Deep learning quantum matter

Machine-learning approaches to the quantum many-body problem

Joaquín E. Drut & Andrew C. Loheac
University of North Carolina
at Chapel Hill

THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL

SAS, September 2018

Outline

Why quantum matter?

What is the challenge?

How machine learning is helping

- Speeding up quantum Monte Carlo
- Detecting phase transitions and critical phenomena
- Our forays with CNNs

Summary and conclusions

Computational Quantum Matter at UNC-CH

A non-perturbative look at quantum matter

https://users.physics.unc.edu/~drut/public_html_UNC/group.html

Graduate Students
Andrew C. Loheac — 5th year
Chris R. Shill — 5th year
Casey E. Berger — 4th year
Josh R. McKenney — 4th year
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Matter whose collective behavior is dominated by the laws of quantum mechanics

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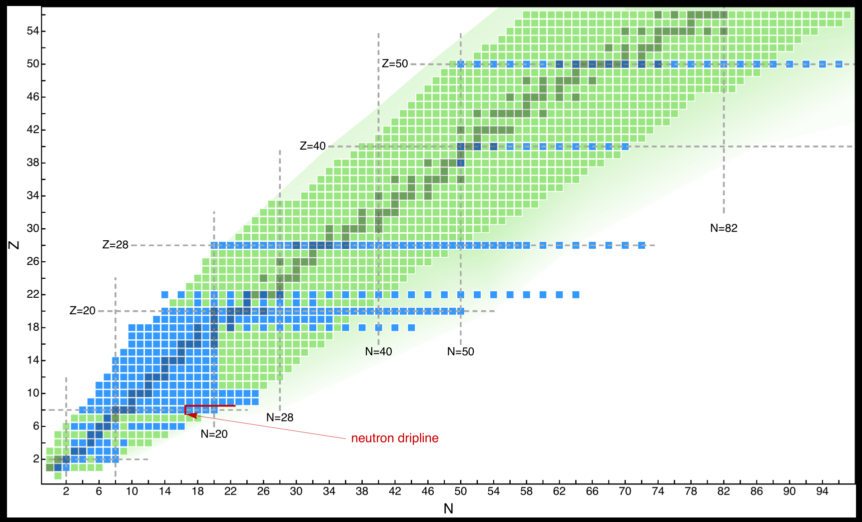
Thermodynamics, phase transitions, response to external perturbations, quantum information,…

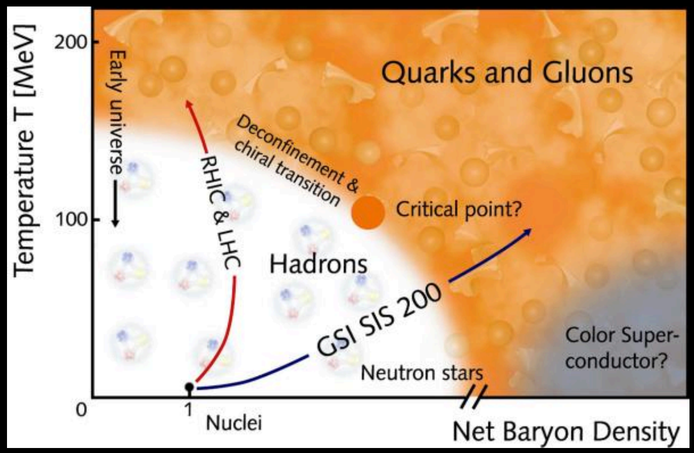
Matter whose collective behavior is dominated by the laws of quantum mechanics

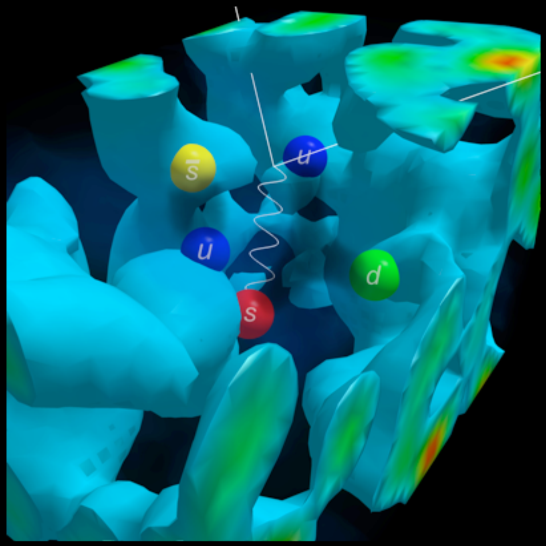
Few to many particles

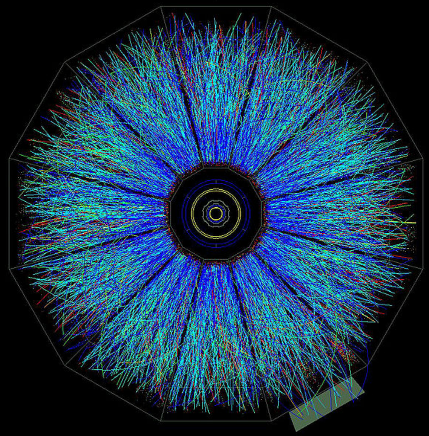
The many-body Schrödinger equation

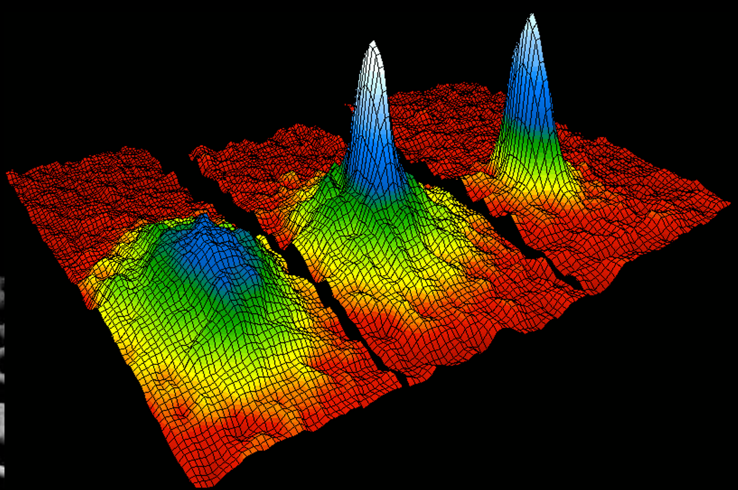
Quantum matter…

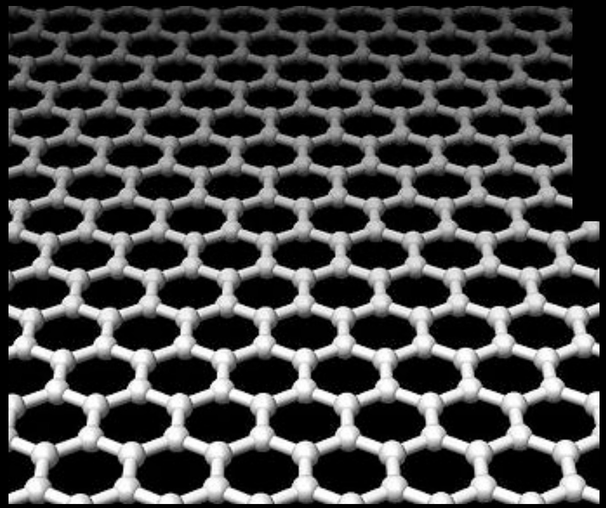


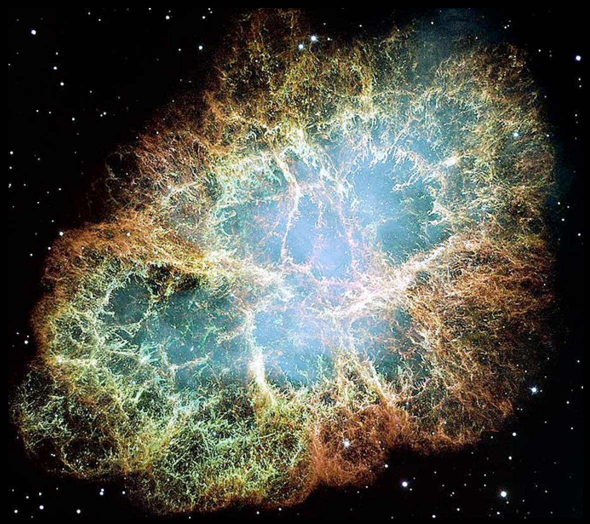


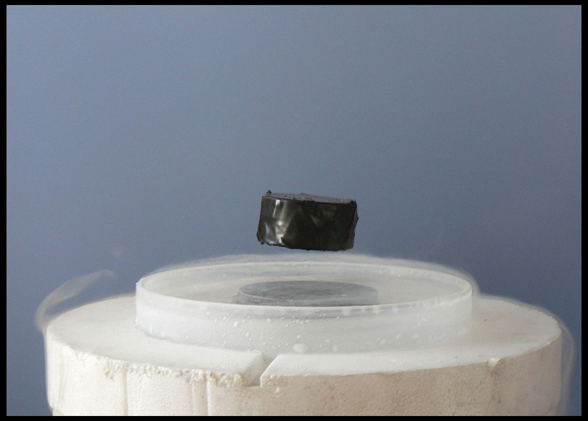












…is everywhere, but…

The challenge*

“Traditional” quantum mechanics

Wavefunction description for N particles requires exponentially as much memory: you need to store a function of N variables

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

Discretize each variable into M points

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Same problem as storing an ***N***-dimensional array

$$\Psi_{ijk\ldots} \qquad \begin{array}{c} i = 1, \ldots, M \\ j = 1, \ldots, M \\ \vdots \end{array} \qquad \Longrightarrow \qquad M^N \text{ elements}$$

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Advantage: knowing the wavefunction amounts to knowing **everything** about the system of interest.

Disadvantage: to good to be true/practical

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“Modern” quantum mechanics, i.e. quantum field theory

We don’t need to know **everything**. Focus on answering specific questions, i.e. computing specific quantities: “observables”.

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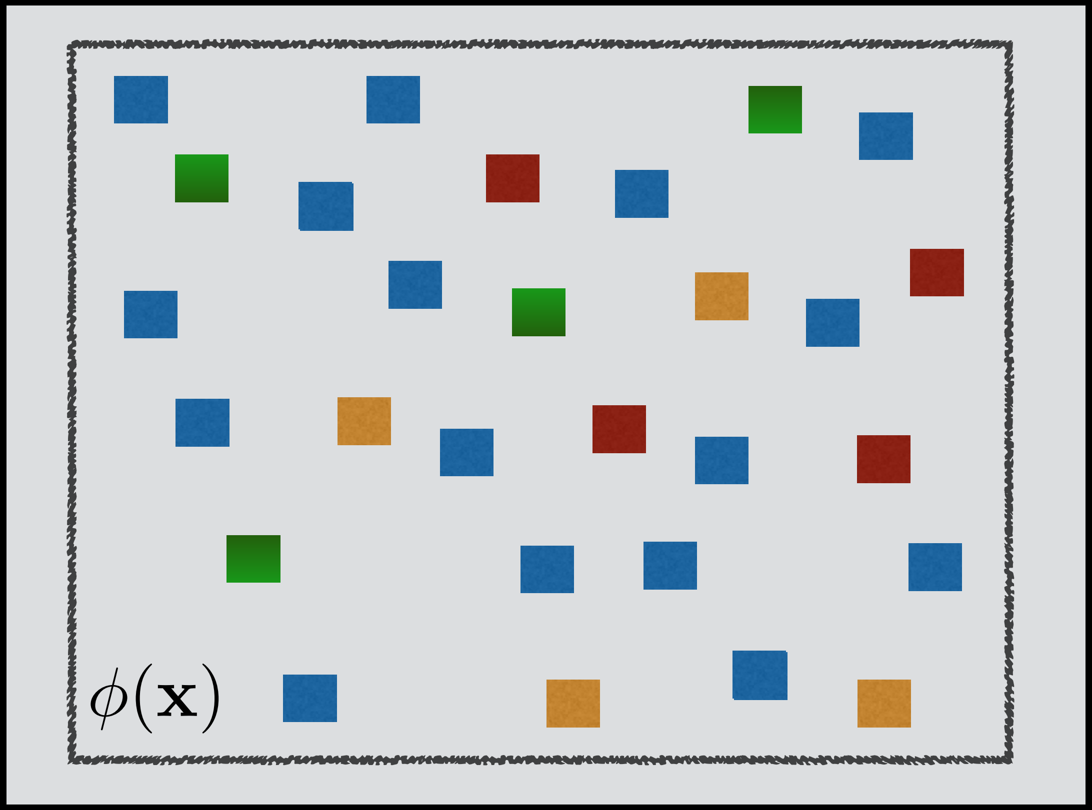
E.g. a correlation function:

$$G(\mathbf{x}) = \int \mathcal{D}\phi \; \mathcal{P}[\phi] \; \mathcal{G}[\phi, \mathbf{x}]$$

Sample with a **random number generator** that obeys $\mathcal{P}[\phi]$

Calculate for each sample



Sum over all possible $\phi(\mathbf{x})$ with weight $\mathcal{P}[\phi]$

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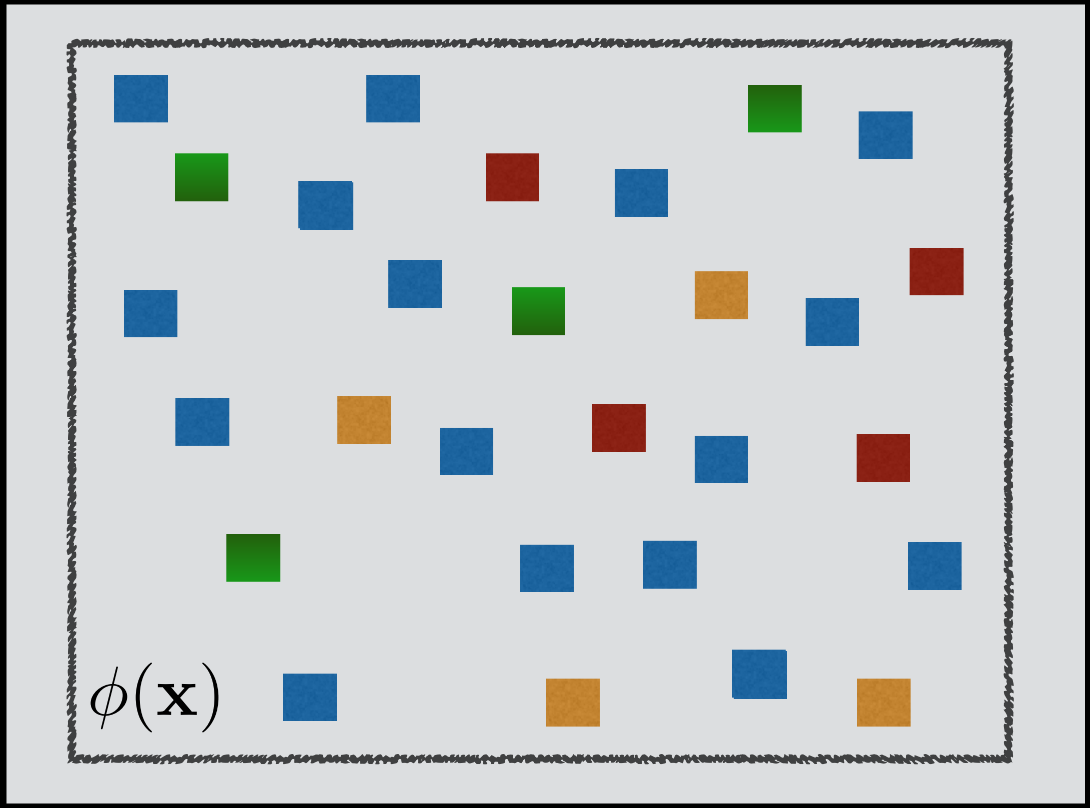

Sum over all possible $\phi(\mathbf{x})$ with weight $\mathcal{P}[\phi]$

Advantage: Doable

Disadvantage: Massive amounts of linear algebra and statistics involved. An important class of systems requires exponentially large statistics.

The challenge*

Random field generator $\mathcal{P}[\phi]$

Typically a very complicated function of the field that requires a large number of linear algebra operations to be evaluated.
(It's the determinant of a large and complicated matrix computed on the fly)

Can we use ML ideas to speed this up?

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Detecting phase transitions

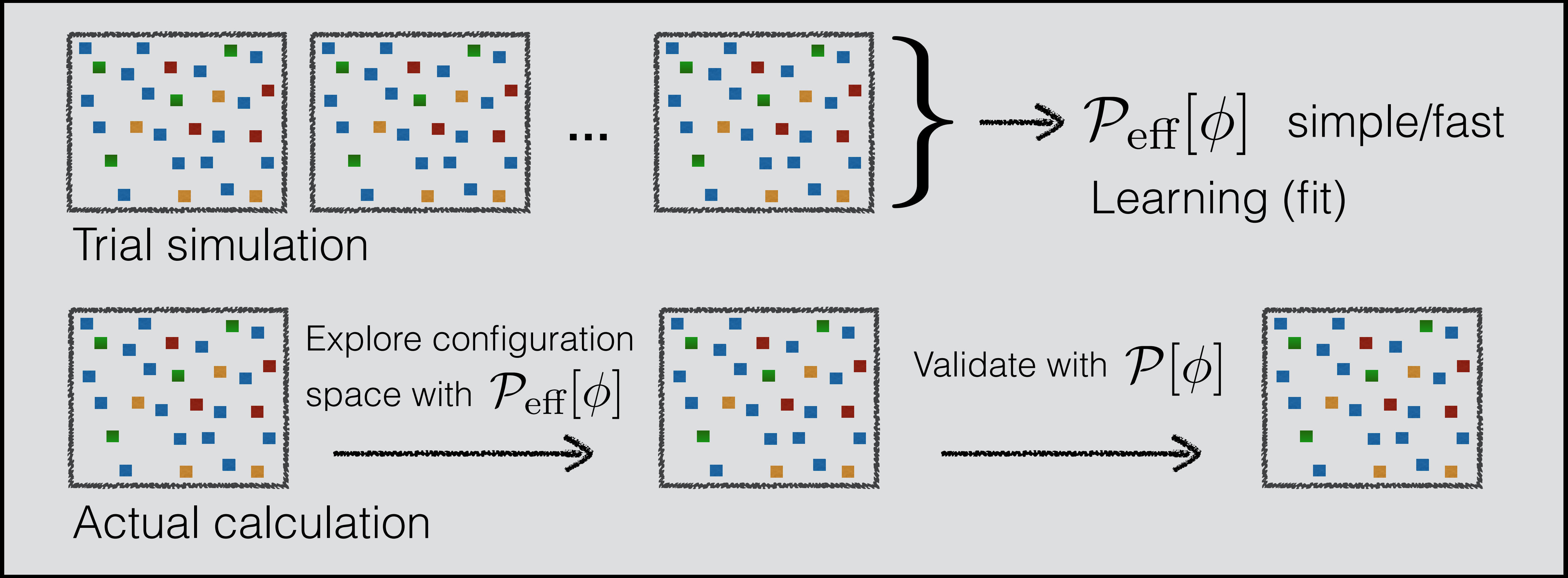
Correlation functions $G(\mathbf{x})$ can be expensive to compute, difficult to analyze, and not always available.

Can neural networks detect phase transitions in the fields ϕ *without computing specific observables?*

How machine learning is helping

Speeding up QMC using ML ideas: "Self-learning QMC"

Not using full-fledged deep learning, but inspired by it.



Fast *and* exact…as long as parametrization is robust

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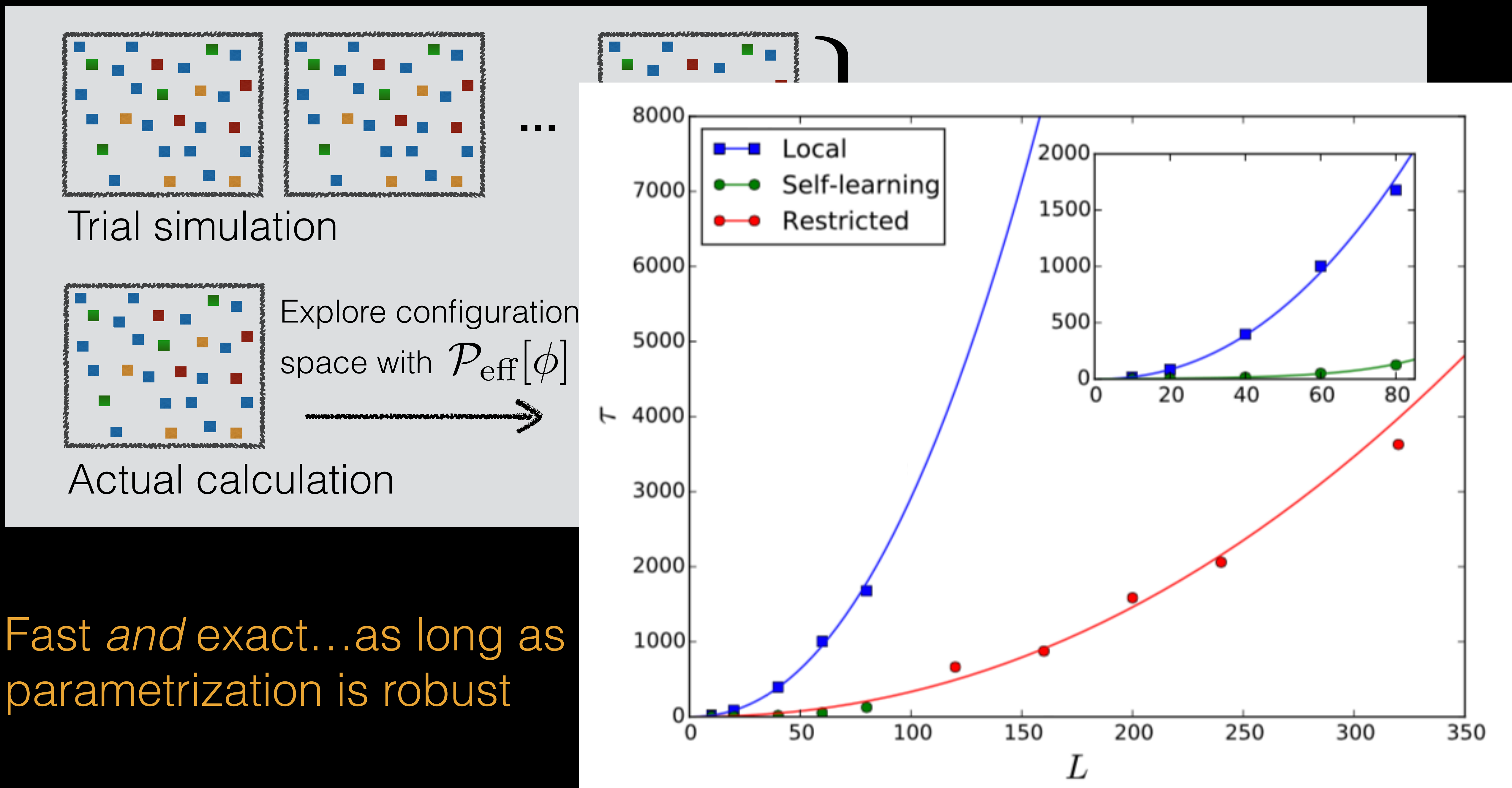

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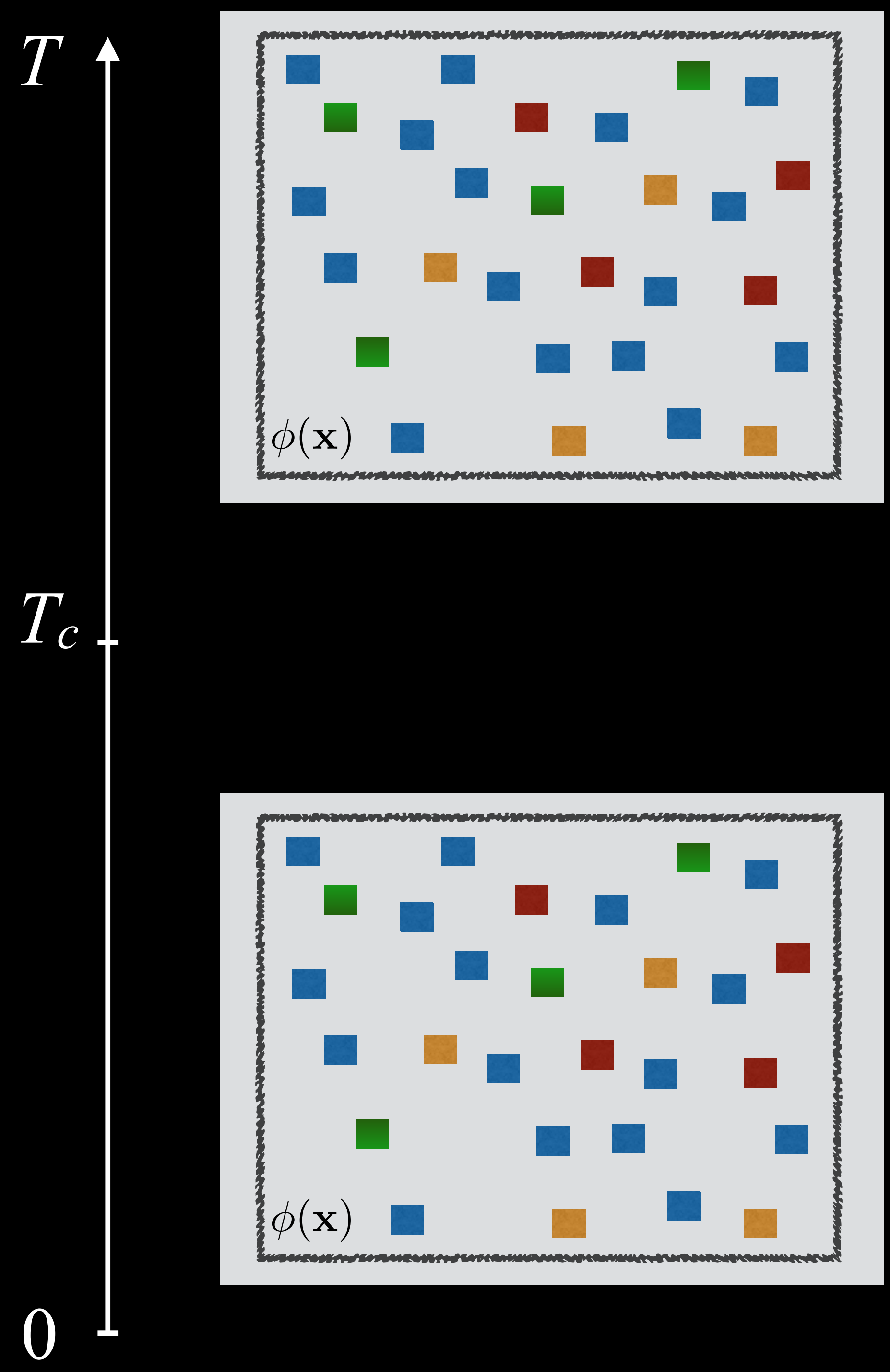
Liu et al. Phys. Rev. B **95**, 041101(R) (2017)

How machine learning is helping

Detecting phase transitions and critical phenomena:
"Machine learning phases of strongly correlated fermions"



"Normal"

"Antiferromagnet"

We can't tell the difference just by looking at the field!

Can a neural network learn to identify phases?

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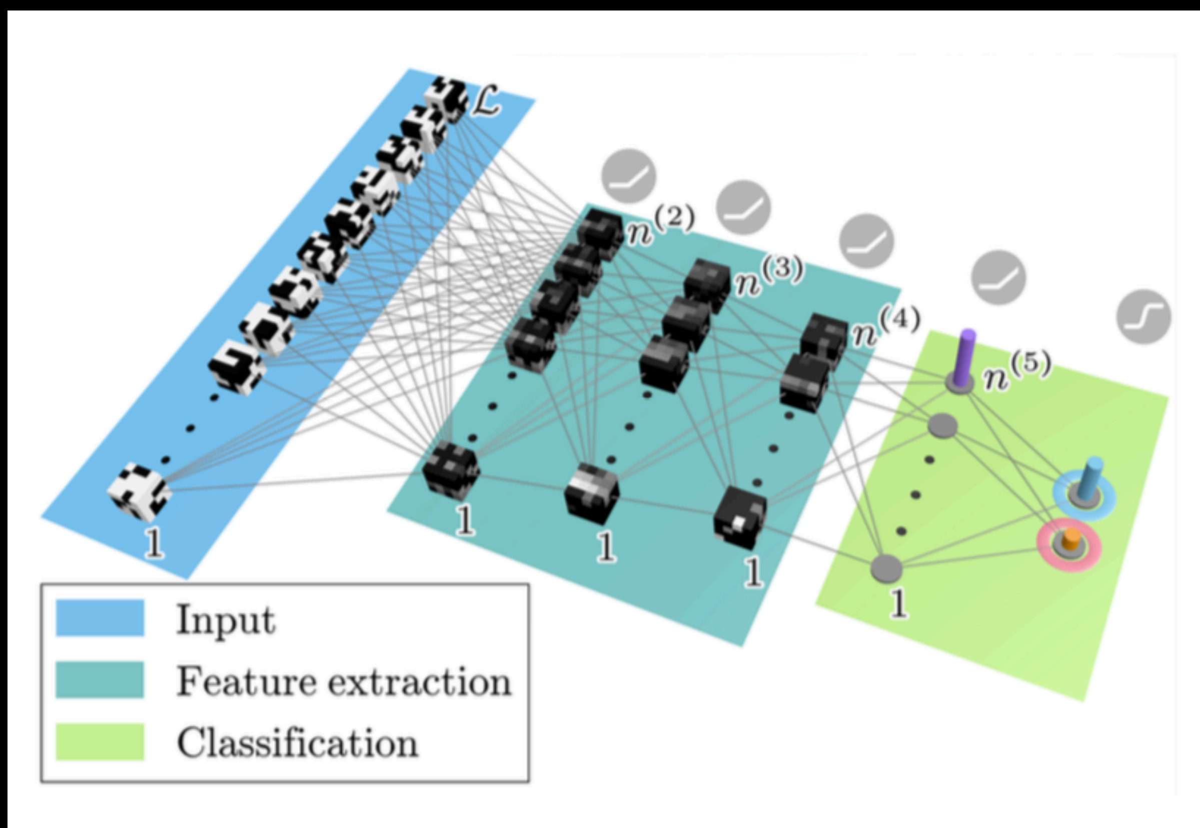
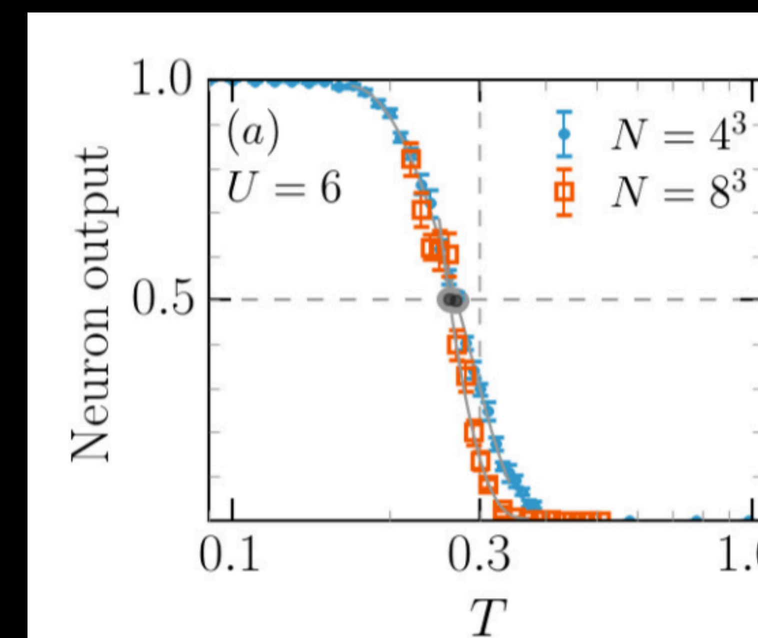


Use a 3D CNN!

Network maximally confused at phase transition temperature



K. Ch'ng, et al. Phys. Rev. X **7**, 031038 (2017)

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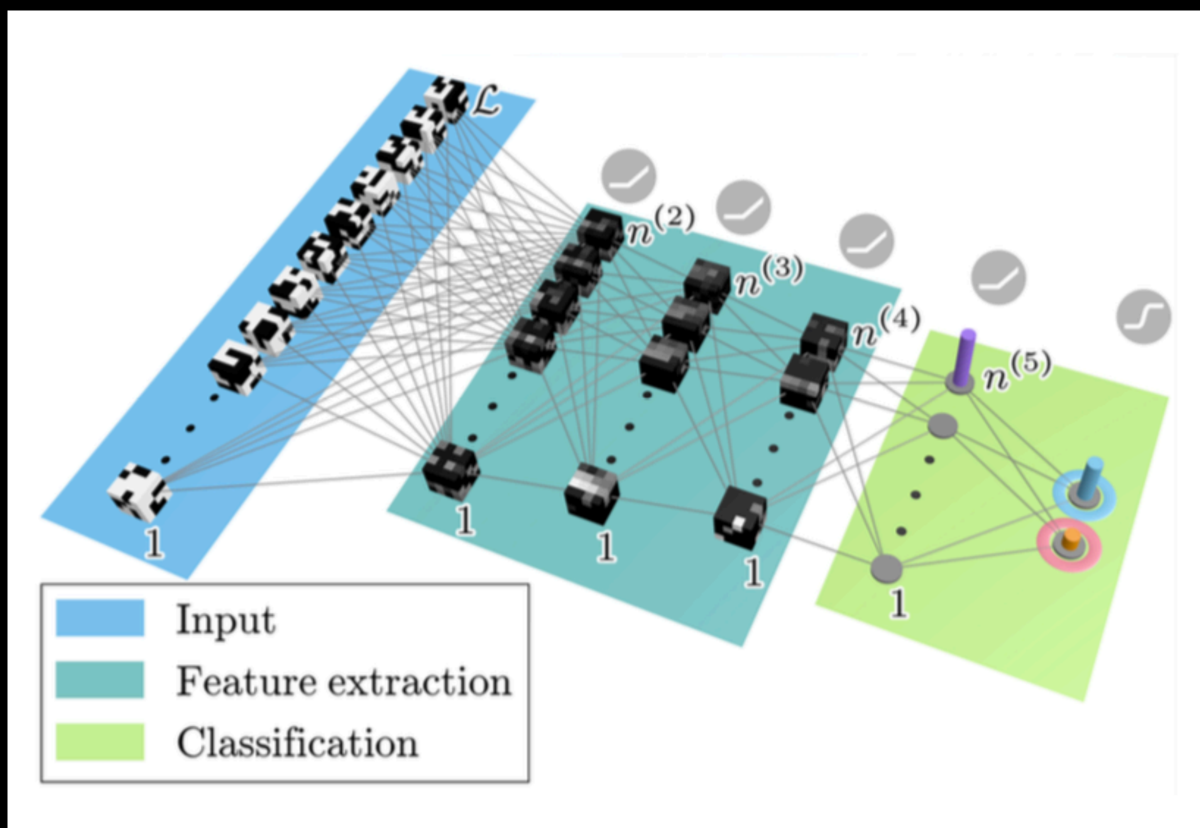

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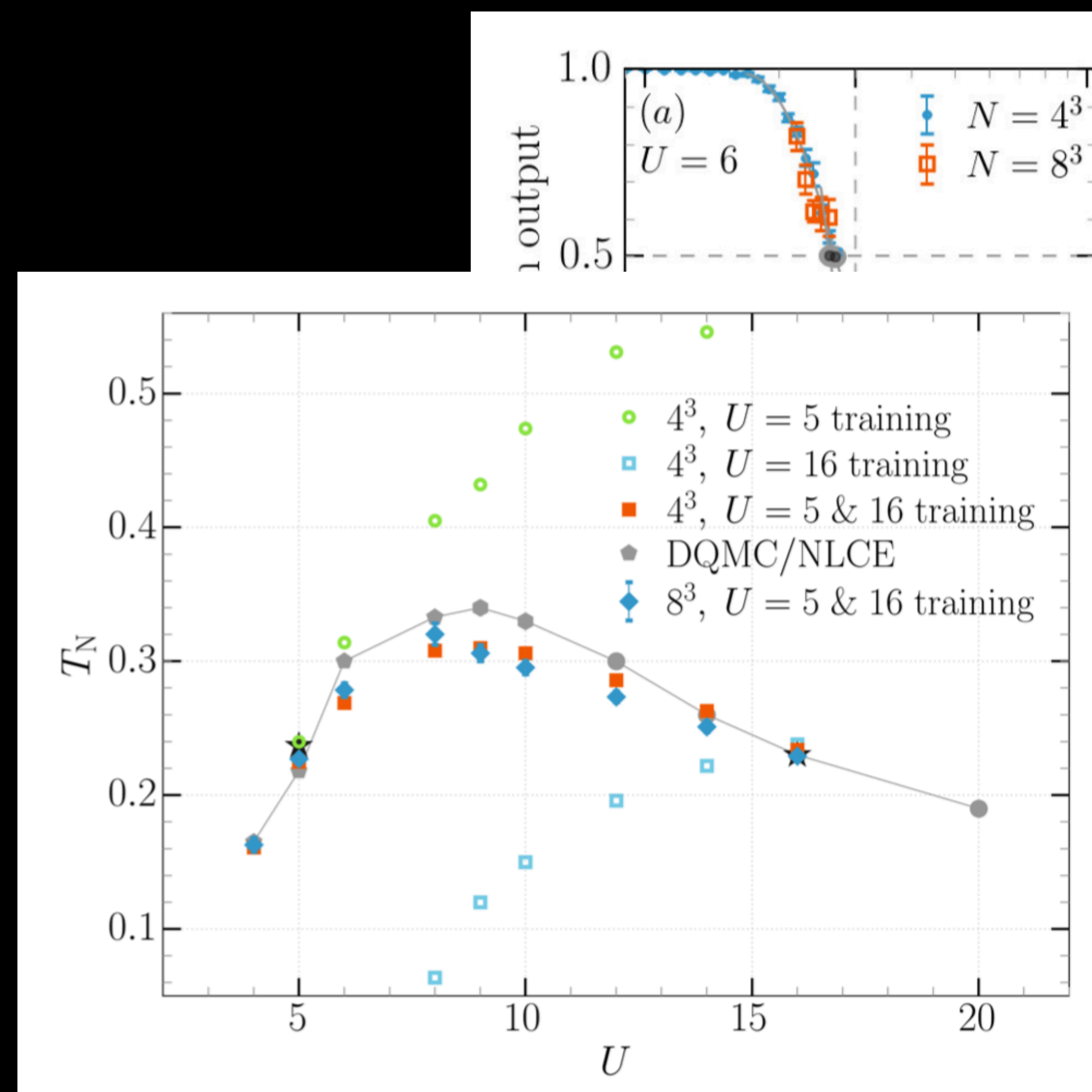


Phase diagram

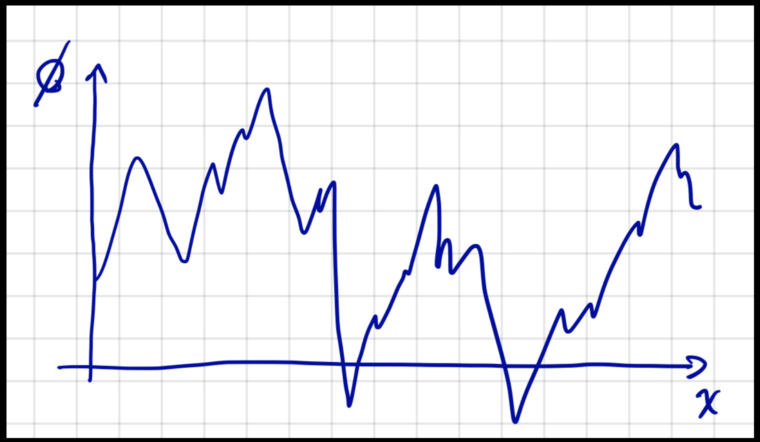
How machine learning is helping

Our forays using CNNs — quieting the sign problem

The **sign problem** is a serious roadblock that prevents important calculations in many areas of physics.

Imagine you would like to estimate an observable using a probability measure $\mathcal{P}[\phi]$, but varies in sign and is not well-defined.

$$\langle \mathcal{O} \rangle = \int \mathcal{D}\phi \, \mathcal{P}[\phi] \, \mathcal{O}[\phi]$$



Determining an accurate estimate for $\langle \mathcal{O} \rangle$ can be like finding a needle in a quantum haystack.

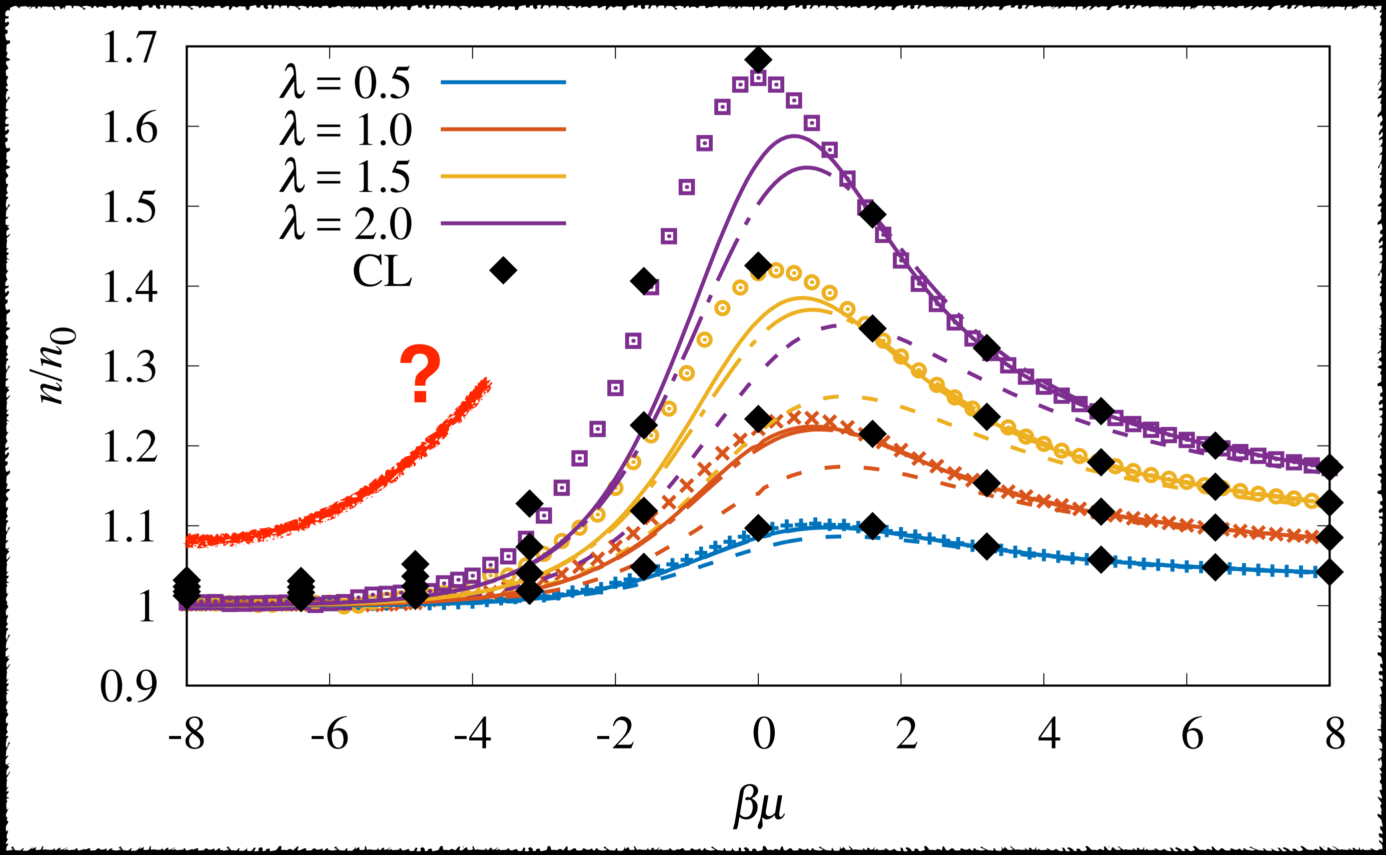
Can we use convolutional neural networks to more cheaply calculate observables when the sign problem worsens?

Learning for dilute quantum matter

The limit of **small densities** (or number of particles) is one region where the sign problem makes calculations difficult.

In our quantum Monte Carlo calculations, we are interested in thermodynamic quantities such as the **density equation of state**.

<u>The goal</u>: CNNs can enable explorations of stronger interactions by *working together* with quantum Monte Carlo algorithms.



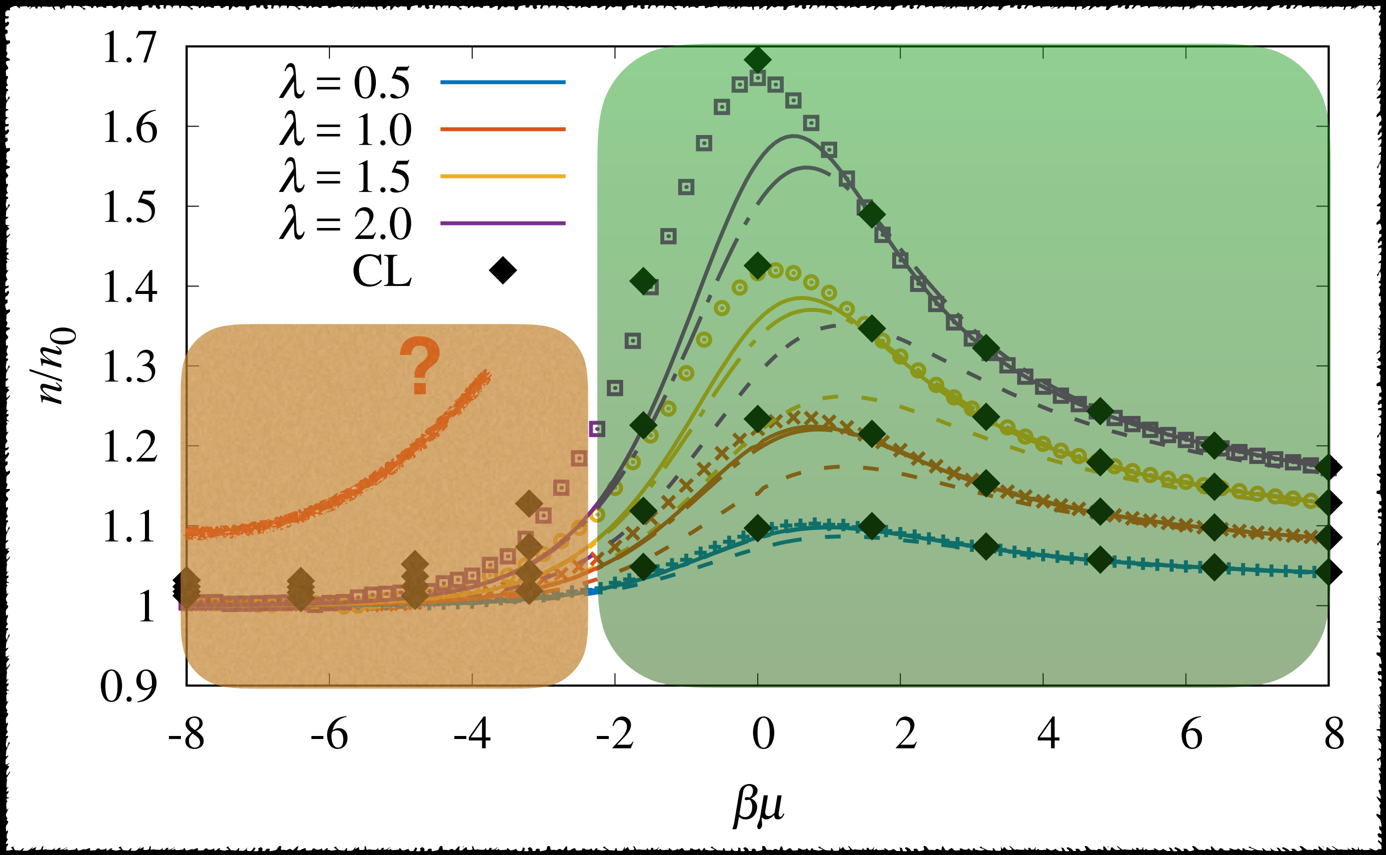
A. C. Loheac and J. E. Drut, Phys. Rev. D **95**, 094502 (2017)

Learning for dilute quantum matter

The goal: CNNs can enable explorations of stronger interactions by *working together* with quantum Monte Carlo algorithms.

Use field configurations from the deep quantum regime (where the signal-to-noise is better) as training data.

Virial region
Can a CNN help QMC make an accurate prediction here?



Deep quantum regime
Can we use this data to train a CNN?

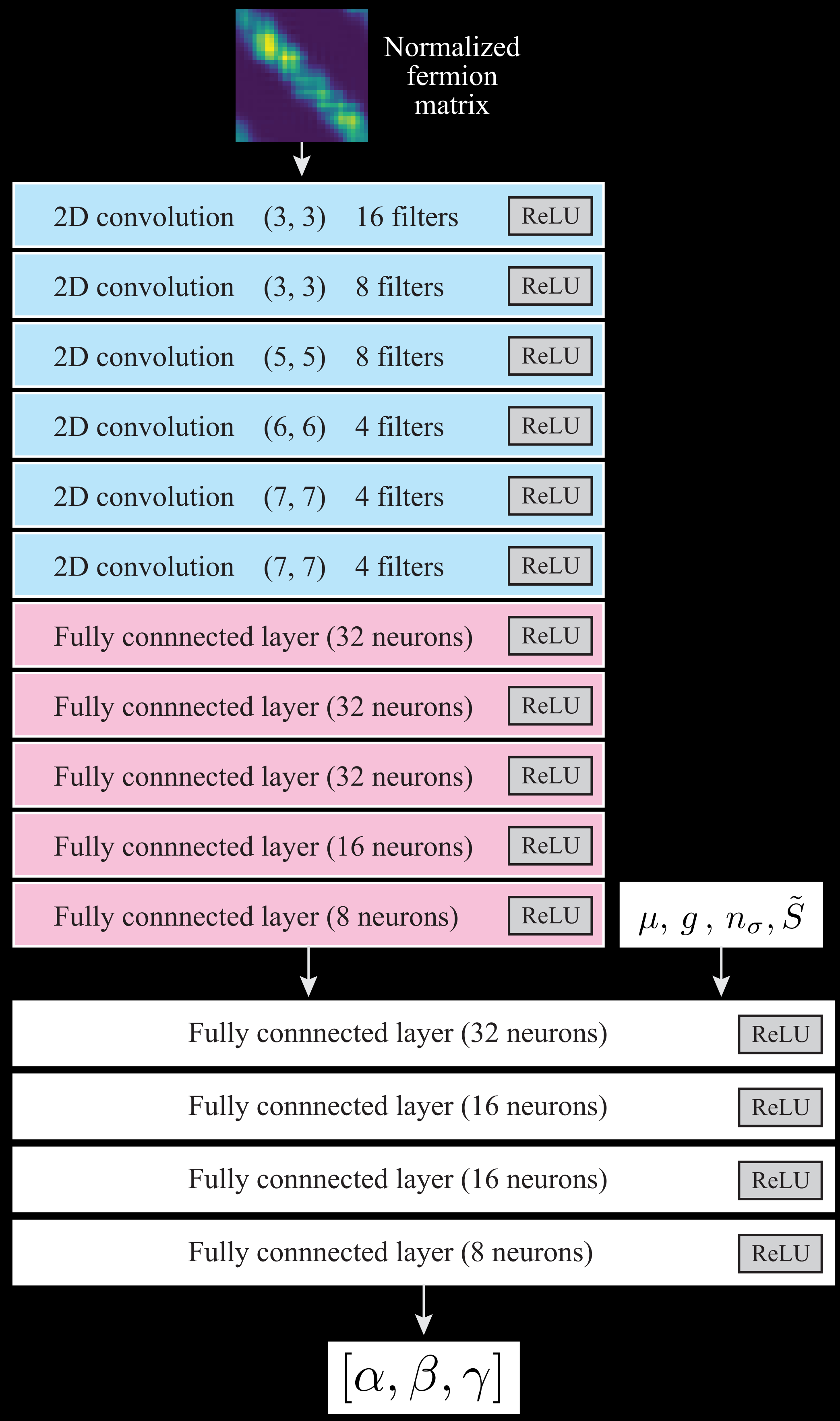
A. C. Loheac and J. E. Drut, Phys. Rev. D **95**, 094502 (2017)

Learning for dilute quantum matter

Network architecture

- Network uses both convolutional and dense layers.
- Implemented in Keras/TensorFlow.
- **Inputs:**
  - normalized form of fermion matrix
  - interaction strength
  - chemical potential
  - value of the fermion determinant
- **Output:** classification of field configuration:
  - $> 20\%$ error in density
  - between 10% and 20% error
  - $< 10\%$ error

~14,500 parameters.
Trained with ~150k - 300k samples.
Design still being optimized.



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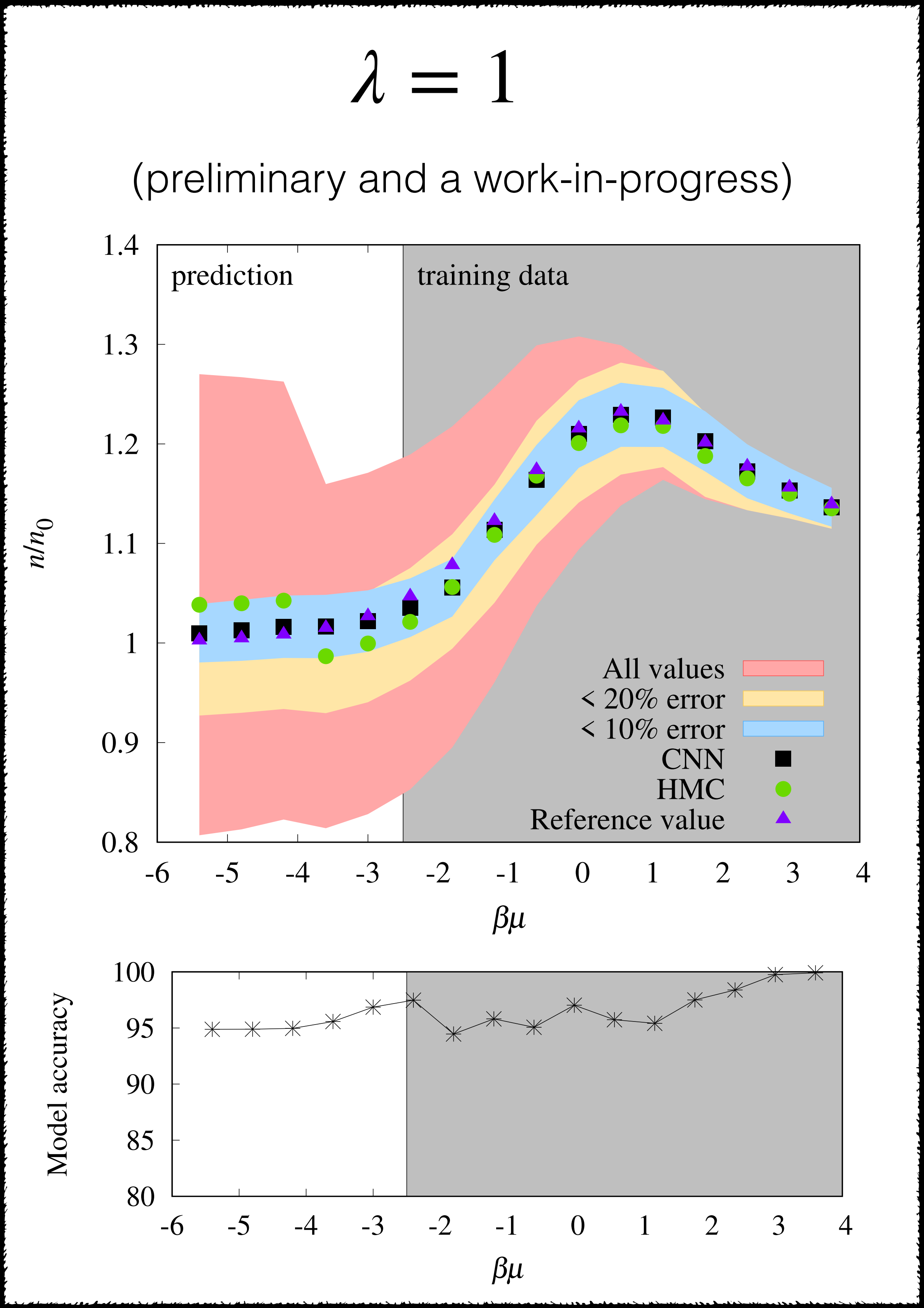


Shaded area shows the standard deviation σ of densities for each bin of field configurations.

The **red** areas show σ for the original Monte Carlo data.

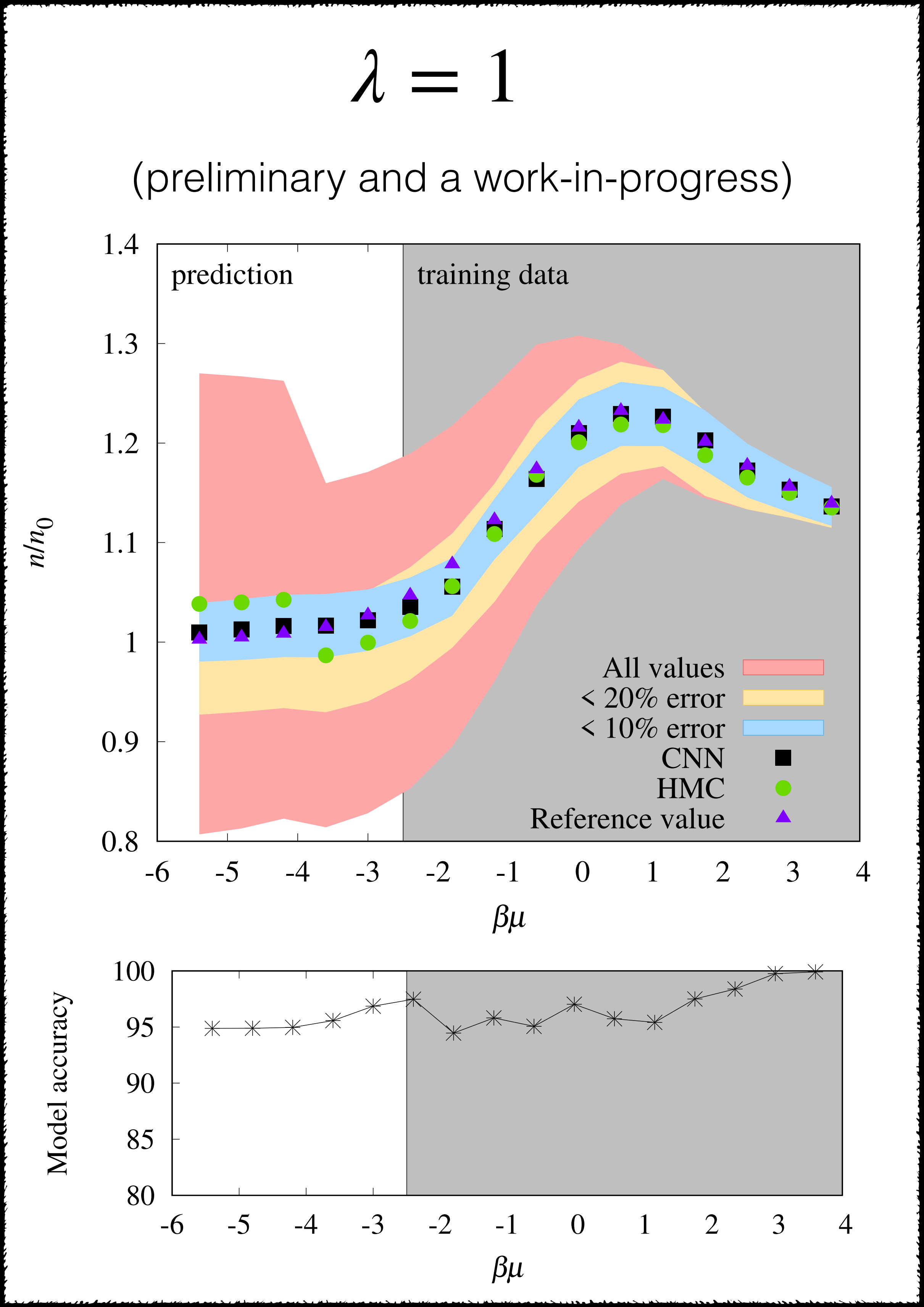
The **yellow** areas show σ for subset of configurations whose error is < 20%.

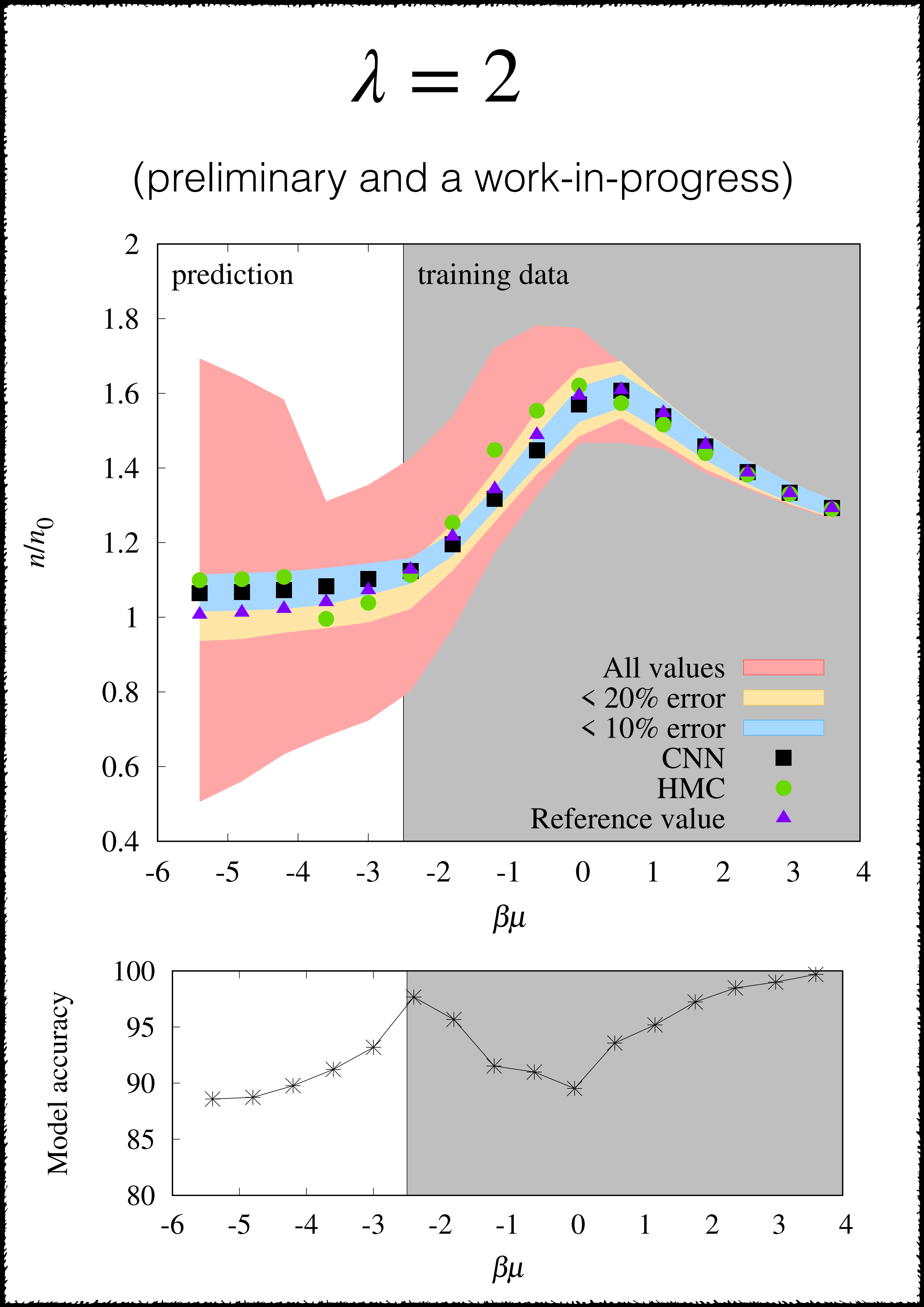
The **blue** areas: error < 10%.

Large σ — severe sign problem.

CNN improves limits drastically.

Learning for dilute quantum matter





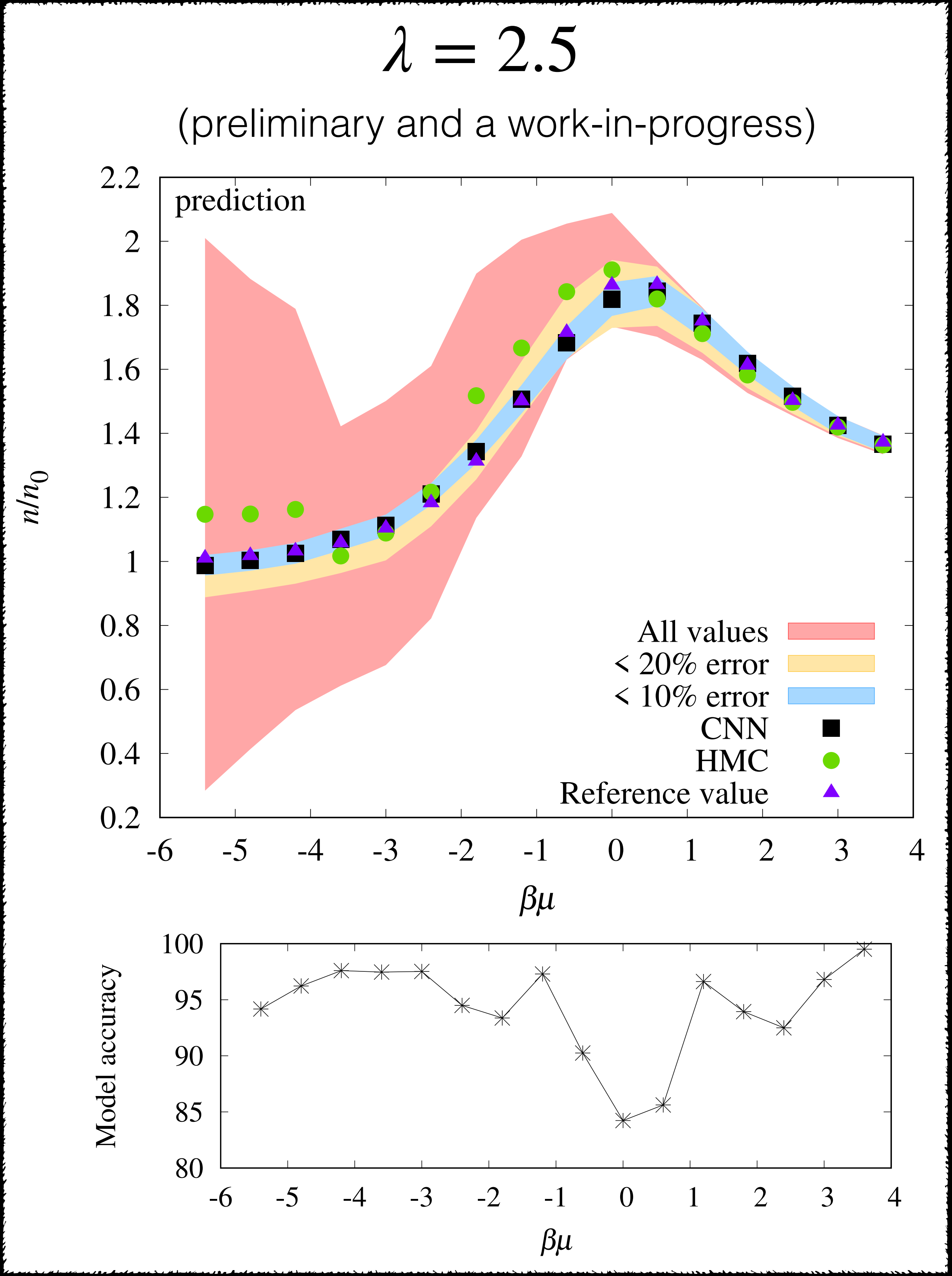
Learning for dilute quantum matter

<u>Entirely a prediction.</u>

The neural network can make small extrapolations to higher interaction strengths it has not seen before.

Potentially very useful for our studies under a severe sign problem!

Step one in a longer-term goal.



Summary & conclusions

Understanding quantum matter is a challenging problem for physics at all scales: **from inside atomic nuclei to materials and star interiors**;

The computational challenge has a **linear algebra** side and a **statistics** side;

Machine learning is helping both sides simultaneously: the essential aspects of **quantum dynamics can be learned with deep networks**;

However, networks work **together** with conventional methods to yield more efficient approaches - they do not replace them.

Thank you!