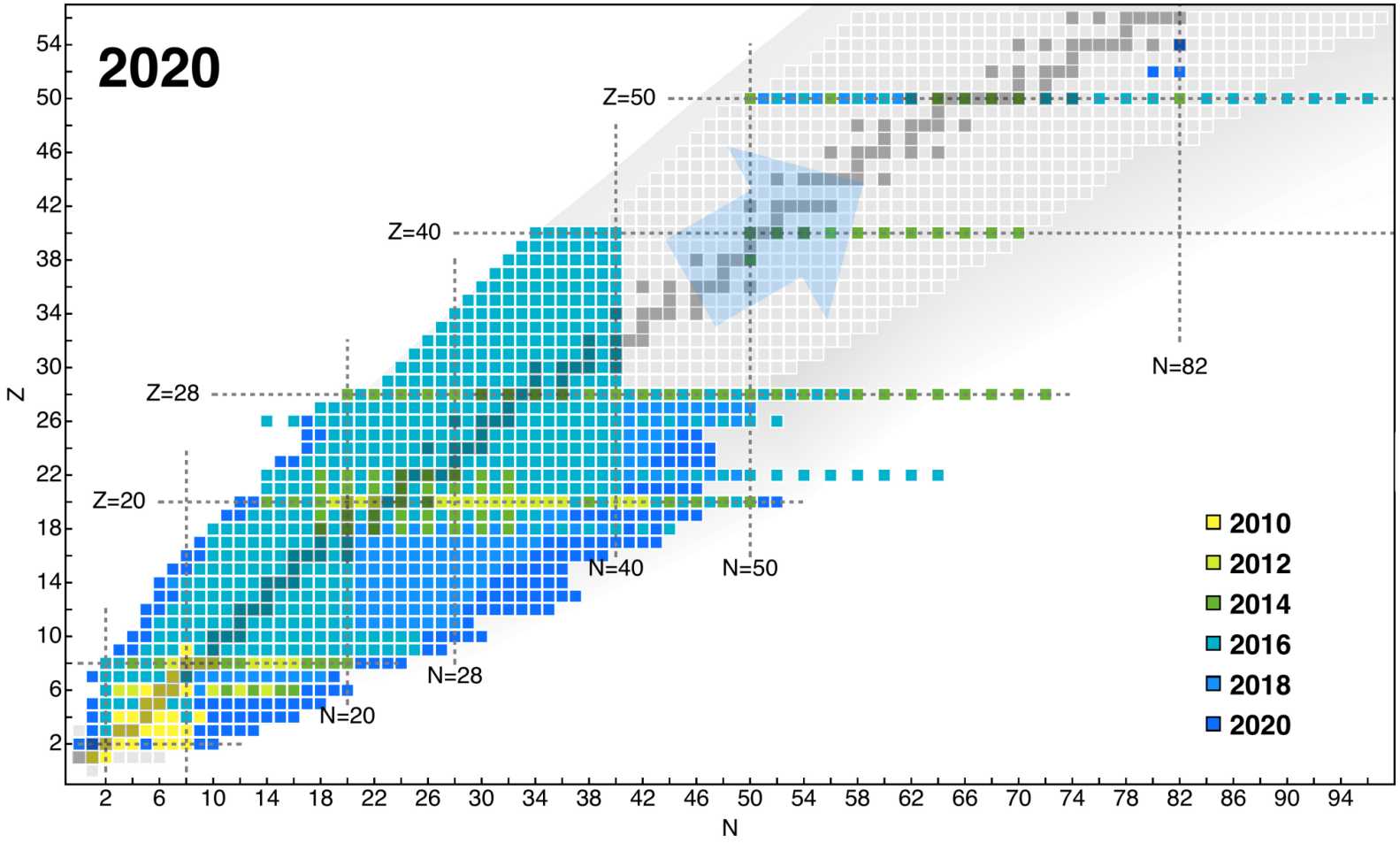
Ab Initio Nuclear Structure

- IT-NCSM
- MR-IMSRG
- VS-IMSRG
- ADC

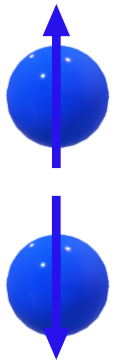


- Lattice EFT
- CCSD
- Λ-CCSD

H. Hergert, Front. Phys. **07** (2020)

Exponential Scaling Problem

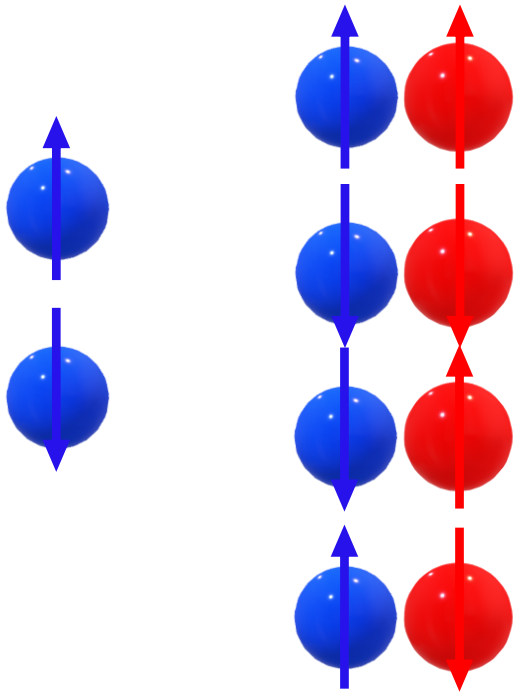
$\mathrm{N}=1$



$2^N=2$

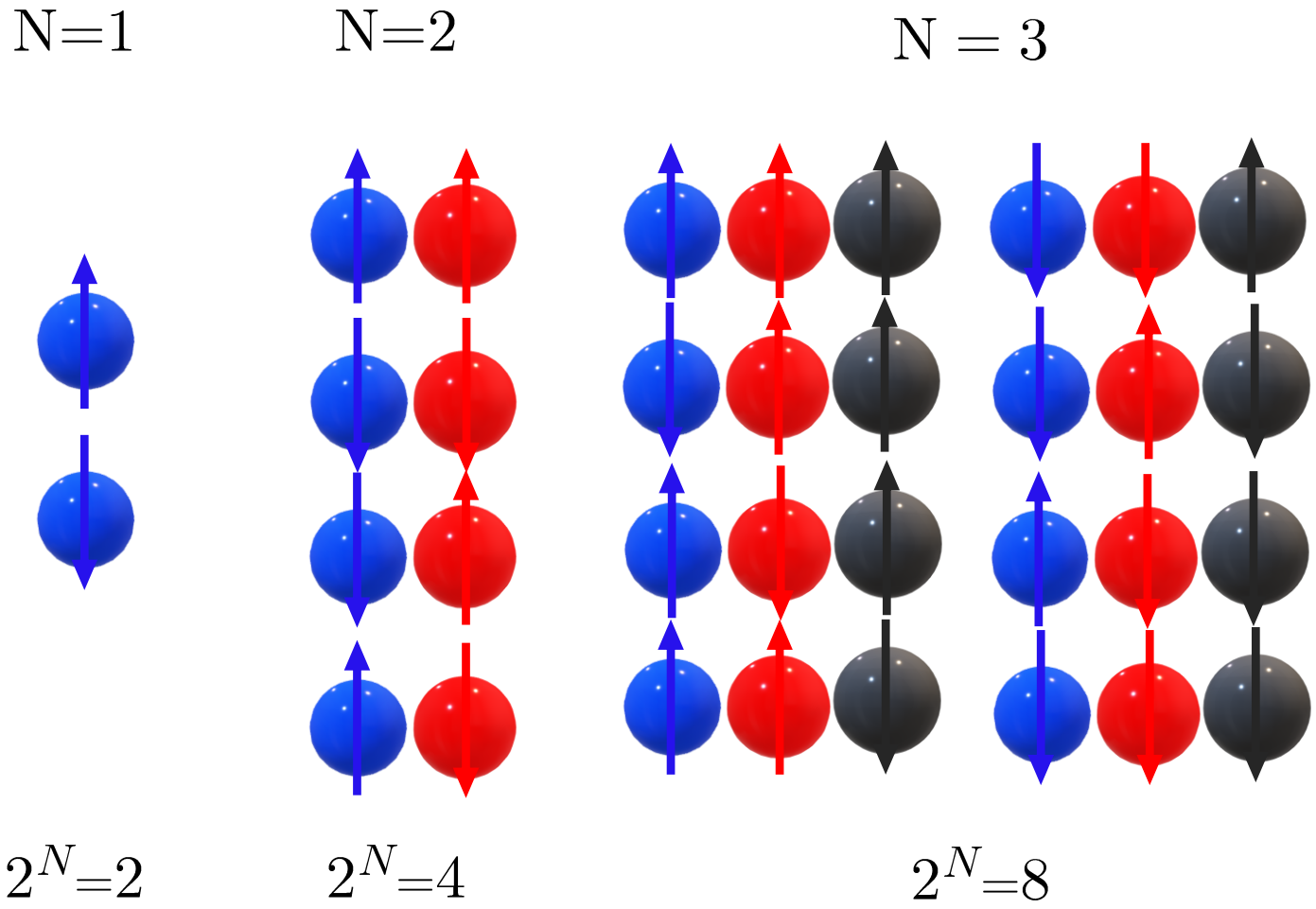
Exponential Scaling Problem

$N=1$ $N=2$



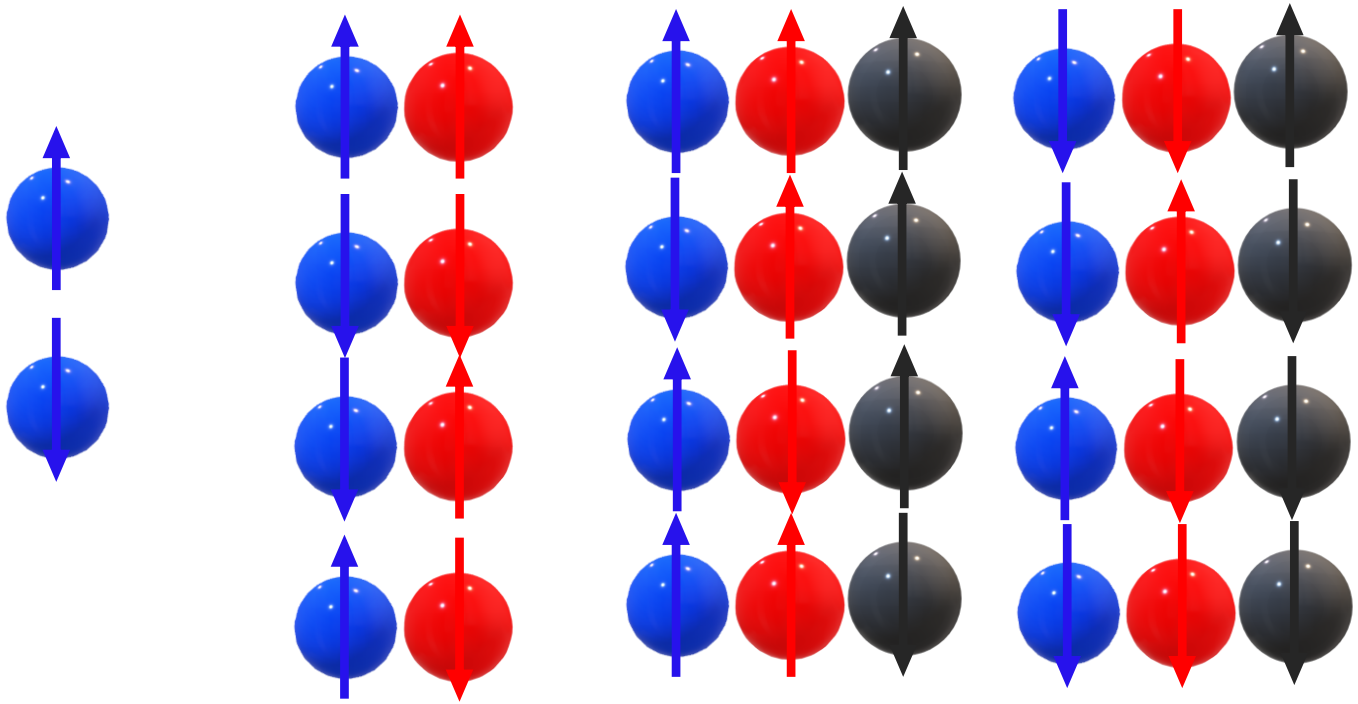
$2^N=2$ $2^N=4$

Exponential Scaling Problem



Exponential Scaling Problem

$N=1$ $N=2$ $N=3$ $N=80$ (Zr)

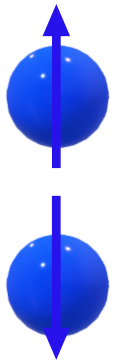


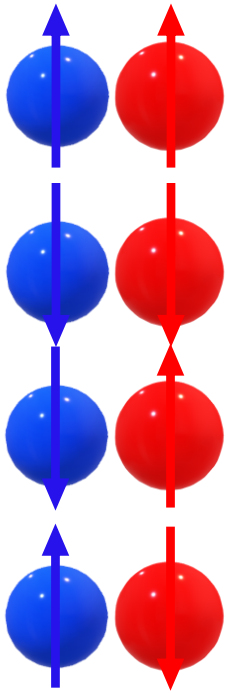
$2^N=2$ $2^N=4$ $2^N=8$ $2^N=1{,}208{,}925{,}819{,}614{,}629{,}174{,}706{,}176$

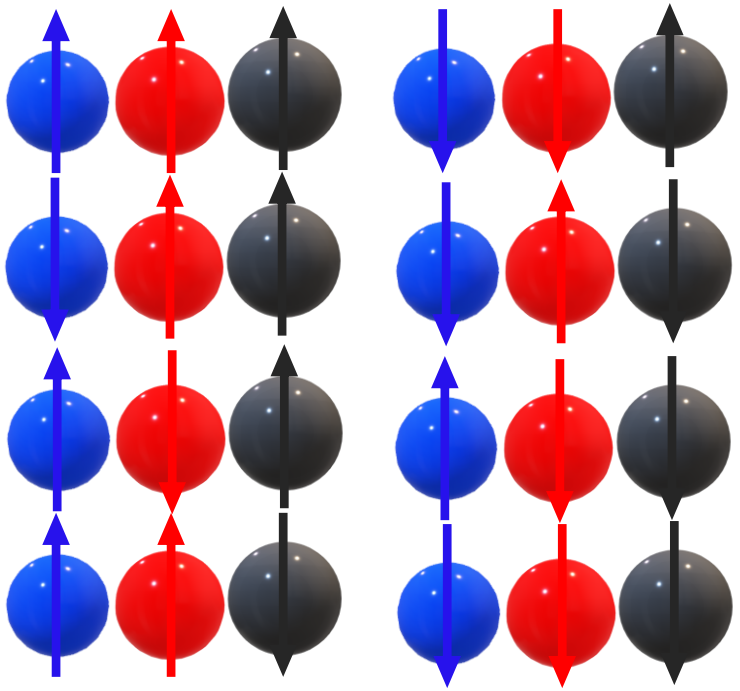
$(1{,}2 \times 10^{24})$

Exponential Scaling Problem

N=1 N=2 N = 3 N = 80 (Zr)







2^N=2 2^N=4 2^N=8 2^N=1,208,925,819,614,629,174,706,176

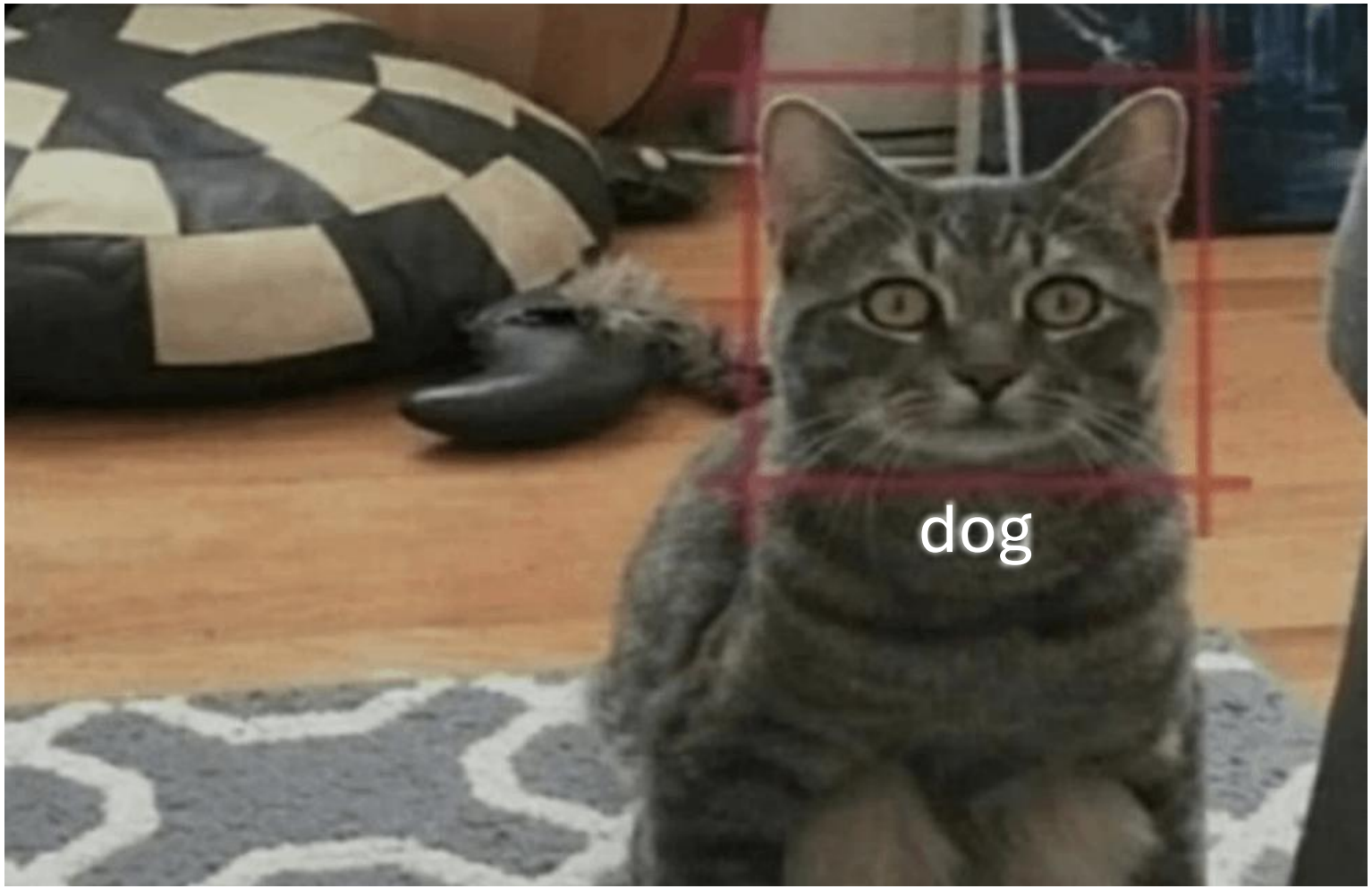
=16B

=32B

=64B

$\sim 10^{25}$B

The Solution: AI



How can AI help us?

Neural Quantum States

- **Variational principle** $\frac{\langle\psi_\theta|\hat{H}|\psi_\theta\rangle}{\langle\psi_\theta|\psi_\theta\rangle} \geq E_{\mathrm{GS}}$ ⟶ Find θ that minimises $\frac{\langle\psi_\theta|\hat{H}|\psi_\theta\rangle}{\langle\psi_\theta|\psi_\theta\rangle}$

G. Carleo and M. Troyer, Science (2017)

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- **Variational Monte Carlo**

$$|\psi_\theta\rangle = \int \psi_\theta(X)dX = \int \psi_\theta(\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_N})d\mathbf{x_1}d\mathbf{x_2}\ldots d\mathbf{x_N}$$

$$\frac{\langle\psi_\theta|\hat{H}|\psi_\theta\rangle}{\langle\psi_\theta|\psi_\theta\rangle} = \mathbb{E}_{X\sim p_\theta}\left[\frac{\langle X|\hat{H}|\psi_\theta\rangle}{\langle X|\psi_\theta\rangle}\right] \simeq \frac{1}{N_s}\sum_{i=1}^{N_s}\frac{\langle X_i|\hat{H}|\psi_\theta\rangle}{\langle X_i|\psi_\theta\rangle}$$

"Local energy"

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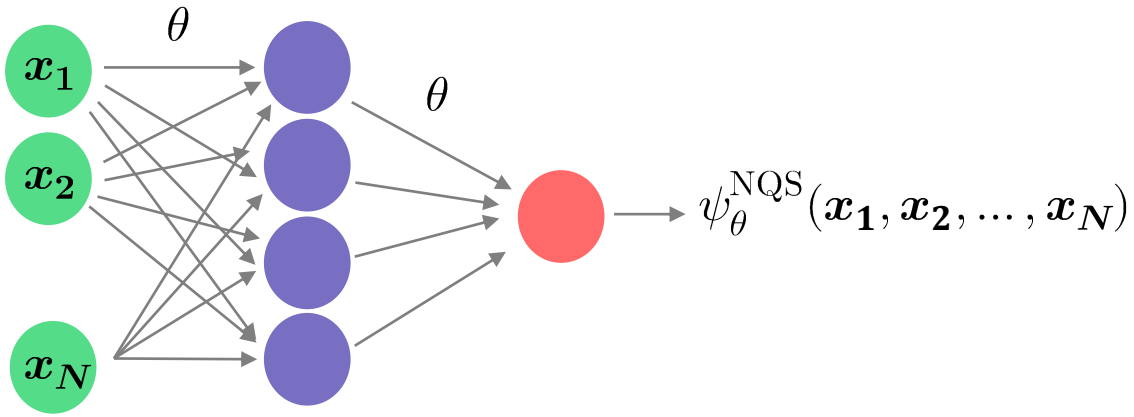
"Local energy"

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



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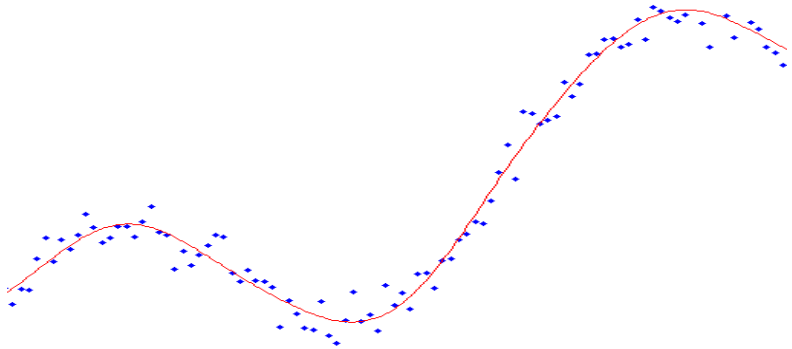
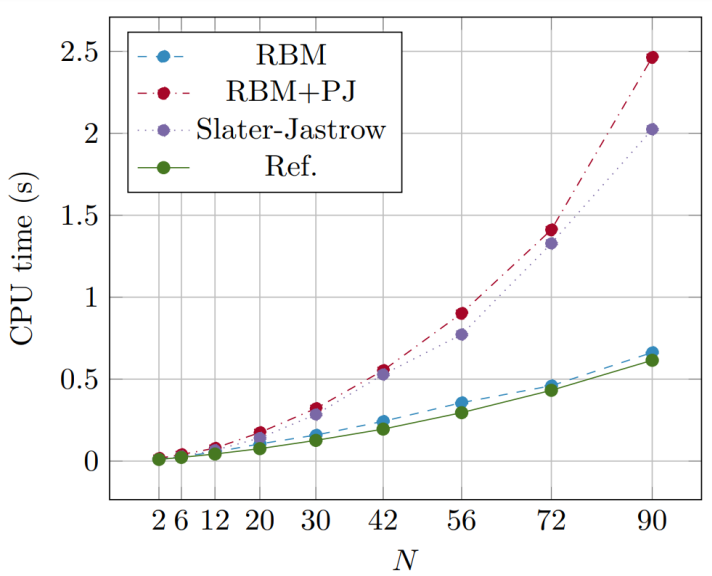
Why Neural Networks?

- **NNs have "∞ power"**: a neural network can approximate any continuous function.



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

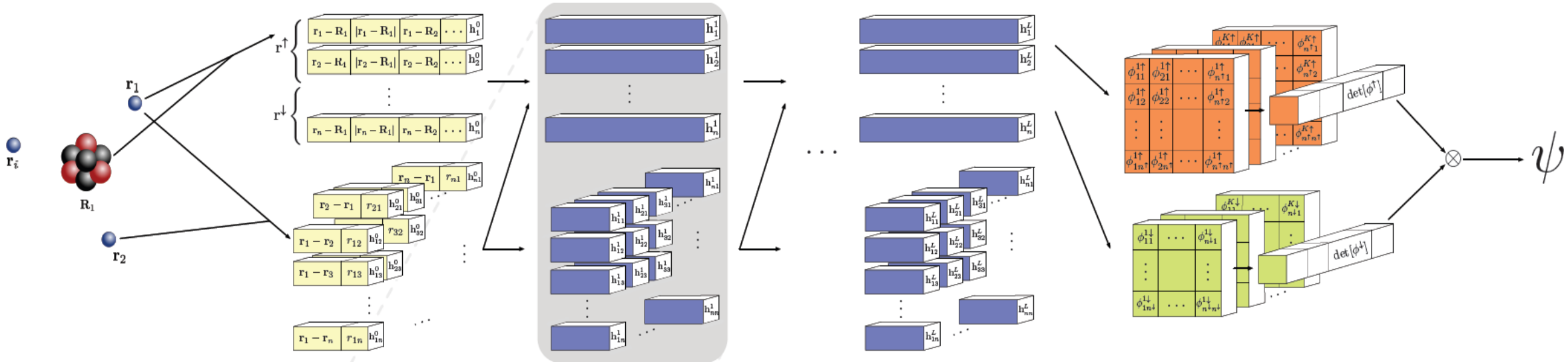
$$\text{Memory}(A) \sim \mathcal{O}(A^n), \quad A = Z + N$$



E M Nordhagen *et al*, arXiv:2210.00365

NQS showcase

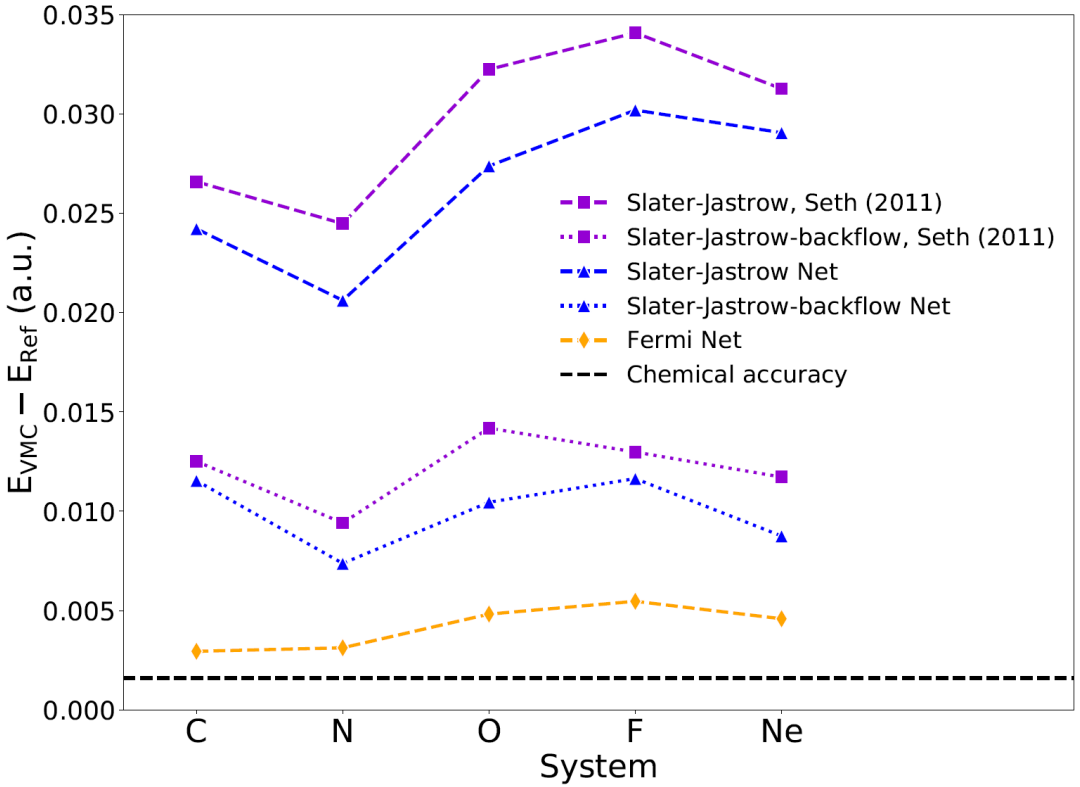
FermiNet (Quantum Chemistry)

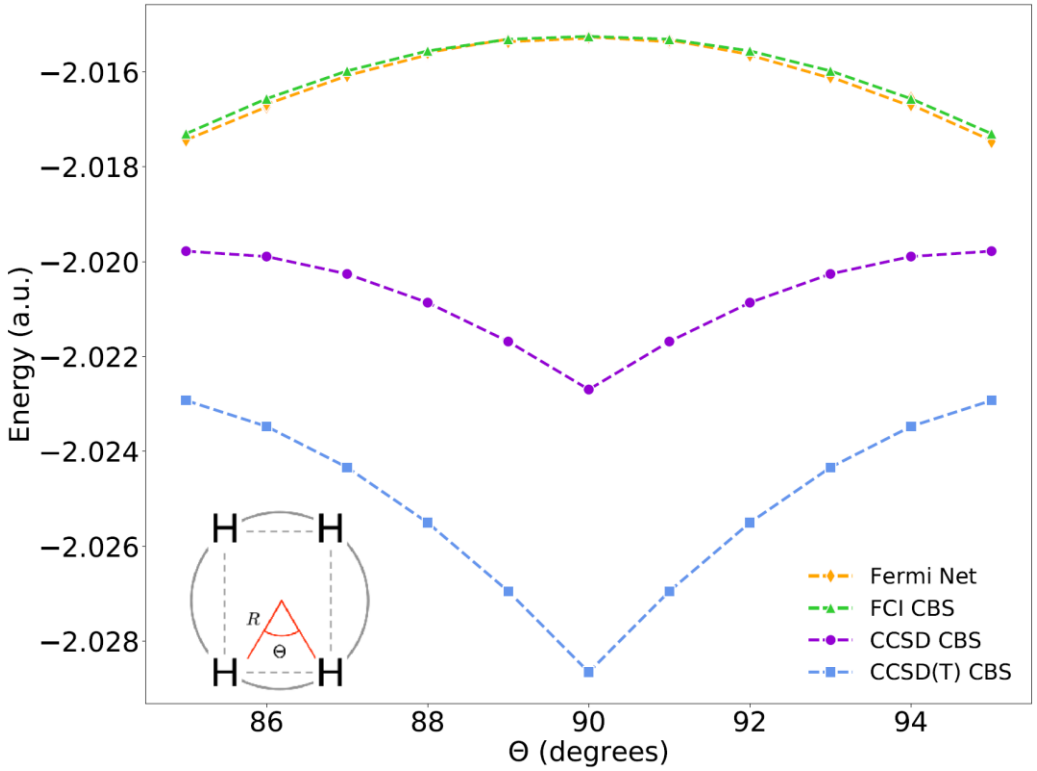


DeepMind

D. Pfau, J. S. Spencer *et al*, 2020, *Phys. Rev. Res.* **2**.

FermiNet (Quantum Chemistry)





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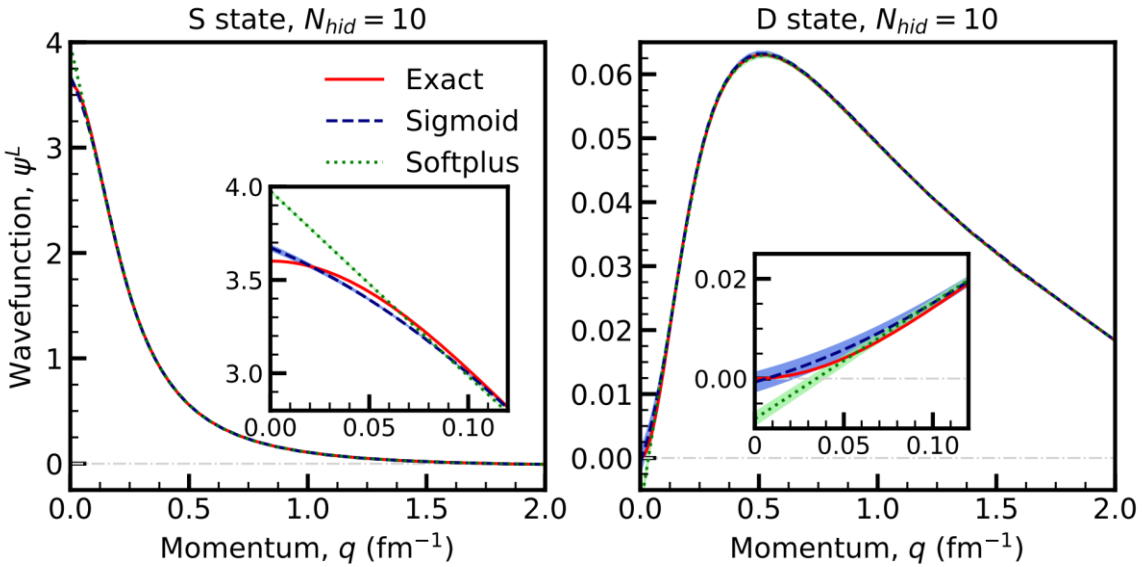
NQS for Nuclei

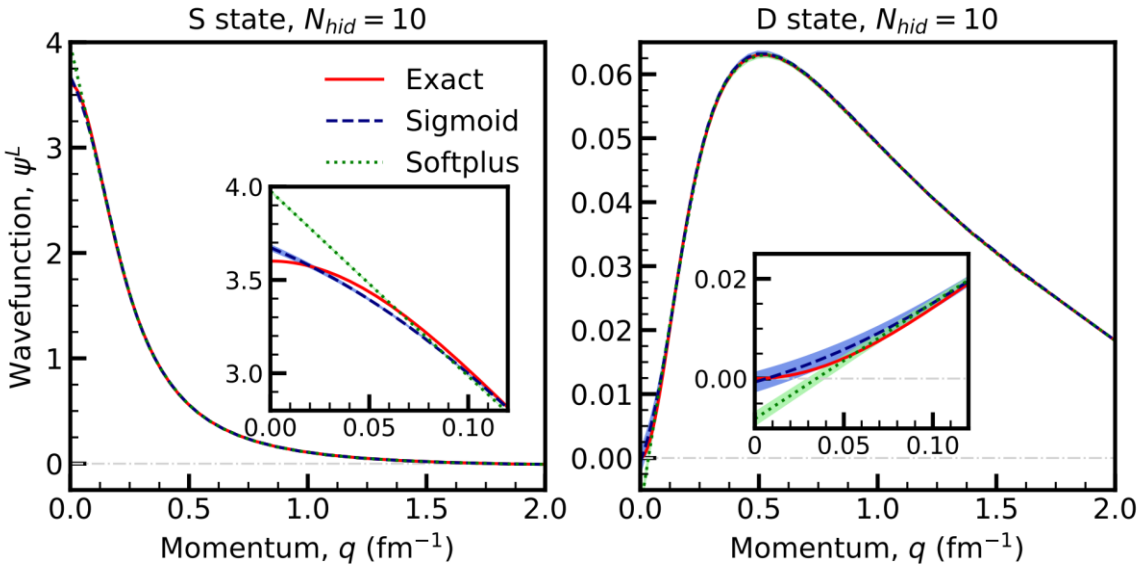
2020

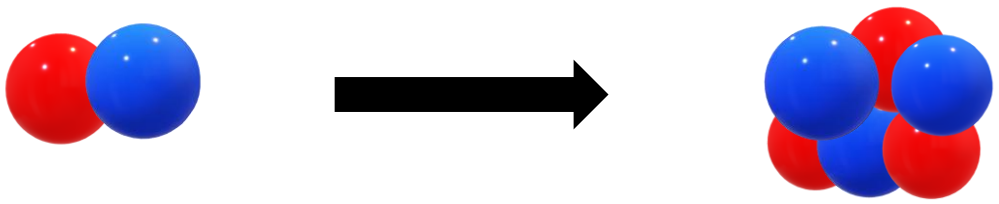


J. Keeble & A. Rios, Phys. Lett. B **809** (2020)

NQS for Nuclei

2020 → …



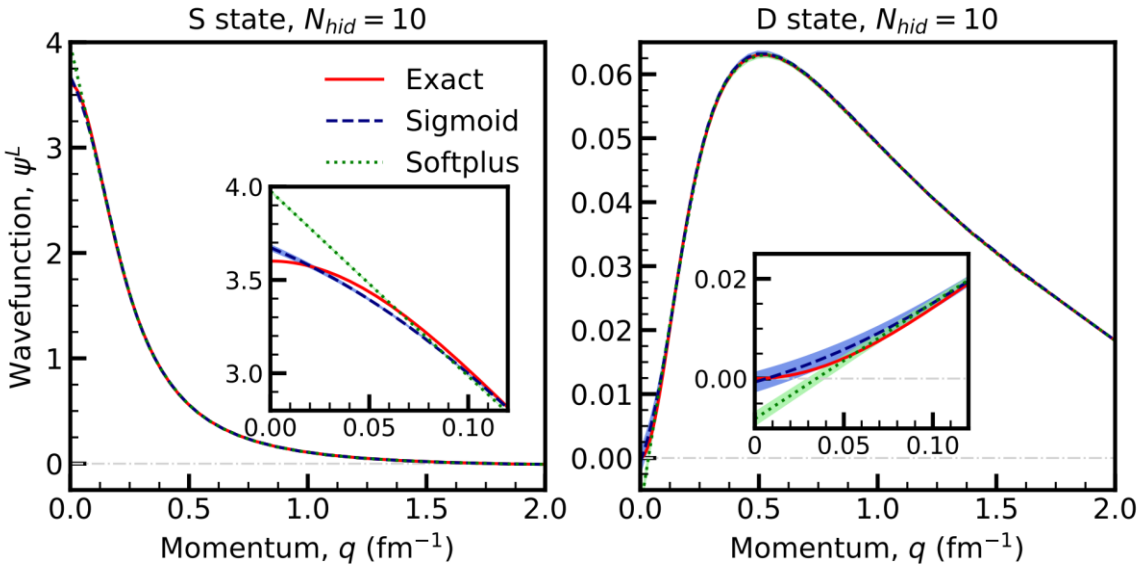


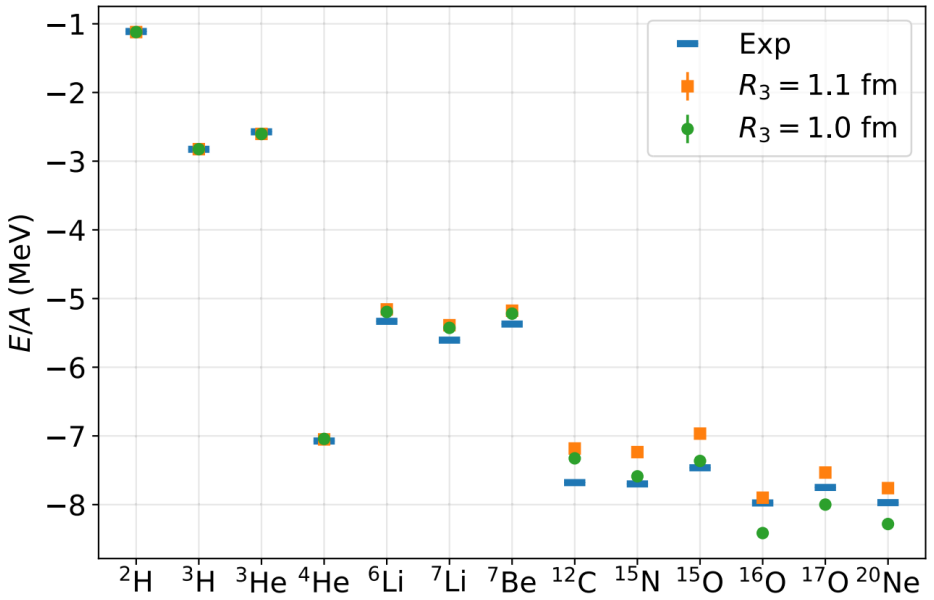
J. Keeble & A. Rios, Phys. Lett. B **809** (2020)

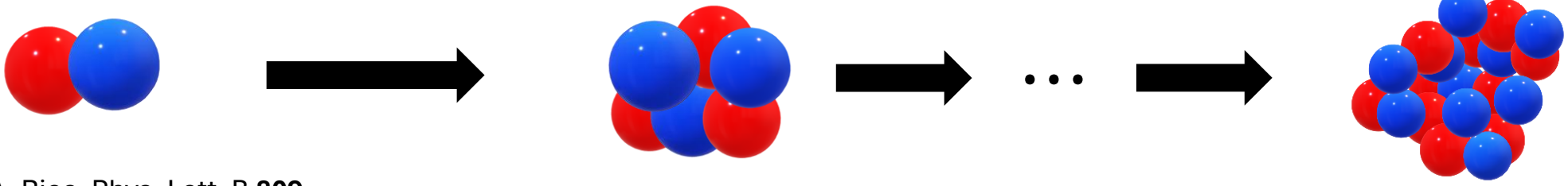
A. Gnech et al, Few-Body Syst. **63** (2022)

NQS for Nuclei

2020 → … → **2024**







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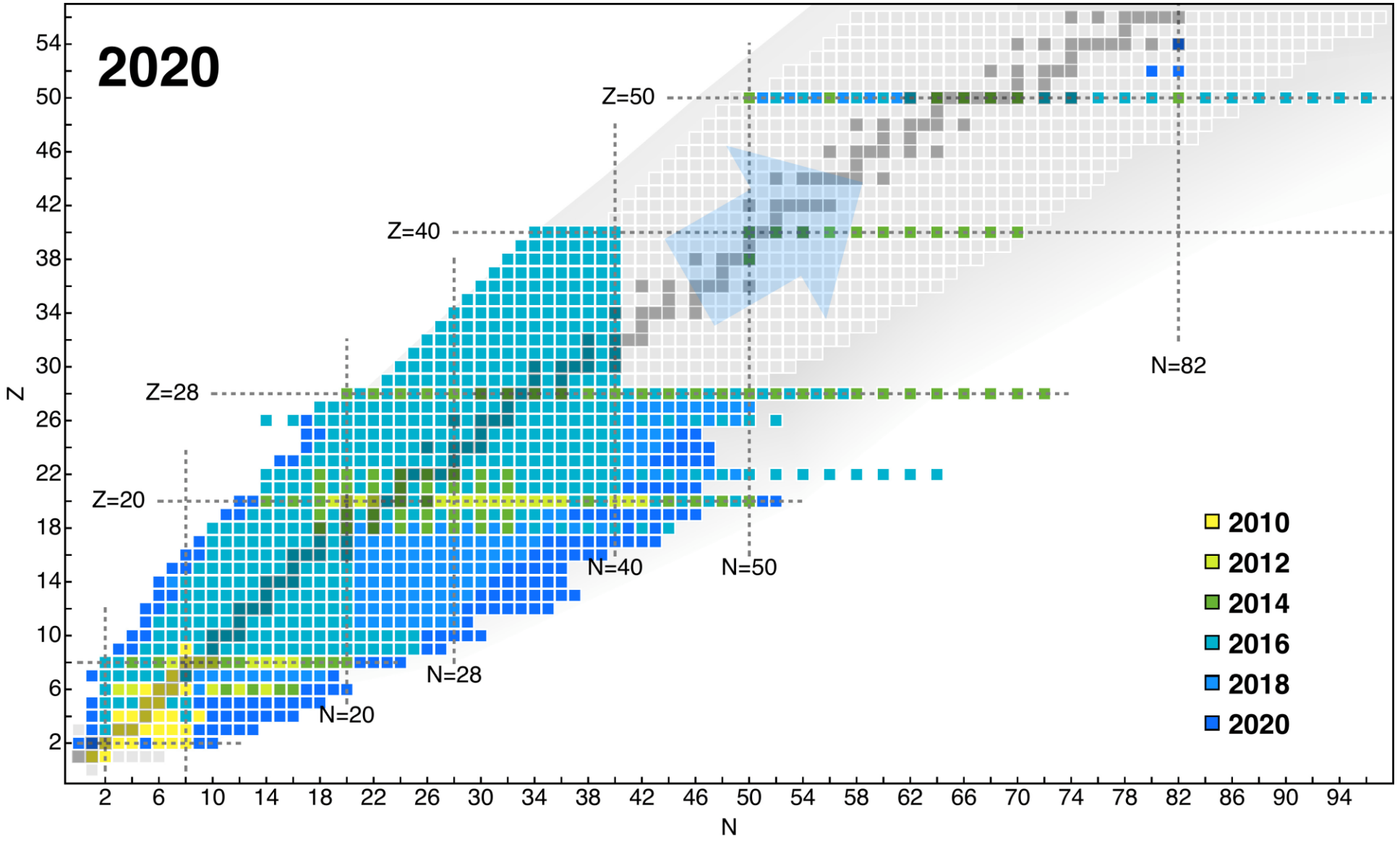
A. Gnech et al, PRL **133** (2024)


2020
Z=50
Z=40
Z=28
Z=20
N=82
N=40
N=50
N=28
N=20
2010
2012
2014
2016
2018
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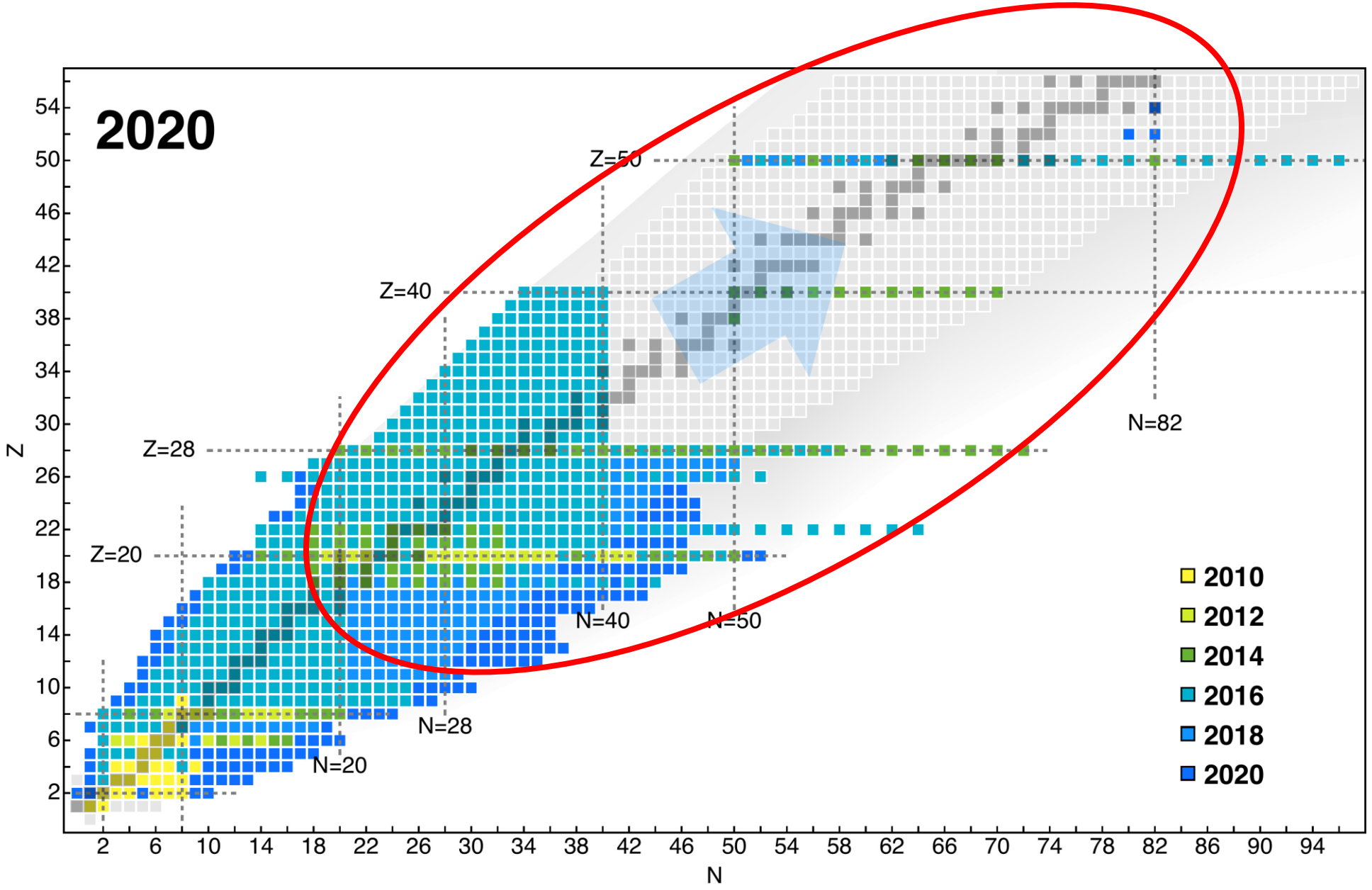
2 6 10 14 18 22 26 30 34 38 42 46 50 54 58 62 66 70 74 78 82 86 90 94
2 6 10 14 18 22 26 30 34 38 42 46 50 54


2020
Z=50
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2 6 10 14 18 22 26 30 34 38 42 46 50 54 58 62 66 70 74 78 82 86 90 94
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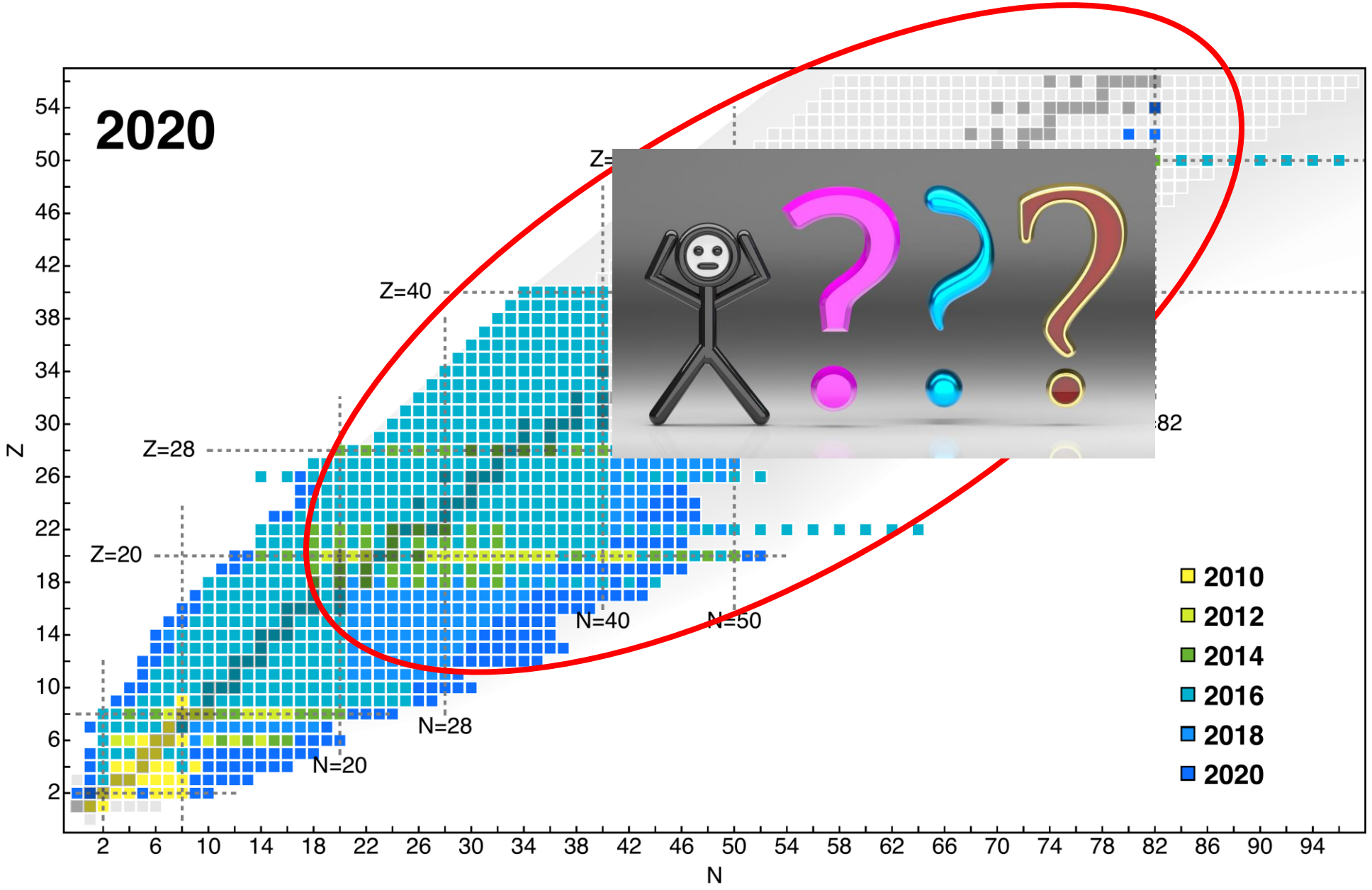
2020
Z=40
Z=28
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N=40
N=50
N=28
N=20
2010
2012
2014
2016
2018
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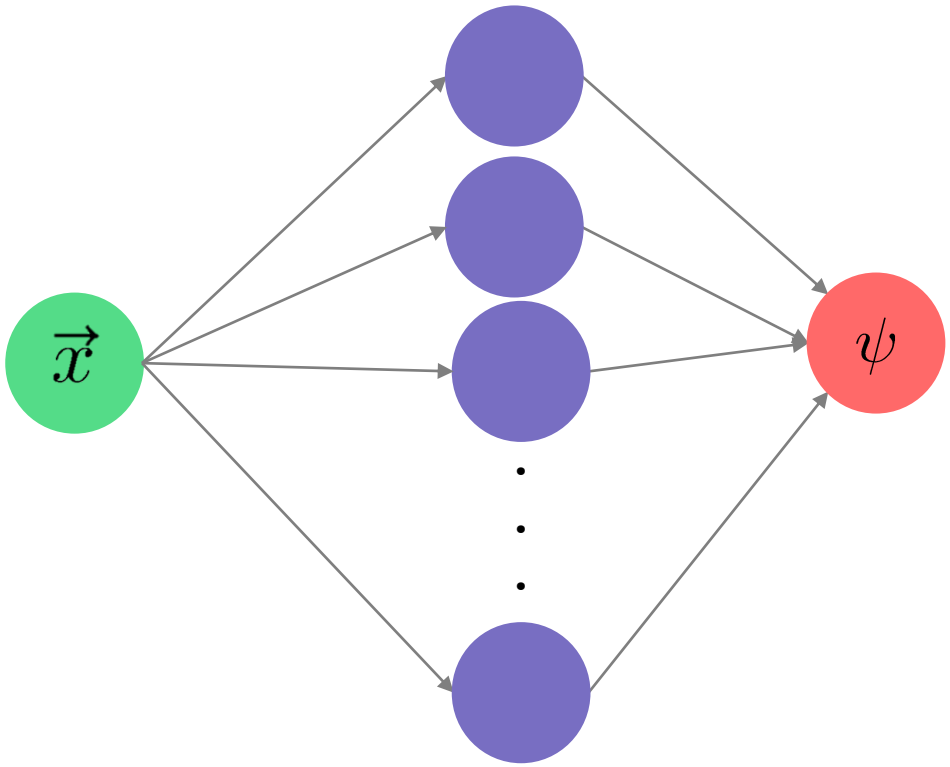
Z
N

1. Neural Network Architecture

Physical properties in NNs



- **Particle exchange symmetry**

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

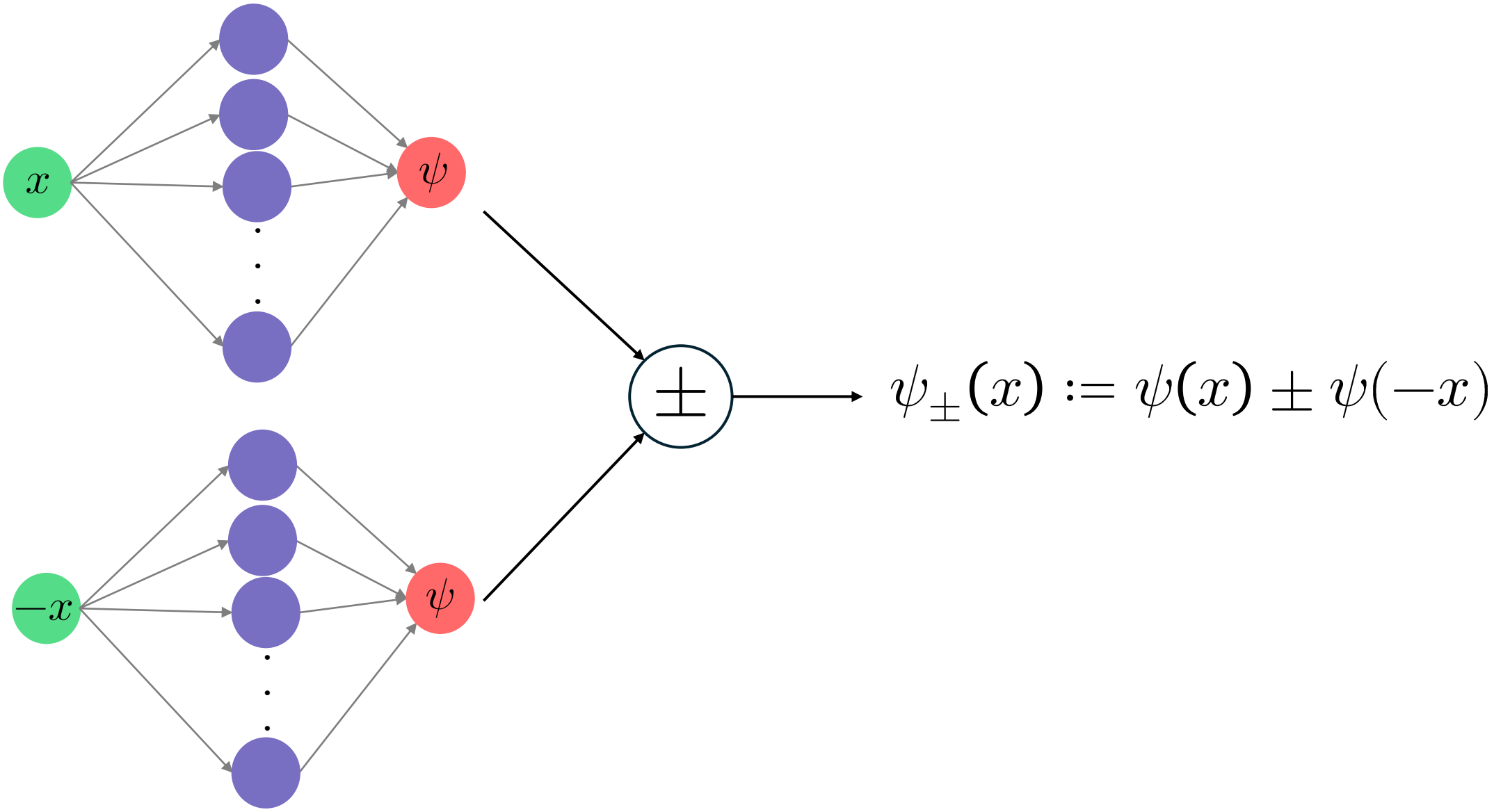
- **Spherical symmetry**

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

- **Time-reversal symmetry**

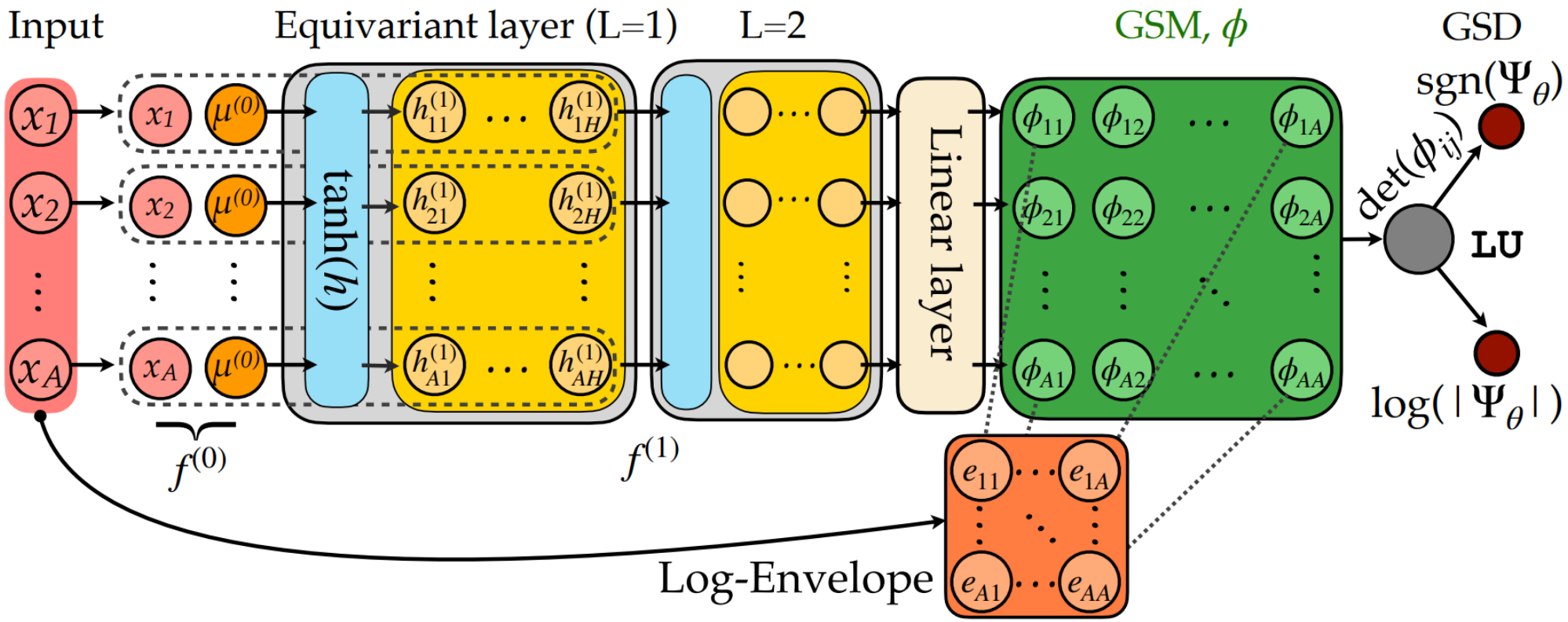
$$\psi(\vec{x}, \sigma) = \psi(T(\vec{x}, \sigma))$$

Reflection Symmetry



Particle Exchange Symmetry

$$\psi_{\mathrm{NQS}}(x_1, x_2, \ldots, x_N) = \varphi_{\mathrm{EQUIV}} \circ \det\, \phi_{\mathrm{GSM}}(x_1, x_2, \ldots, x_N)$$



J.W.T Keeble, M. Drissi , A. Rojo-Francàs, B. Juliá-Díaz & A. Rios, Phys. Rev. A. **108** (2023)

Towards a universal recipe...

- **Continous groups:** what about Lie groups? $SU(2)$ $SO(3)$
- **Mixed groups:** what about product groups? $SU(2) \times S_N$

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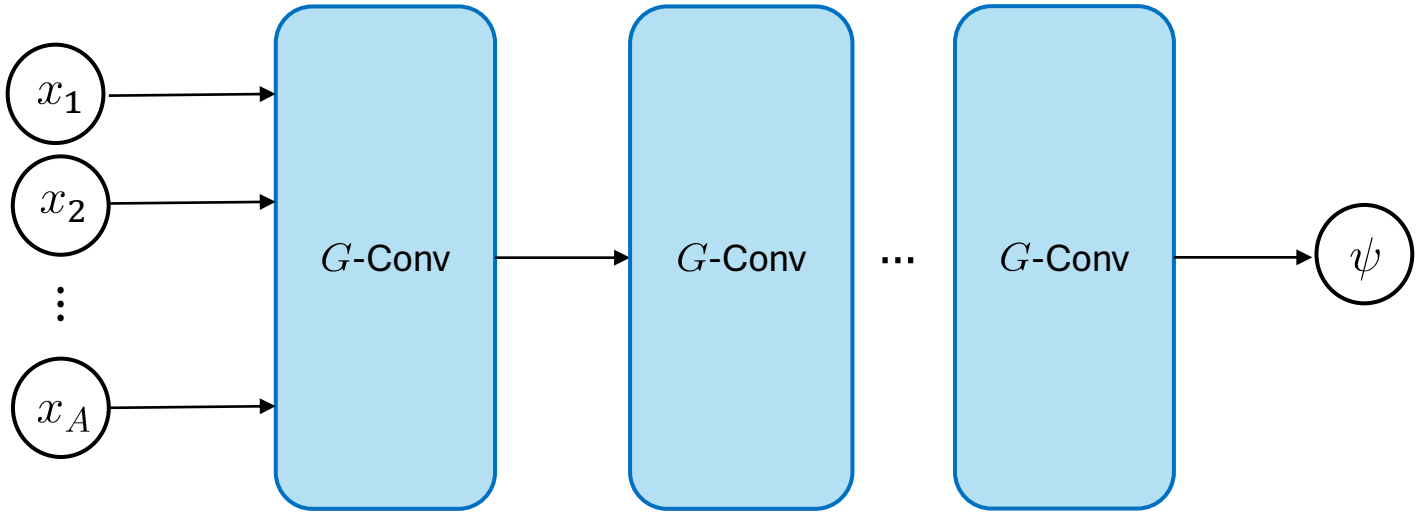

R. Kondor & S. Trivedi, arXiv:1802.03690

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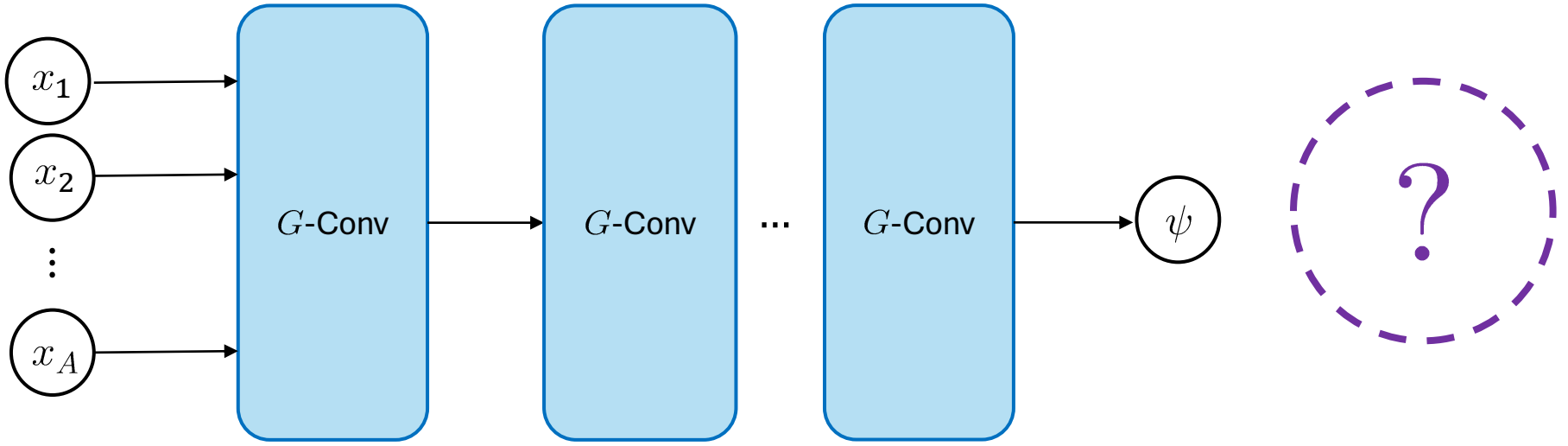

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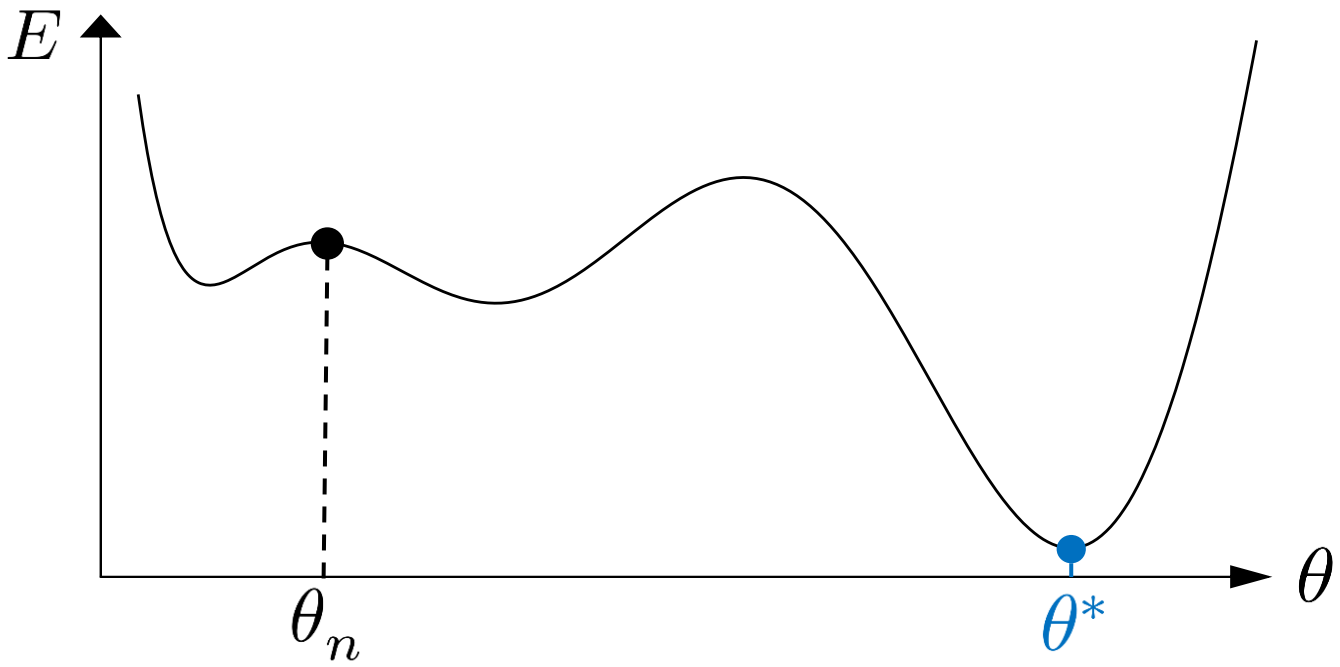
2. Optimisation Strategy

Gradient Descent

- **Local Linear Model:** $M_n(\delta) = L^T\delta + C$
- **Update:** $\theta_{n+1} = \theta_n + \delta_n$ where $\delta_n \equiv \text{argmin}_{\delta \in T_n} M_n(\delta)$



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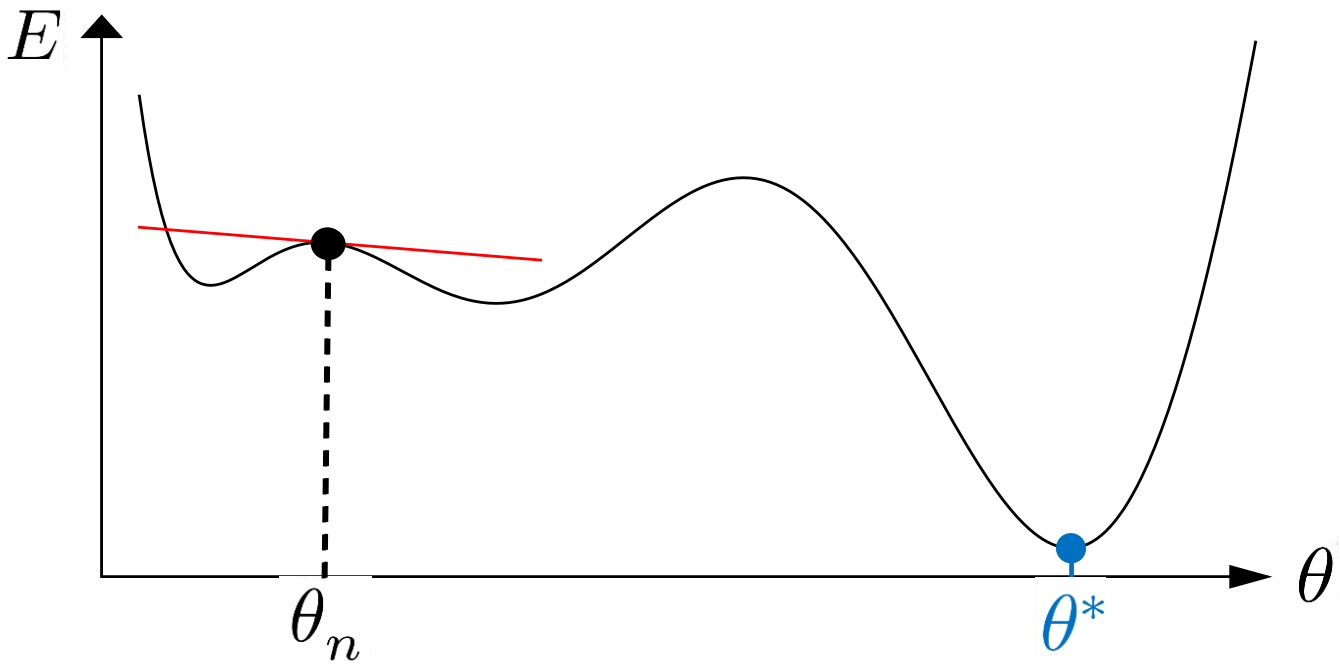
$$\delta_n = -\alpha \nabla E(\theta_n) \qquad \theta_{n+1} = \theta_n - \alpha \nabla E(\theta_n)$$



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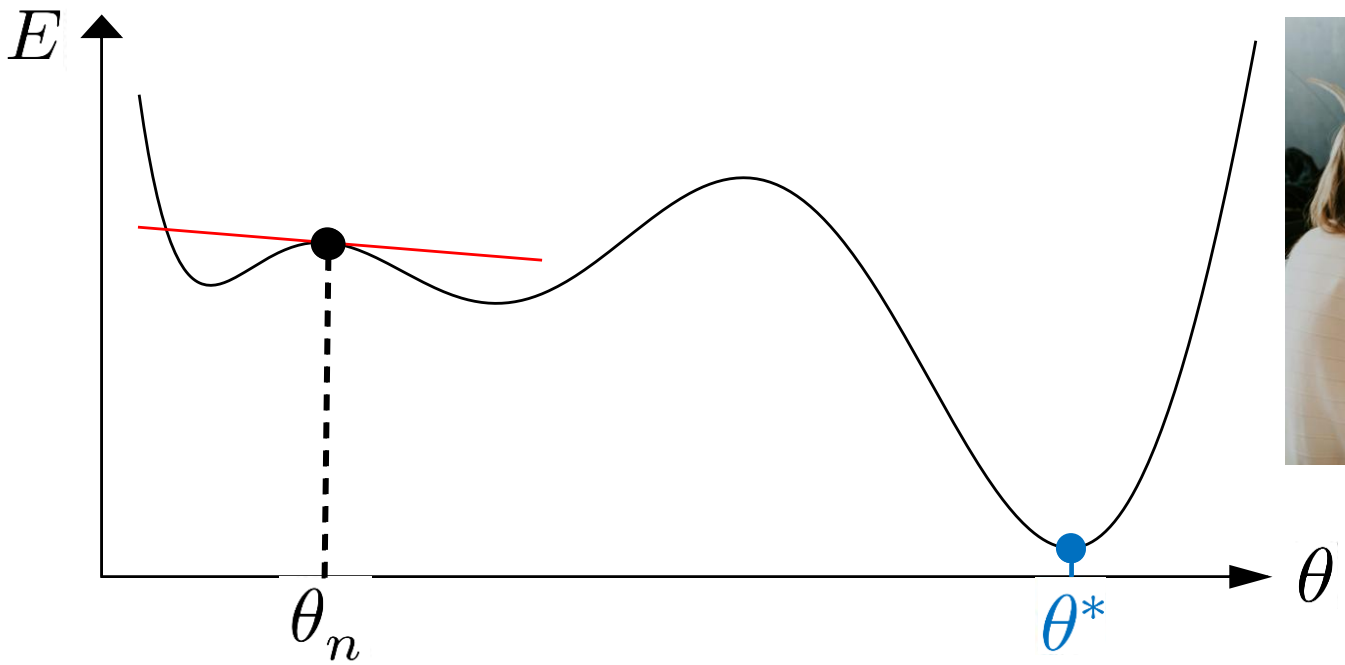

Second-order optimisation

- **Local Quadratic Model:** $M_n(\delta) = \frac{1}{2}\delta^T Q \delta + L^T \delta + C$
- **Trust region:** $T_n = \{\delta : \delta^T R_n \delta \leq r^2\}$
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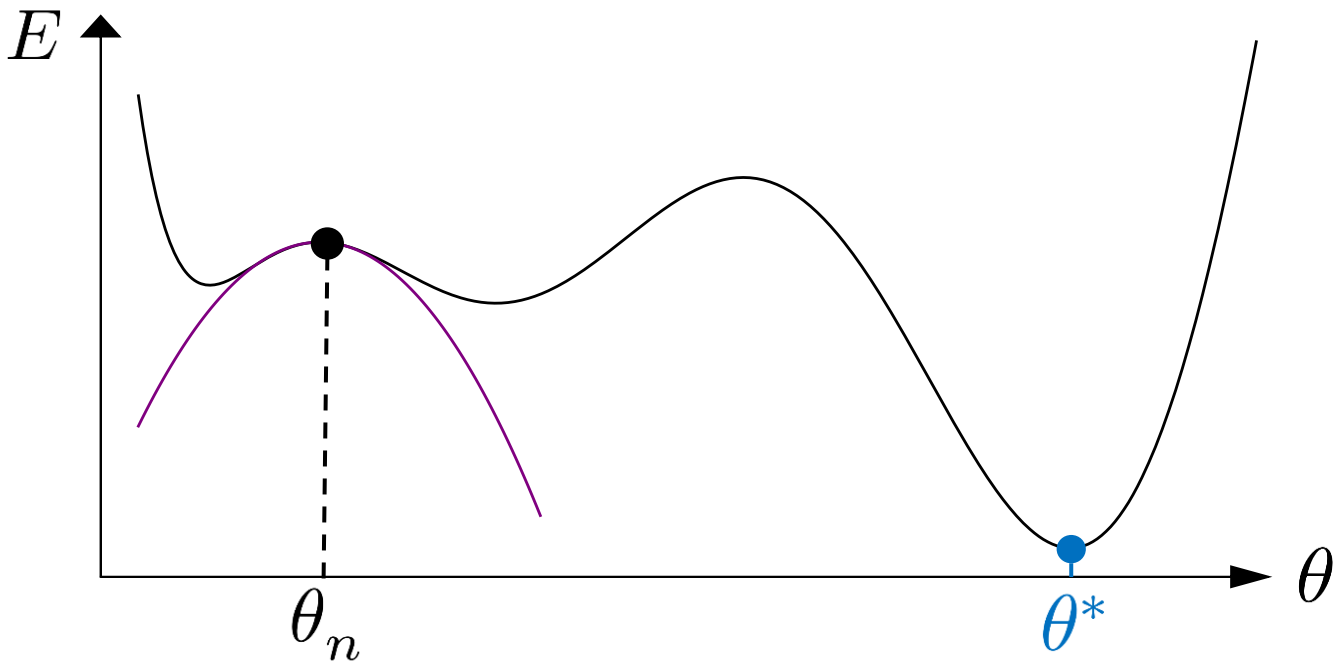

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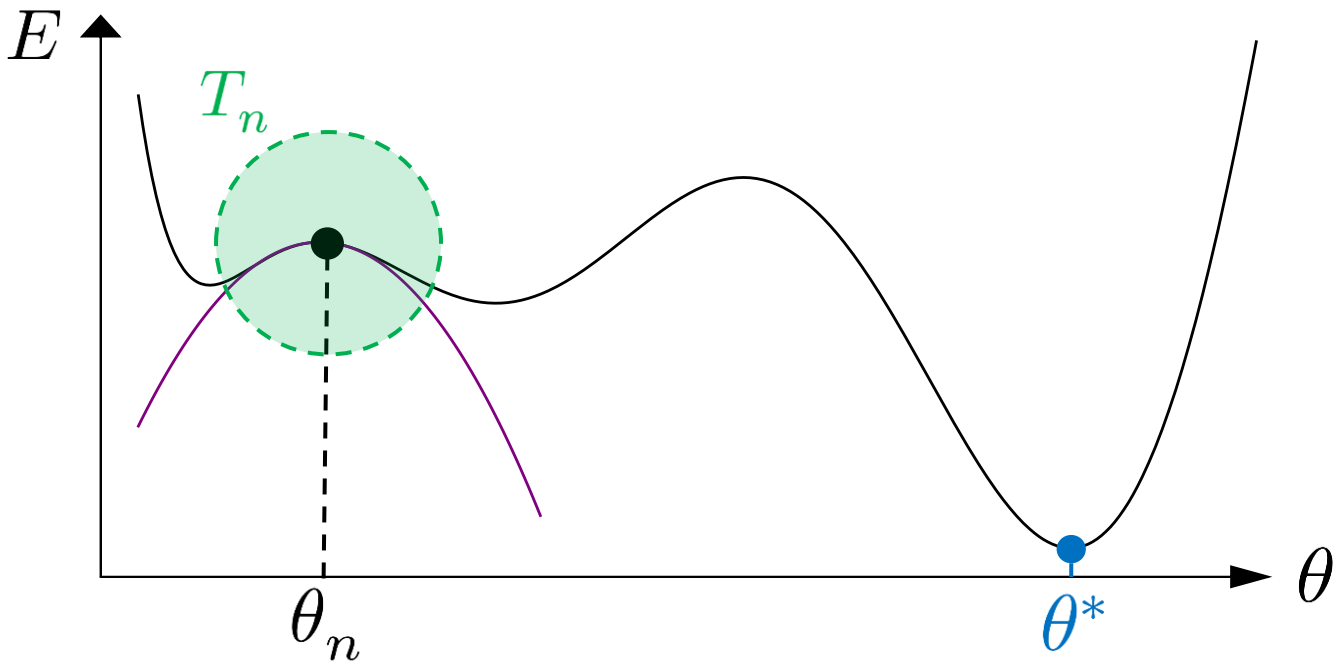

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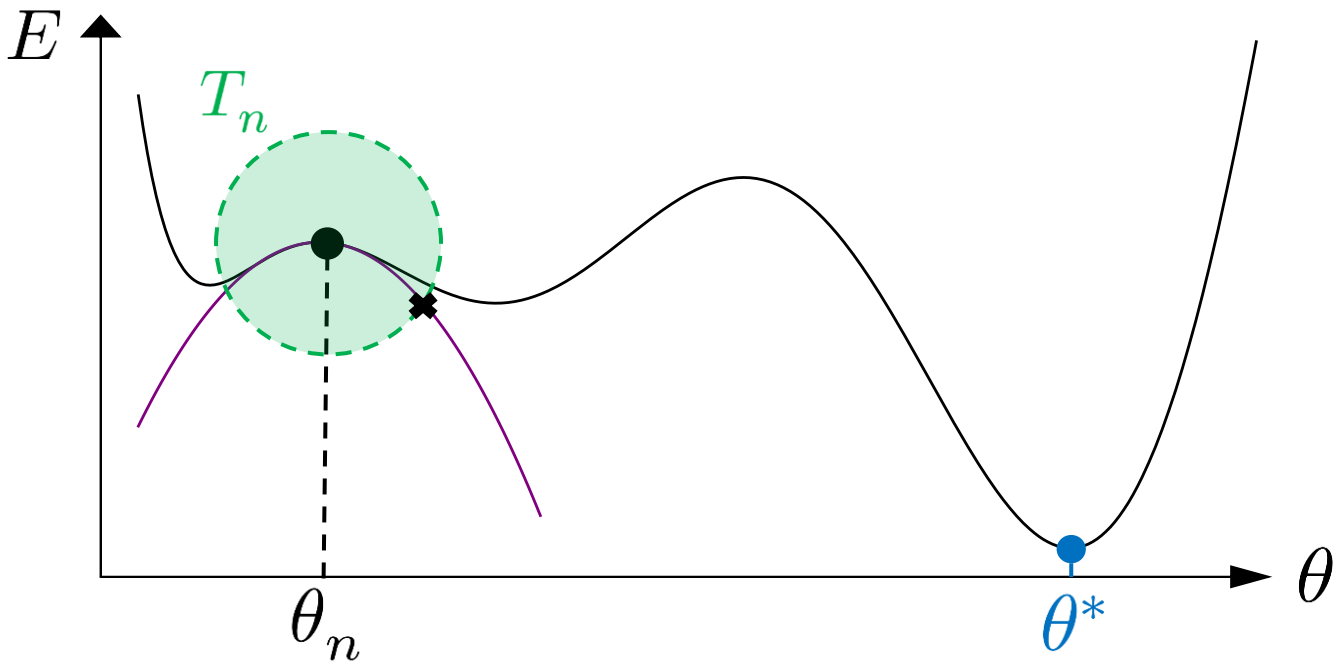

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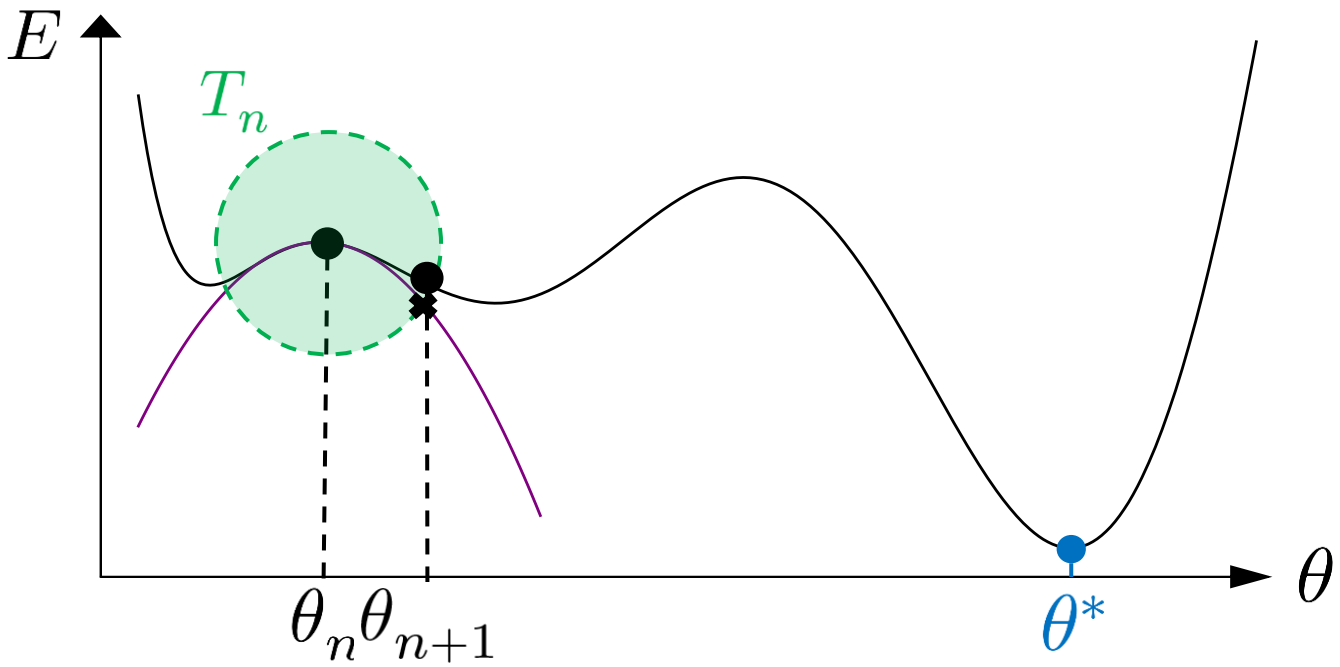

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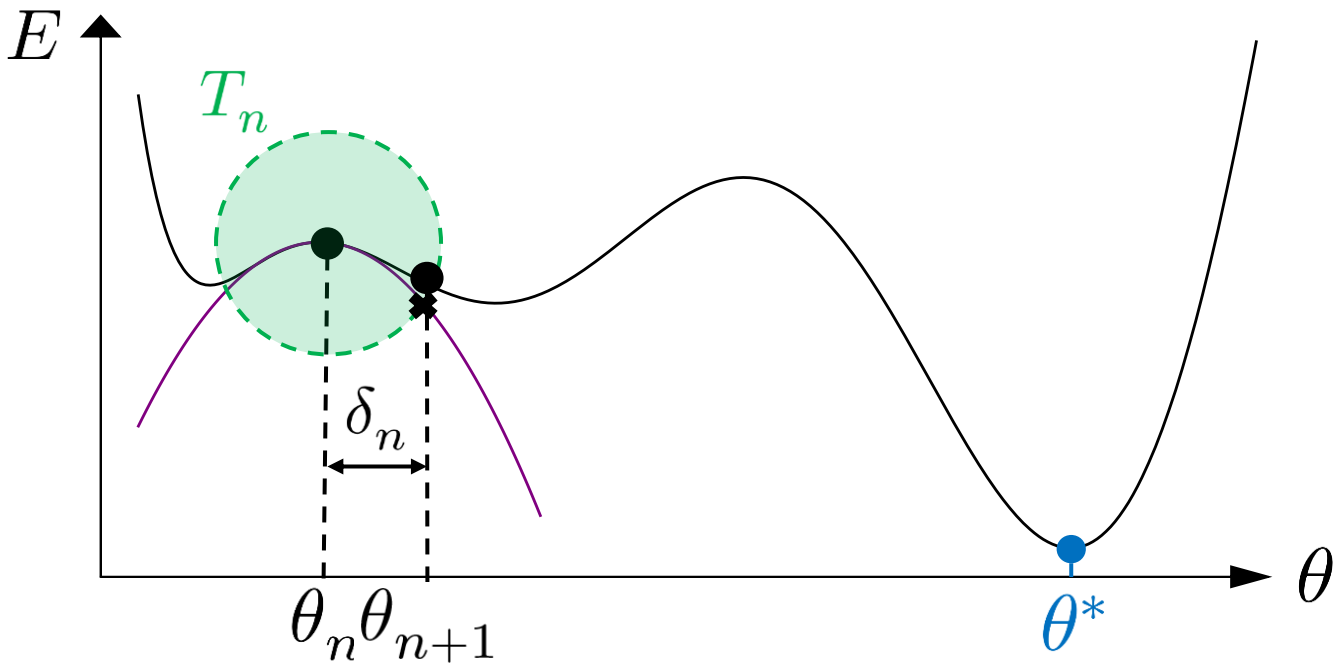

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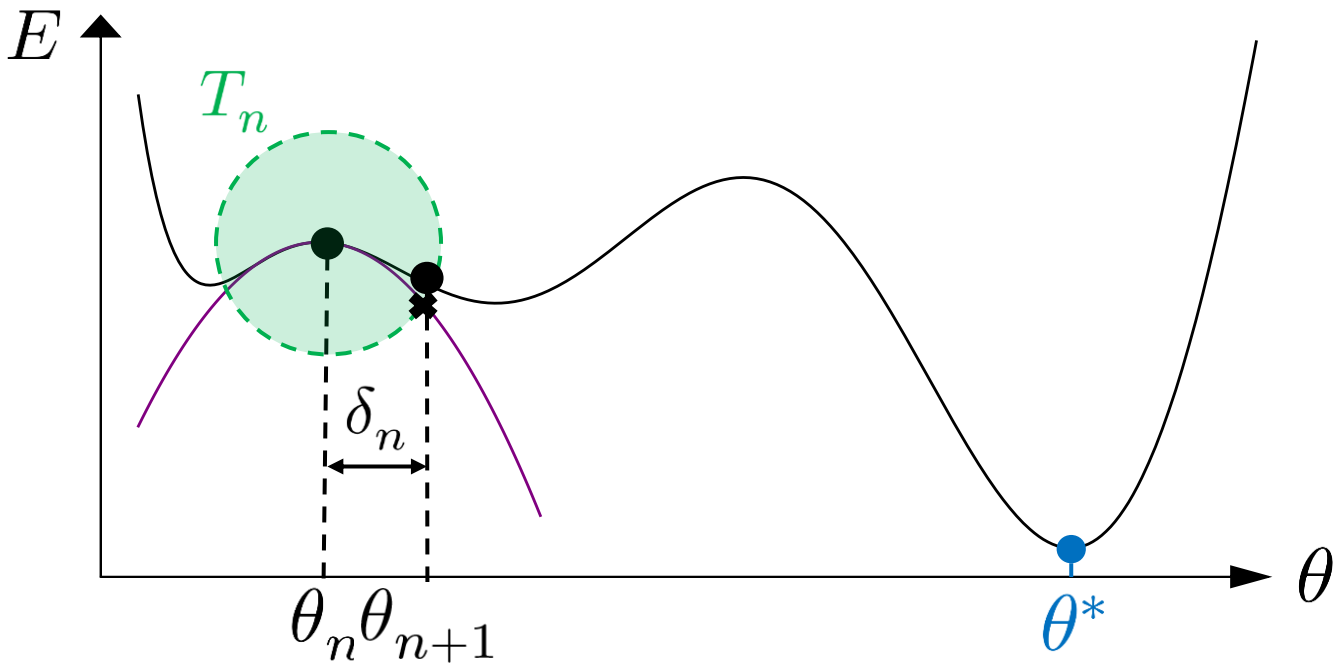

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$$L = \nabla_\theta E$$

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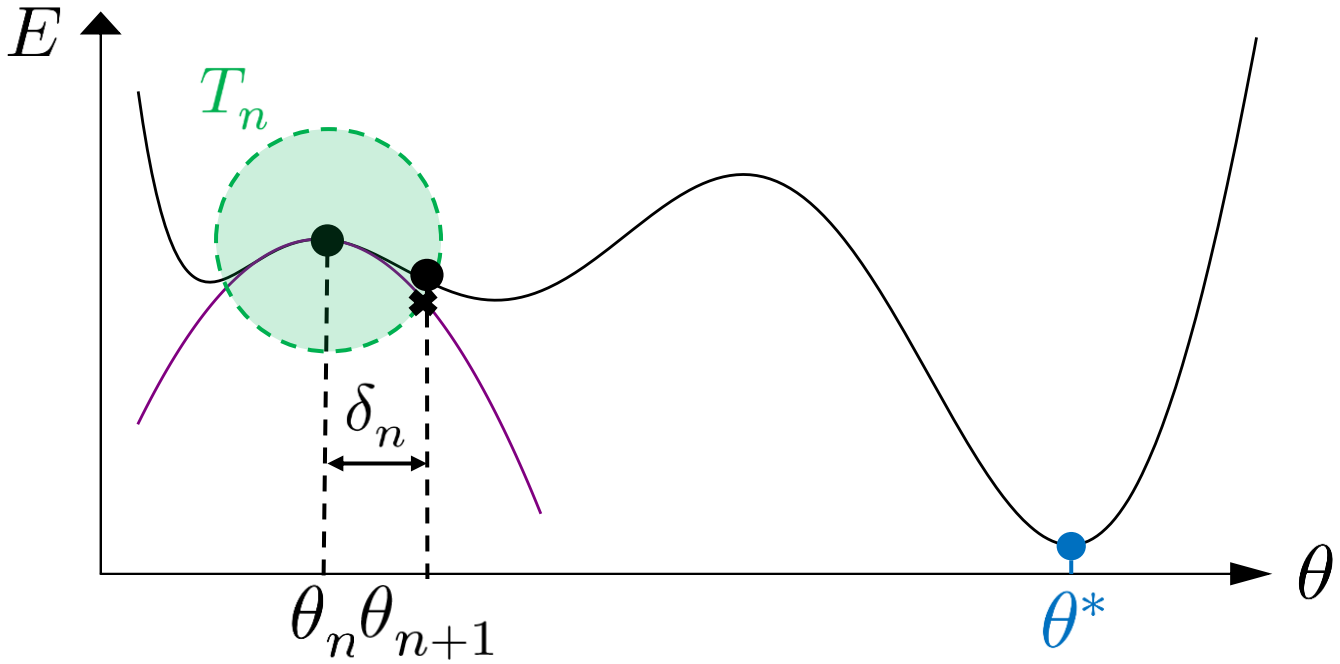

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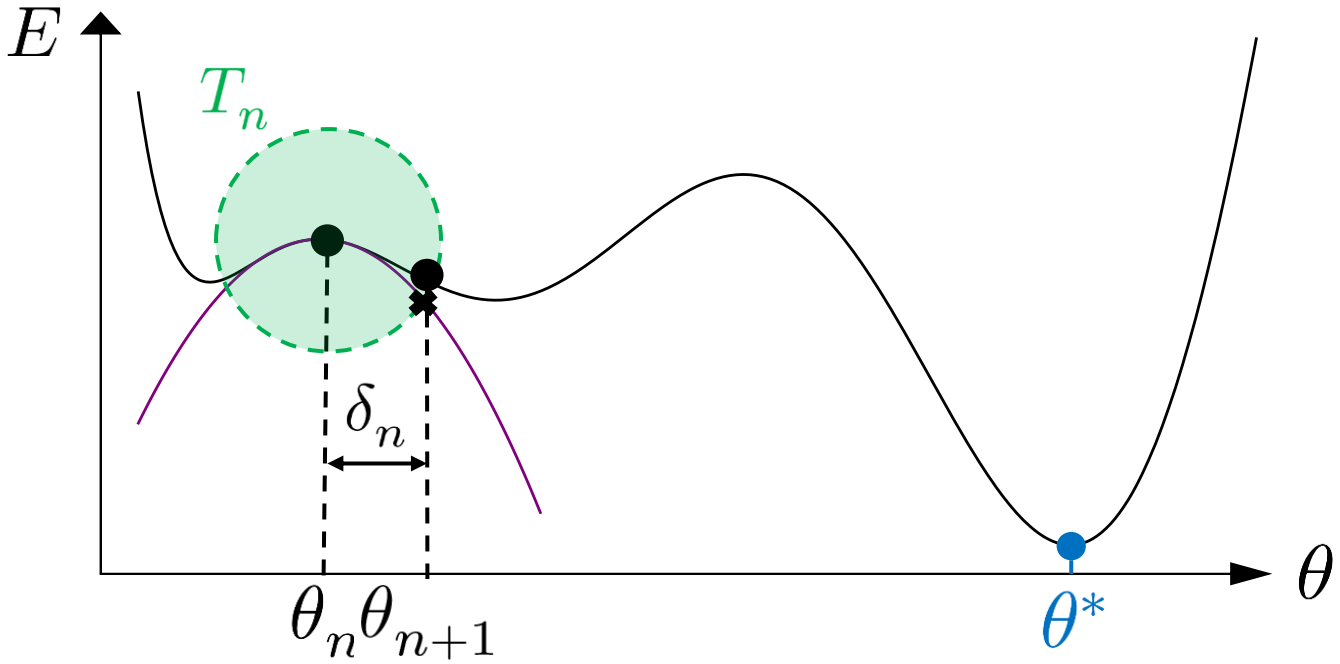

Stochastic Reconfiguration

"Quantum Geometric Tensor"

- **Local Quadratic Model:** $M_n(\delta) = \frac{1}{2}\delta^T Q \delta + L^T \delta + C, \quad Q_{ij}(\theta) = \left\langle \frac{\partial \psi_\theta}{\partial \theta_i}, \frac{\partial \psi_\theta}{\partial \theta_j} \right\rangle - \left\langle \frac{\partial \psi_\theta}{\partial \theta_i}, \psi_\theta \right\rangle \left\langle \psi_\theta, \frac{\partial \psi_\theta}{\partial \theta_j} \right\rangle$
- **Trust region:** $T_n = \{\delta : \delta^T R_n \delta \leq r^2\}, \quad R_n = 1$
- **Update:** $\theta_{n+1} = \theta_n + \delta_n$ where $\delta_n = -\left(Q_n + \lambda_n R_n\right)^{-1} \nabla E(\theta_n)$

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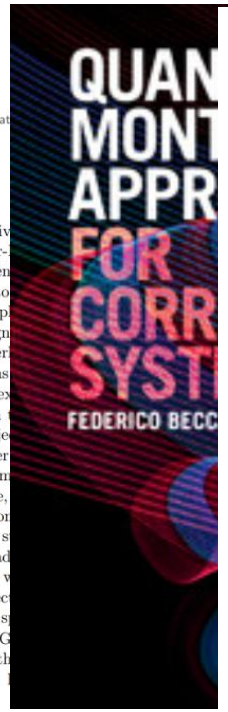

02108v3 [quant-ph] 14 May 2020

Quantum Natural Gradient

James Stokes[1], Josh Izaac[2], Nathan Killoran[2], and Giuseppe Carleo[3]

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10010 USA
[2]Xanadu, 777 Bay Street, Toronto, Canada
[3]Center for Computational Quantum Physics, Flatiron Institute, New York, NY 10010 USA

A quantum generalization of Natural Gradient Descent is presented as part of a general-purpose optimization framework for variational quantum circuits. The optimization dynamics is interpreted as moving in the steepest descent direction with respect to the Quantum Information Geometry, corresponding to the real part of the Quantum Geometric Tensor (QGT), also known as the Fubini-Study metric tensor. An efficient algorithm is presented for computing a block-diagonal approximation to the Fubini-Study metric tensor for parametrized quantum circuits, which may be of independent interest.

1 Introduction

Variational optimization of parametrized quantum circuits is an integral component for many hybrid quantum-classical algorithms, which are arguably the most promising applications of

rameters, including deriv
methods such as Nelder-
[12] or SPSA [33]. Recen
ploiting direct access to
formation has been exp
circuits have been design
dients with minimal over
tive function evaluations

One motivation for ex
dients is theoretical: in
pected error in the obje
best known zeroth-order
algorithm scales polynon
d of the parameter space,
dient Descent (SGD) co
d. Another motivation s
success of stochastic grad
deep neural networks, w
tion of non-convex objec
dimensional parameter s

The application of SG
fers from the caveat th
tion hinges on careful

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A simple
Large-Sca

Riccardo Rende,[1,*] Luciano Loris V
[1]International School for Ad
[2]Dipartimento di Fisica,

Neural-network architecture
functions. These networks req
optimize using traditional met
effective with a limited numb
parameters. Here, we leverag
even in the deep learning scen
a Deep Transformer architect
energy in the J_1-J_2 Heisenber
benchmark in highly-frustrate
scalability and efficiency of S
method to investigate unknow

I. INTRODUCTION

Deep learning has become crucial in
fields, with neural networks being the ke
pressive results. Well-known examples in
volutional Neural Networks for image r
and Deep Transformers for language-rel
The success of deep networks comes fr
ents: architectures with a large numbe
(often in the billions), which allow for
and training these networks on large a
However, to successfully train these large
tice, one needs to navigate the complic
non-convex landscape associated with th
rameter space.

The most used methods rely on stocha
scent (SGD), where the gradient of the
estimated from a randomly selected sub
ing data. Over the years, variations of t
such as Adam [6] or AdamW [7] hav

2163v2 [quant-ph] 13 Oct 2020

Geometr

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Combining insights from m
ration method with neural n
ground state estimation of q
in practice, little is known al
hidden details of the algorith
of the quantum Fisher matrix
initial dynamics, but the conv
contrast to the spectral prope
at convergence do not reveal
identify a new measure of co
show that, generically, the le
value, suggesting that correlat
stable representations of the

I. INTRODUCTION

Recently the fields of machine learni
information science have seen a lot
On the one hand, a number of promis
been obtained suggesting the potentia
quantum or classical machine learning
tum computer [1]. In particular, the variational quan-
tum eigensolver [2]–perhaps the most promising quan-
tum algorithms for first generation quantum computers–
is based on the variational optimization of a cost func-
tion to be evaluated on a quantum device, providing
a new playground for hybrid quantum-classical learning
[3, 4]. However, arguably the most significant advances

v2 [cond-mat.dis-nn] 21 Feb 2023

Efficient optimization of deep neural quantum states toward machine precision

Ao Chen and Markus Heyl
Center for Electronic Correlations and Magnetism,
University of Augsburg, 86135 Augsburg, Germany

Neural quantum states (NQSs) have emerged as a novel promising numerical method to solve the quantum many-body problem. However, it has remained a central challenge to train modern large-scale deep network architectures to desired quantum state accuracy, which would be vital in utilizing the full power of NQSs and making them competitive or superior to conventional numerical approaches. Here, we propose a minimum-step stochastic reconfiguration (MinSR) method that reduces the optimization cost by orders of magnitude while keeping similar accuracy as compared to conventional stochastic reconfiguration. MinSR allows for accurate training on unprecedentedly deep NQS with up to 64 layers and more than 10^5 parameters in the spin-1/2 Heisenberg J_1-J_2 models on the square lattice. We find that this approach yields better variational energies as compared to existing numerical results and we further observe that the accuracy of our ground state calculations approaches different levels of machine precision on modern GPU and TPU hardware. The MinSR method opens up the potential to make NQS superior as compared to conventional computational methods with the capability to address yet inaccessible regimes for two-dimensional quantum matter in the future.

As a fundamental concept in quantum physics, the ground state wave function plays a central role in understanding the behavior of many-body quantum systems. The accurate numerical solution of ground states, however, becomes an extraordinary challenge for existing numerical methods, especially in complex and large two-dimensional systems. The respective challenges depend on the individual utilized method, such as the "curse of dimensionality" in exact diagonalization (ED) [1], the notorious sign problem [2] in quantum Monte Carlo (QMC) [3], or the entanglement growth and matrix contraction complexity in tensor network (TN) methods [4].

Recently, the neural quantum state (NQS) has been introduced as a promising alternative for the calculation of ground states of quantum matter by means of artifi-
nature of entanglement in the spin chain. We are far
form such a detailed understanding of machine learning
inspired methods.

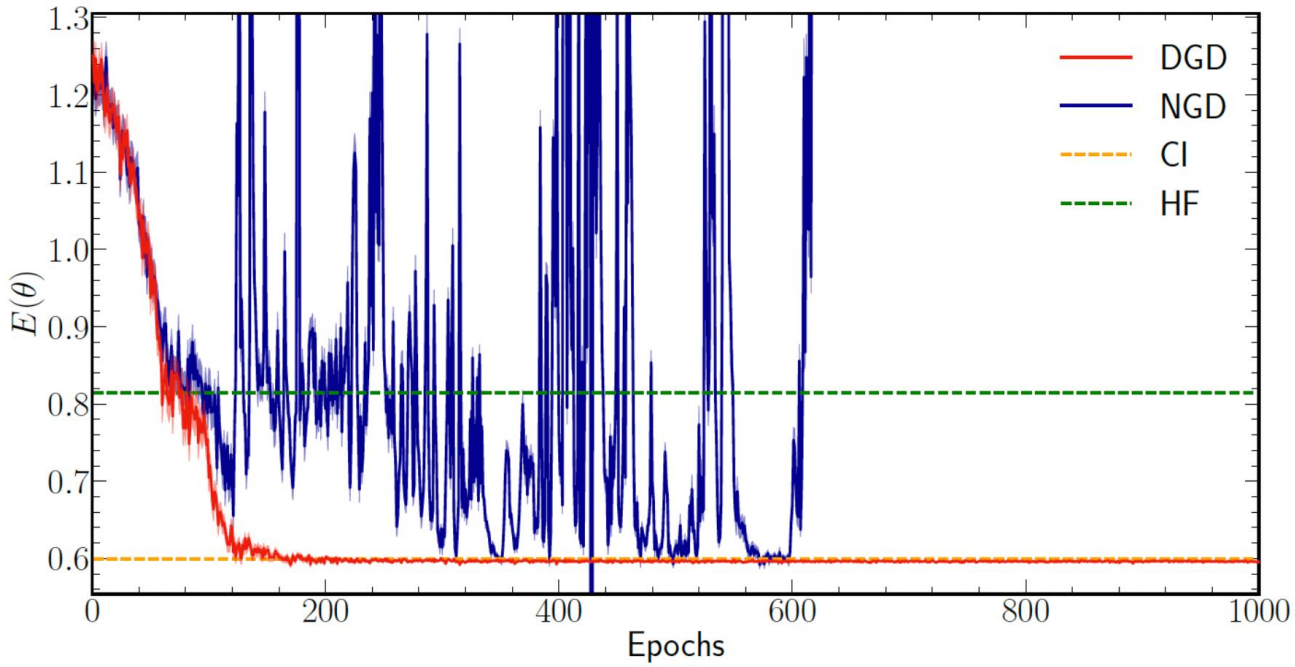
Thus it is natural that some studies have related complex RBM states to tensor network states [17, 18]. But these studies are mostly based on constructing abstract mappings between RBM wave functions and tensor net-

networks, we find significantly lower variational energies outperforming conventional numerical approaches up to lattice sizes of 16×16 spins. Most importantly, we observe that our ground state results reach different levels of machine precision. Thus, with MinSR we are able to reach the frontier where the sole limitation of applying the NQS approach to complex two-dimensional quantum matter is not anymore the expressive power of the neural network but rather the inherent numerical precision of the computing device. This is of key importance to exploit the full power of NQS for the calculation of ground states in the future opening up the potential to address yet inaccessible regimes of quantum many-body systems also in higher spatial dimensions.

Decisional Gradient Descent

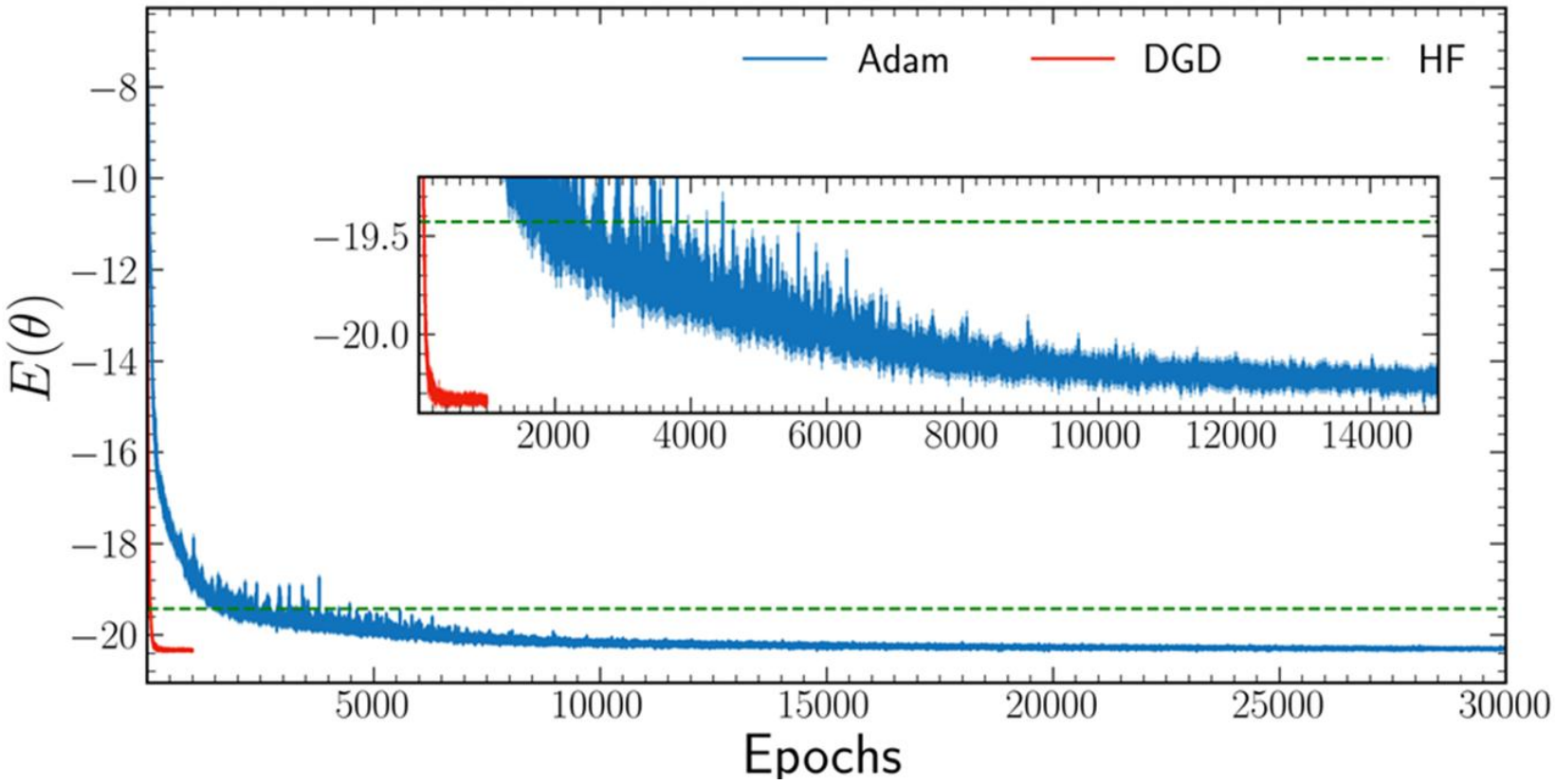
- **System:** chain of **1D spin-polarized fermions** $H = -\frac{1}{2}\sum_{i=1}^{A}\nabla_i^2 + \frac{1}{2}\sum_{i=1}^{A}x_i^2 + \frac{V_0}{\sqrt{2\pi}\sigma_0}\sum_{i<j}e^{-\frac{(x_i-x_j)^2}{2\sigma_0^2}}$

- **Quadratic term:** $\mathrm{Q}_{\mathrm{VMC}}(\theta)_{\theta_i\theta_j} \equiv \frac{1}{4}\sum_{k=1}^{A} E_{X\sim p_\theta}\left[\partial_{\theta_i}\partial_{x_k}\ln p_\theta(X)\partial_{\theta_j}\partial_{x_k}\ln p_\theta(X)\right]$



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

DGD vs. ADAM



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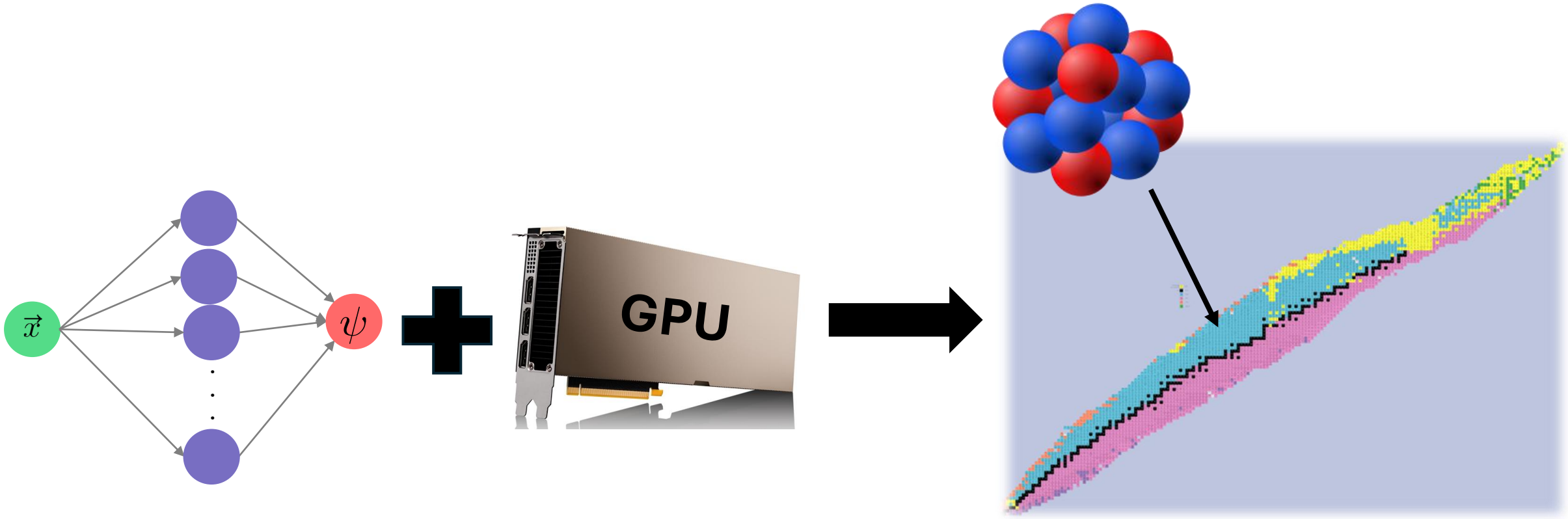
Conclusions

Takeaway



Thank you

J. Rozalén Sarmiento, A. Rios

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