

Using Machine Learning to Calculate the Energy of Infinite Nuclear Matter Systems

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Outline

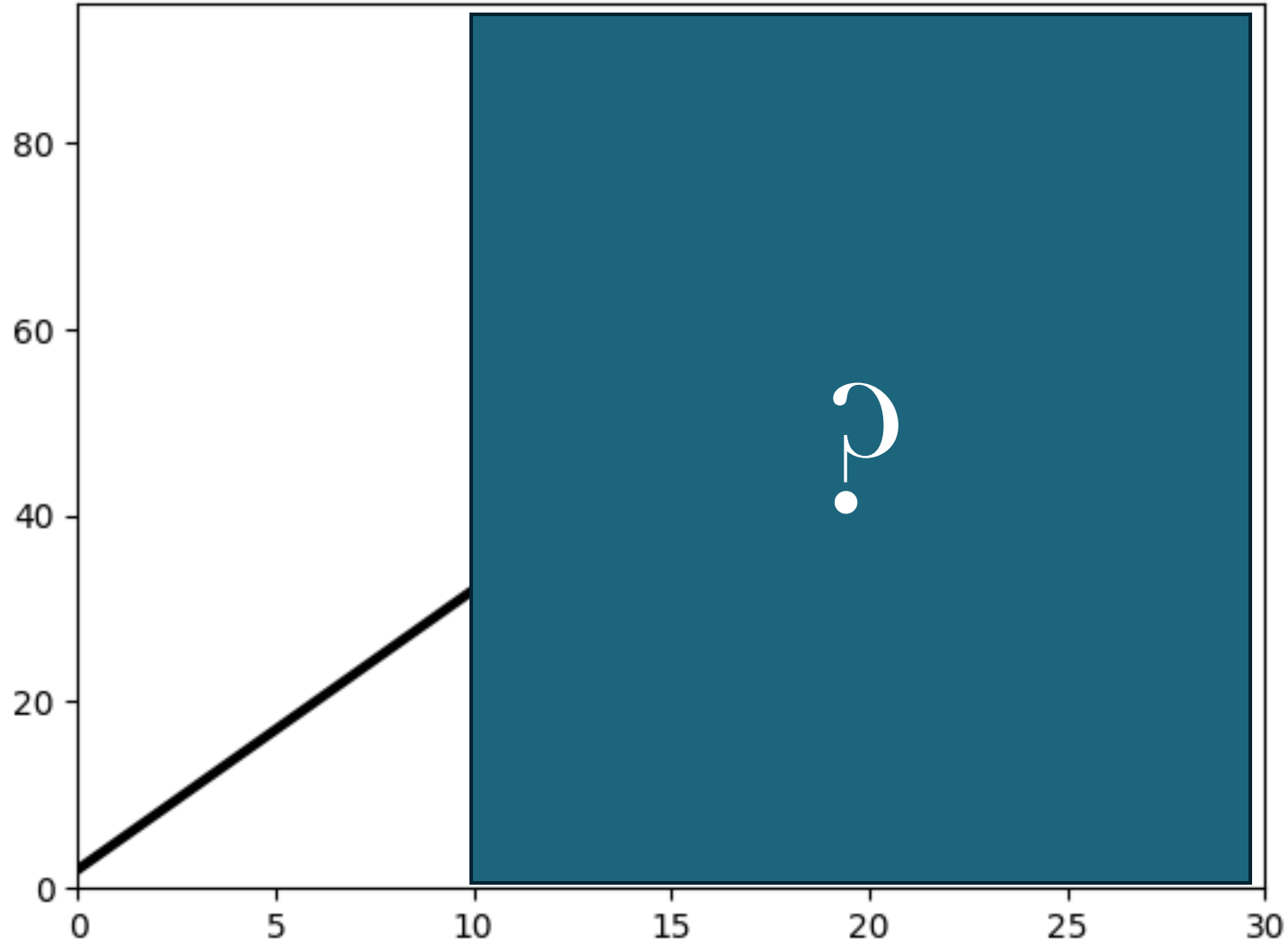
- What is Extrapolation?
- Introduction to Many-Body Physics
- Sequential Regression Extrapolation (SRE)
- Conclusion and Applications



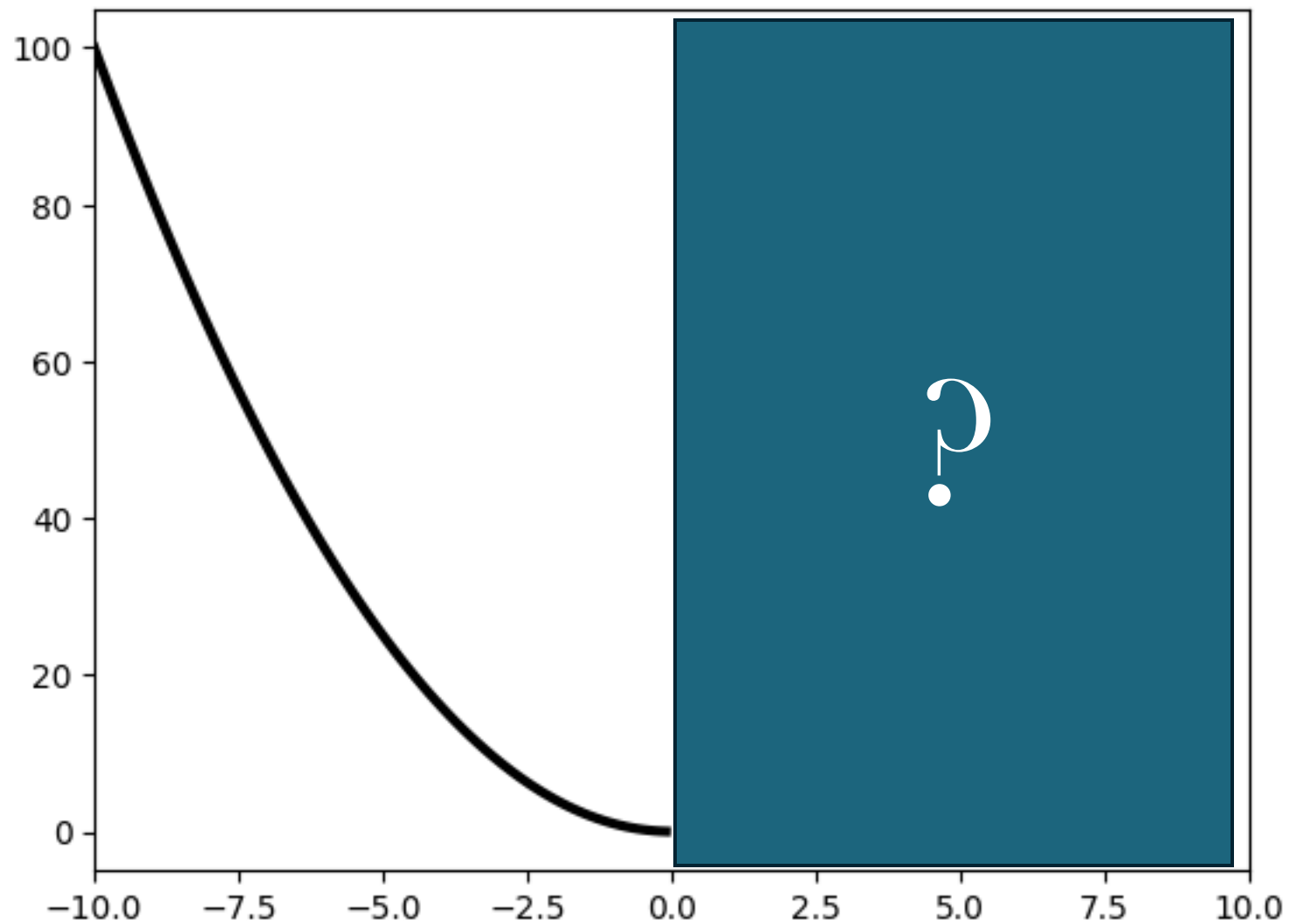
What is Extrapolation?

The action of estimating or concluding something by assuming that existing trends will continue or a current method will remain applicable. -Oxford Dictionary

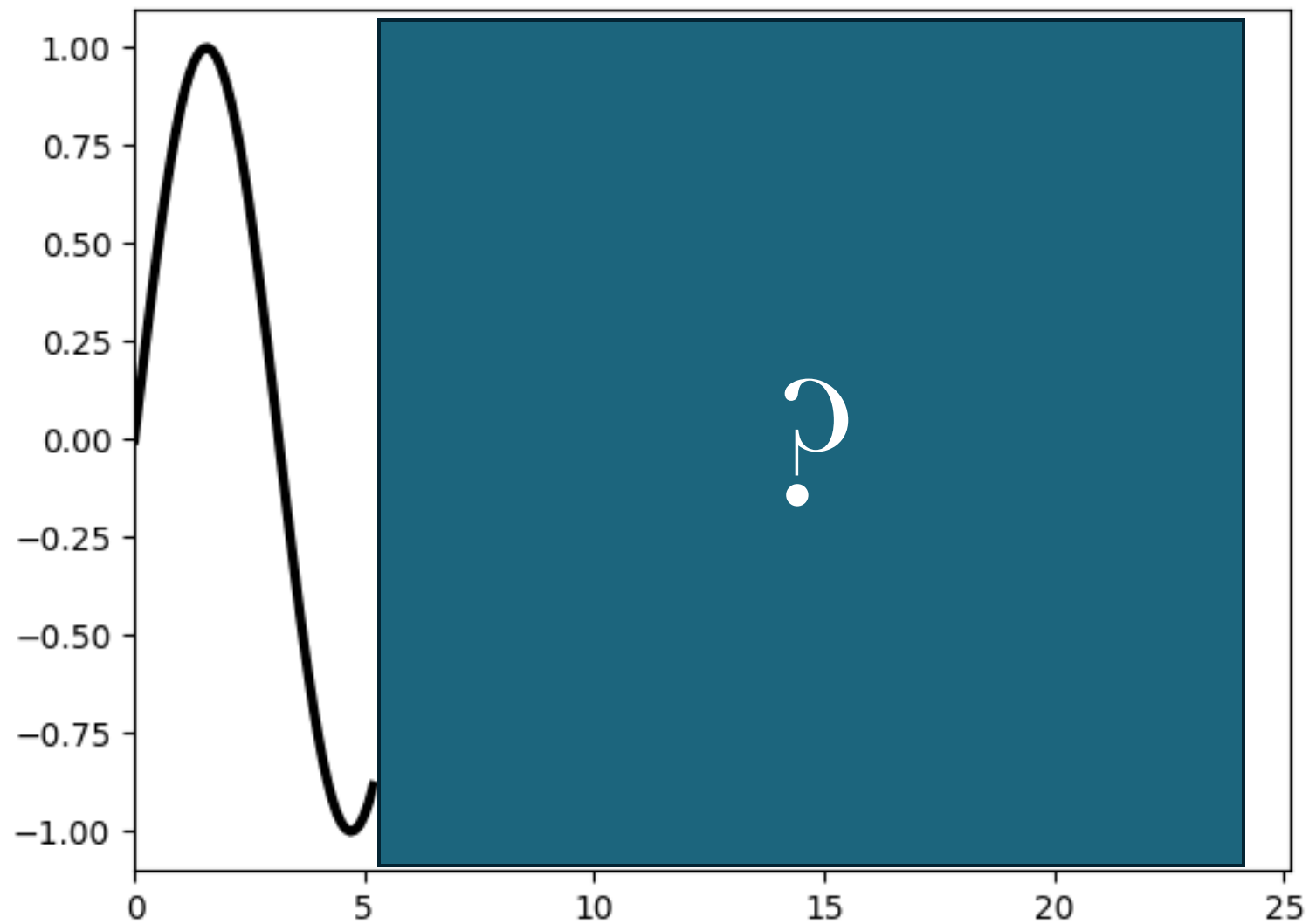
Extrapolation Example 1



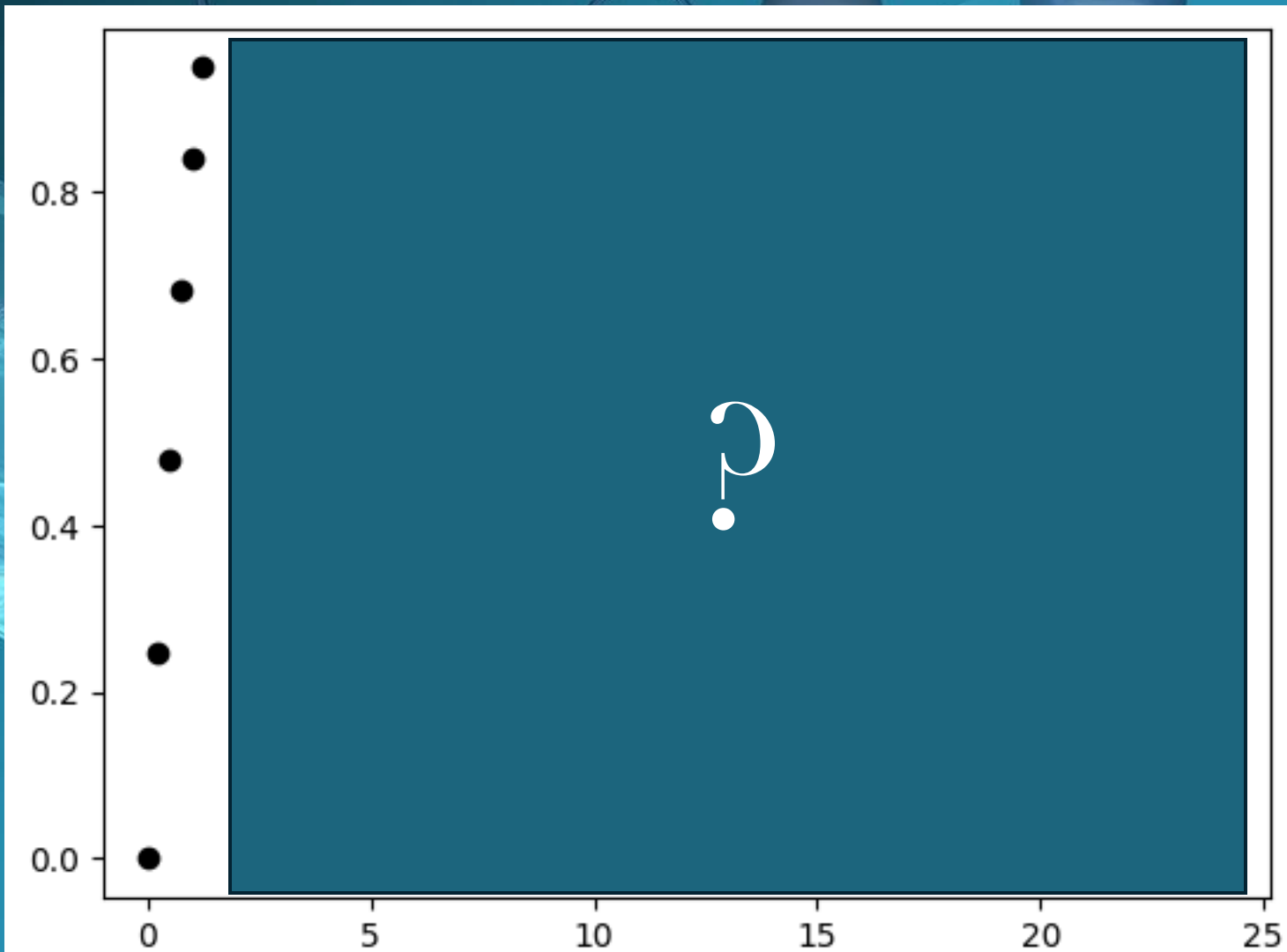
Extrapolation Example 2



Extrapolation Example 3



Example Extrapolation 4

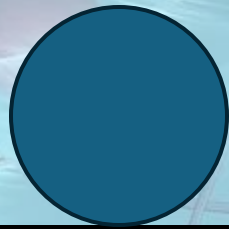


Introduction to Many-Body Physics

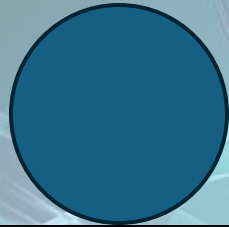
Particle (Proton or Neutron)

Single Particle State

How many configurations?



Introduction to Many-Body Physics



Excitation: Moving to a higher single particle state

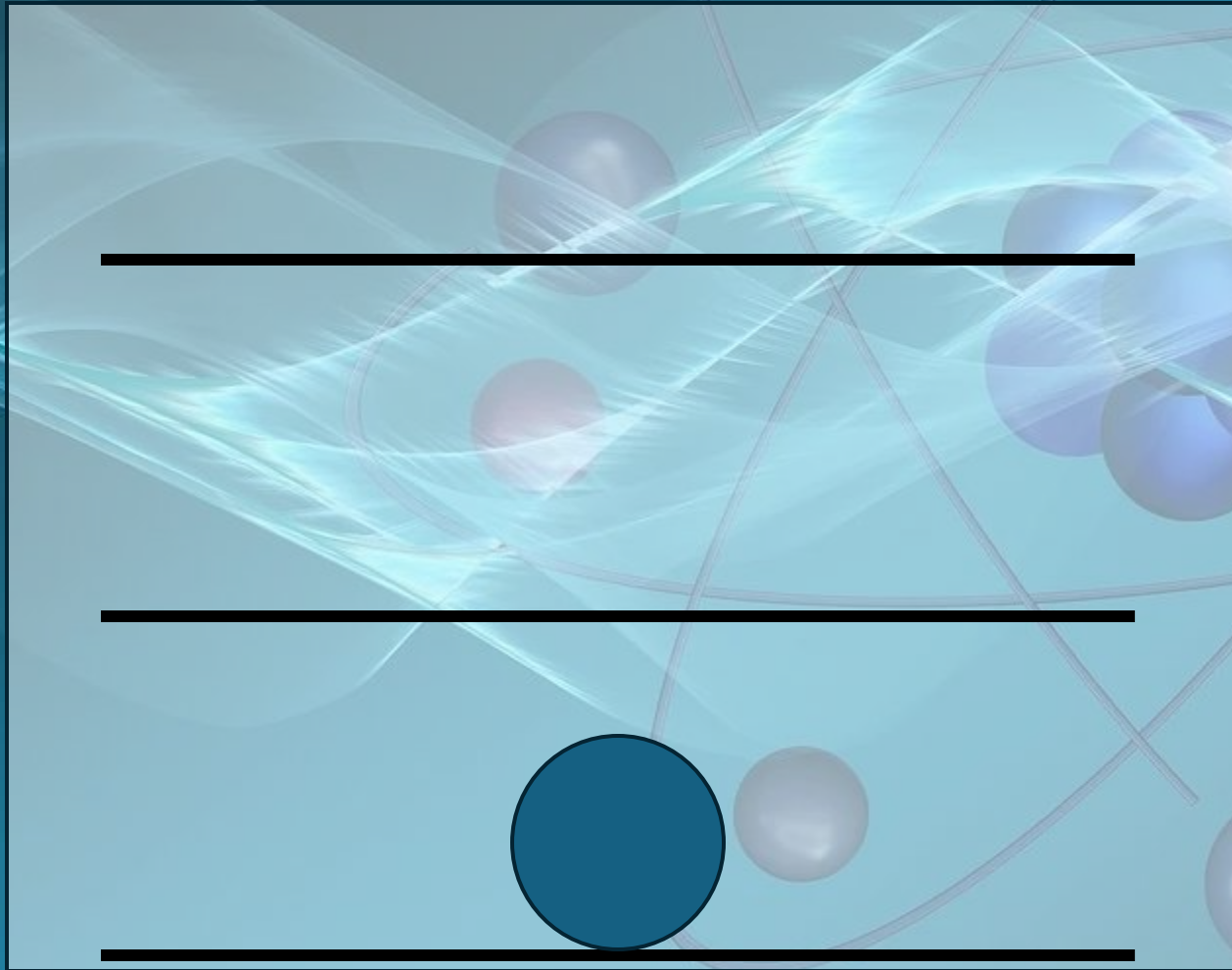
How many configurations?

Introduction to Many-Body Physics

Deexcitation: Moving to a higher single particle state

How many configurations?

Three configurations

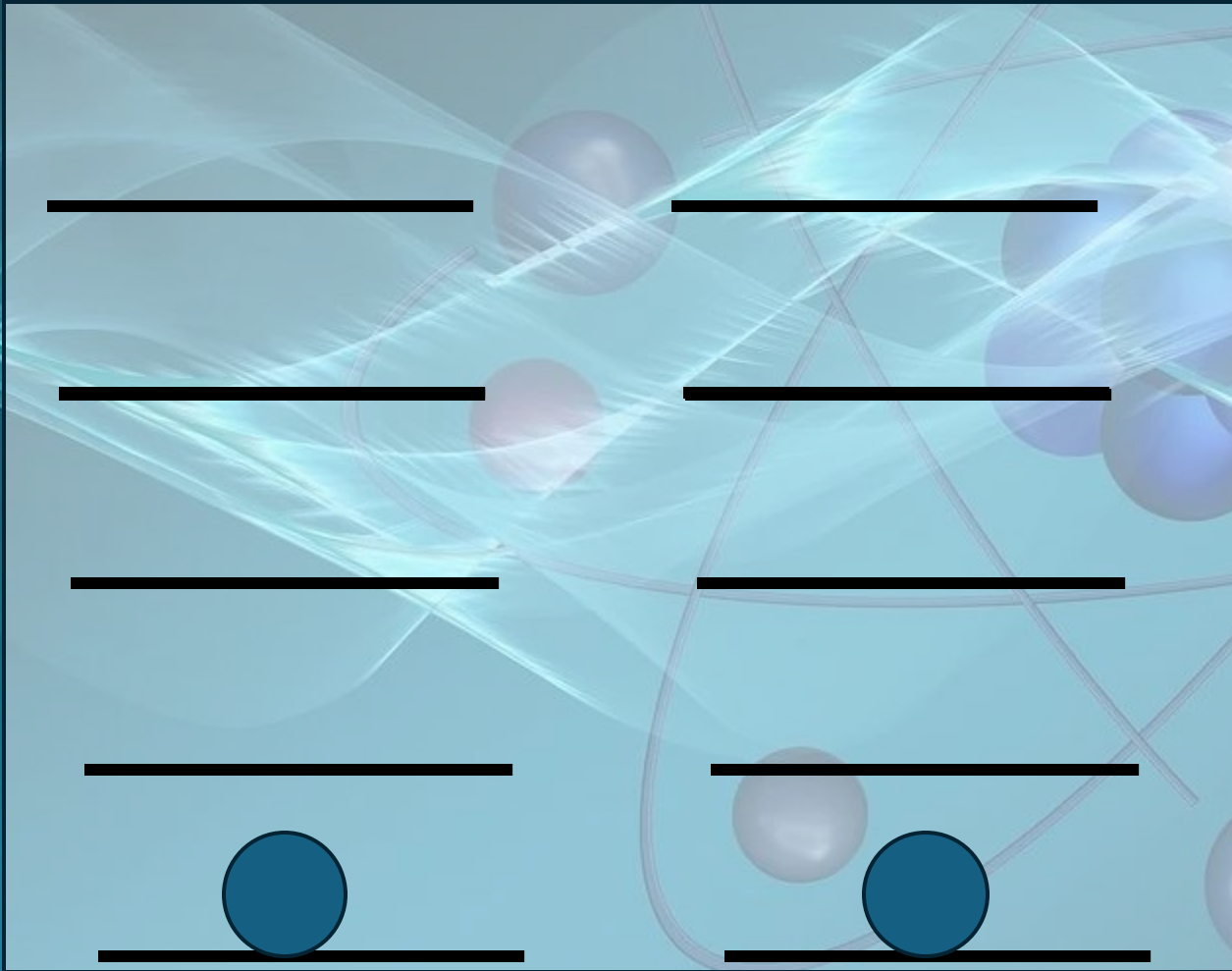


Introduction to Many-Body Physics

Two-Particle Example

Degenerate Single Particle States

How many configurations?

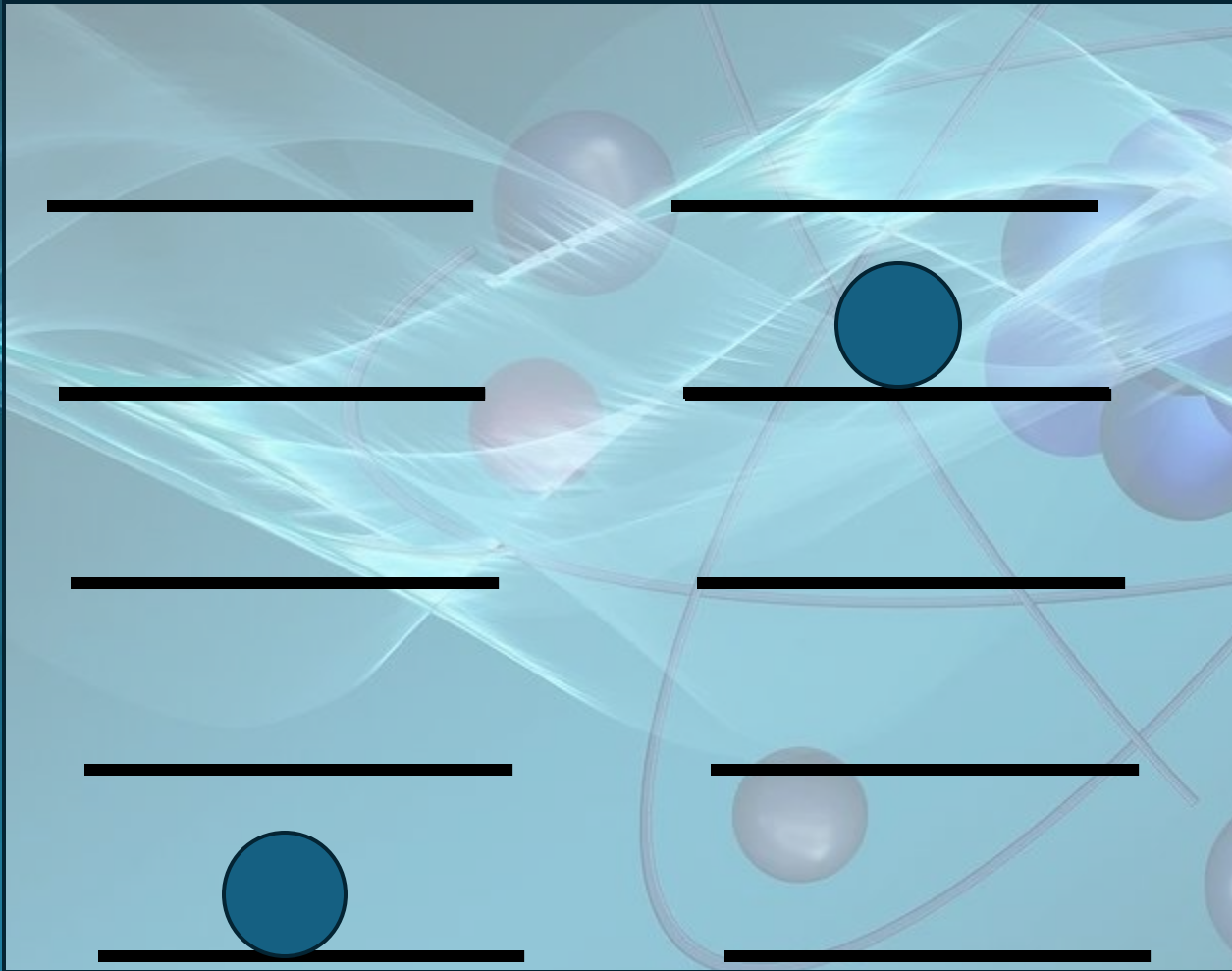


Introduction to Many-Body Physics

Two-Particle Example

Degenerate Single Particle States

How many configurations?

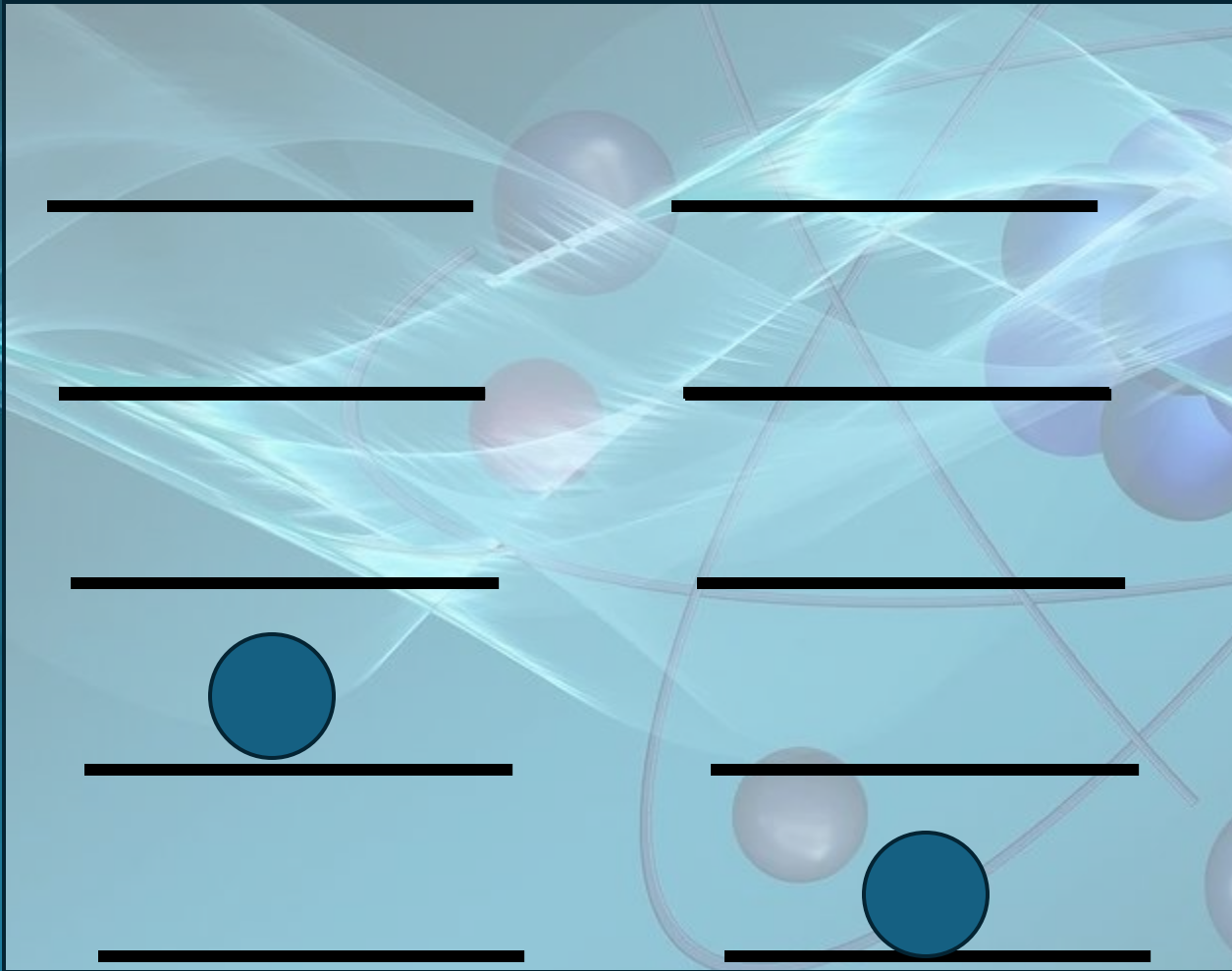


Introduction to Many-Body Physics

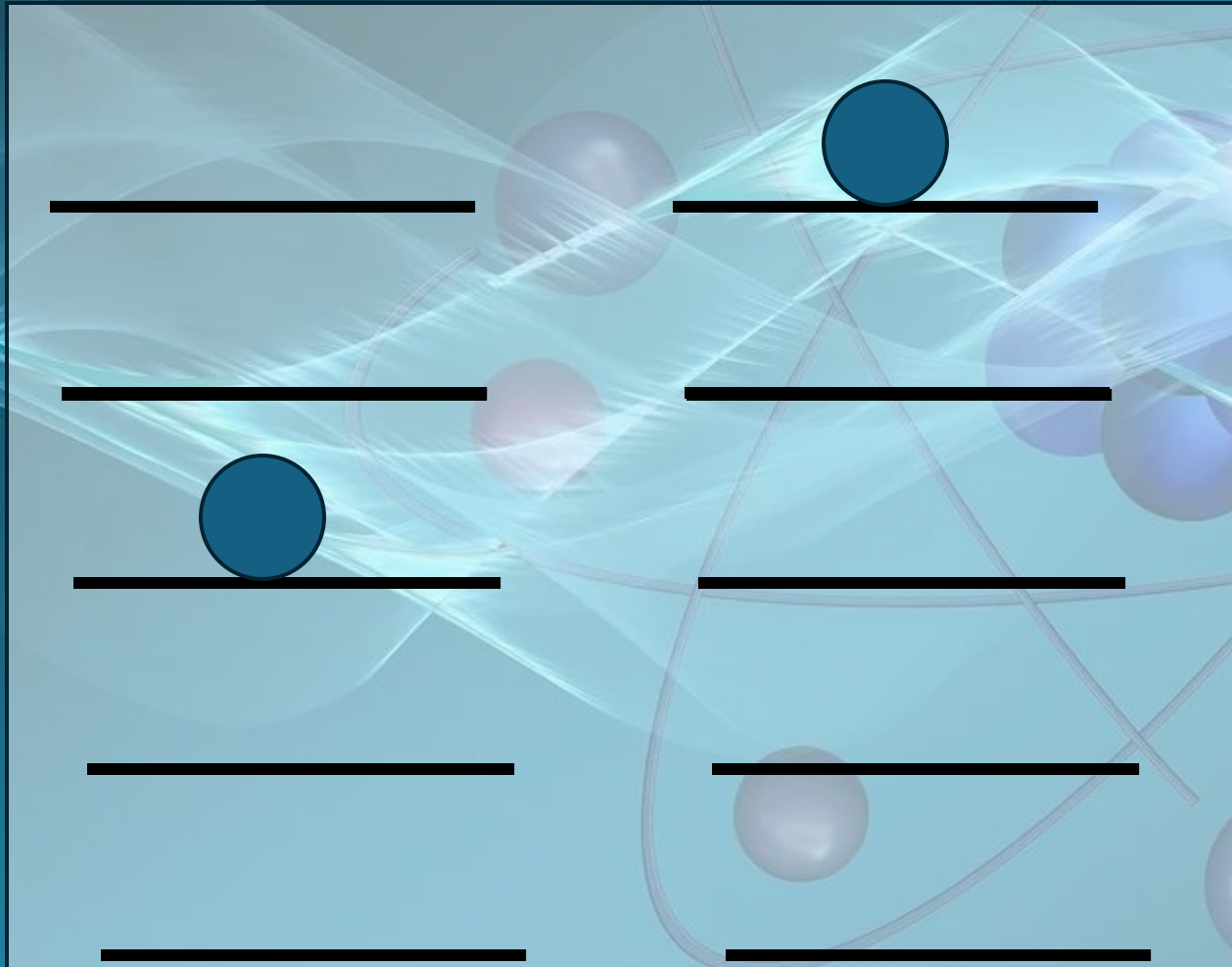
Two-Particle Example

Degenerate Single Particle States

How many configurations?



Introduction to Many-Body Physics



Two-Particle Example

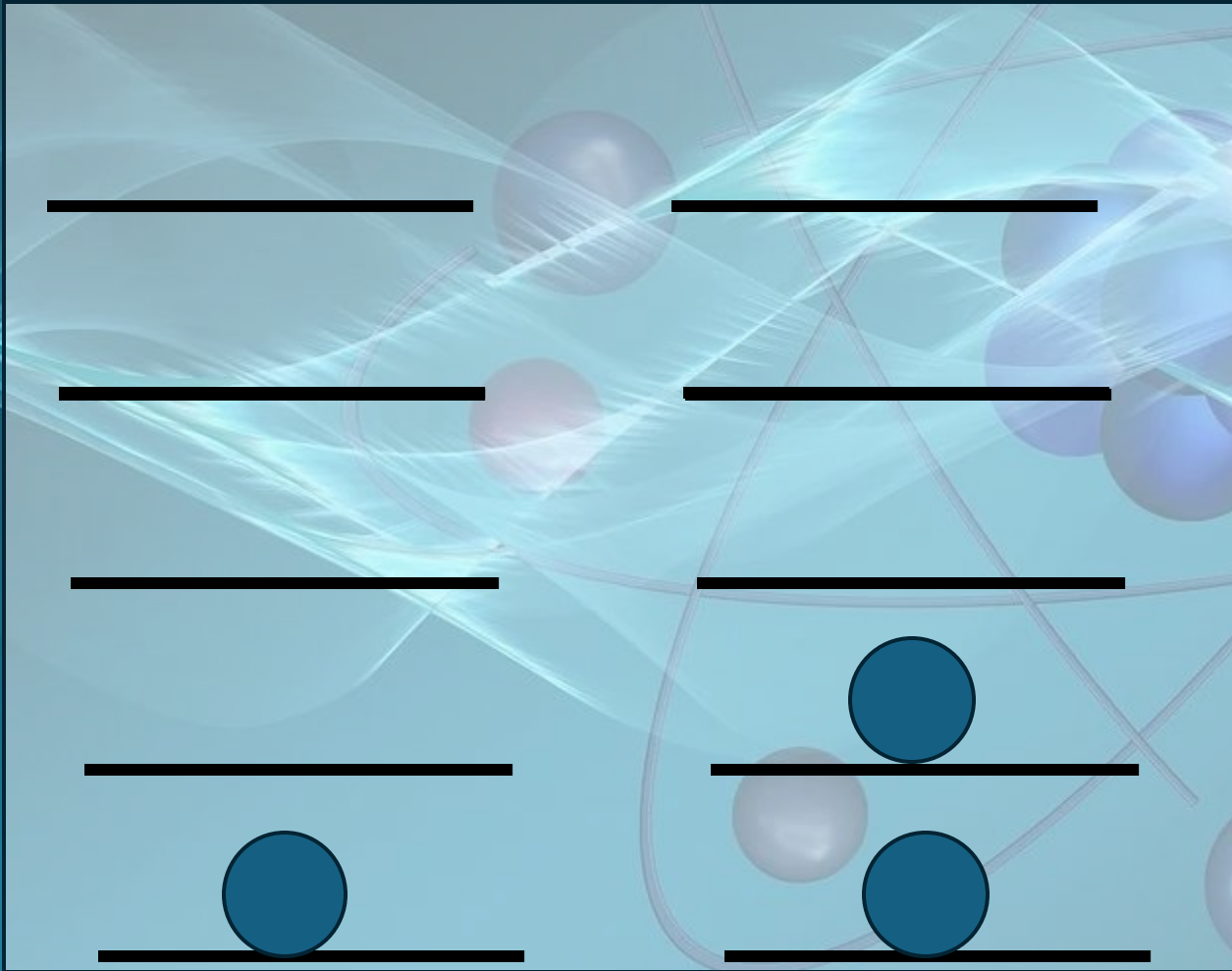
Degenerate Single Particle States

How many configurations?
45 configurations

Introduction to Many-Body Physics

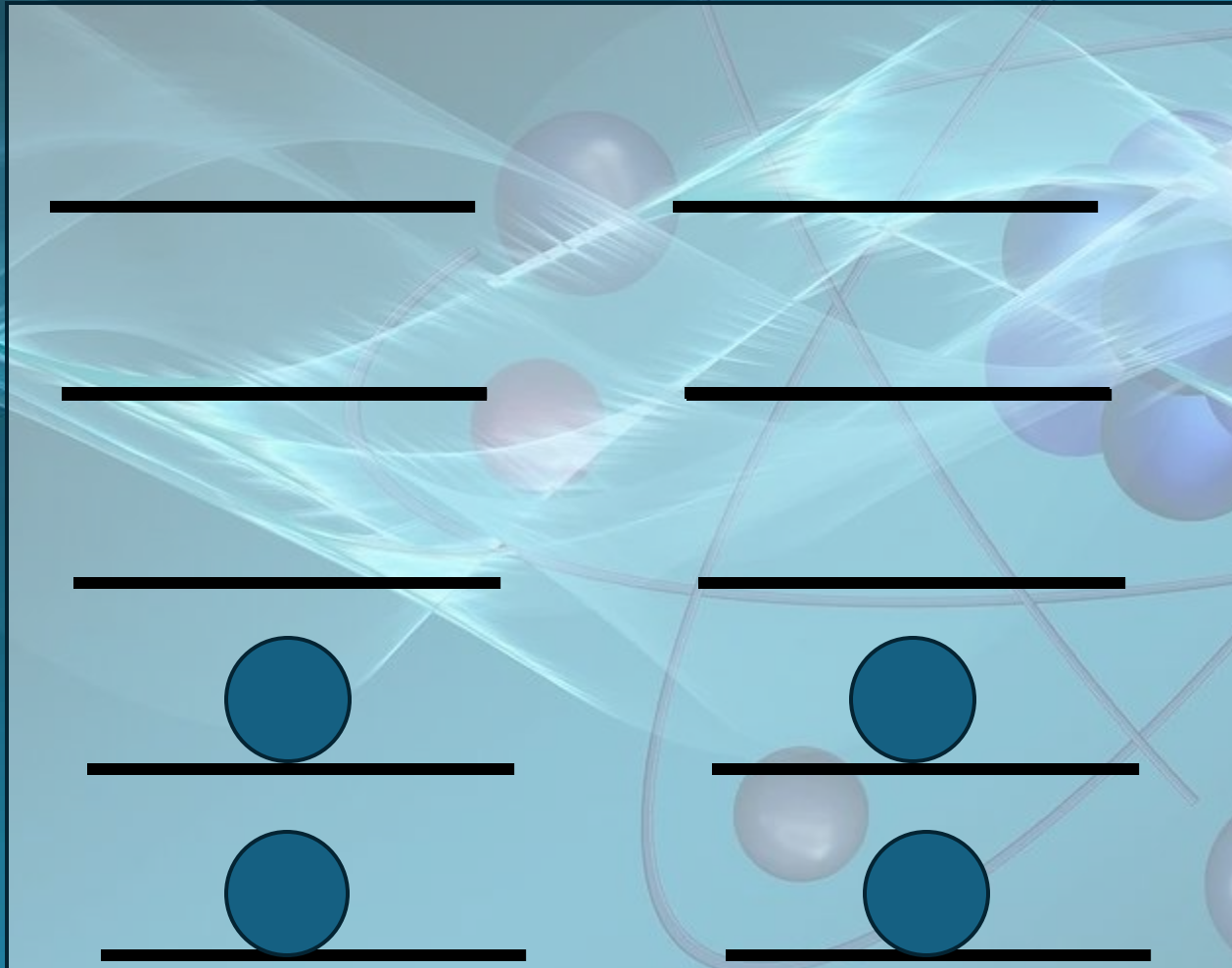
Three-Particle Example

How many configurations?
120 configurations



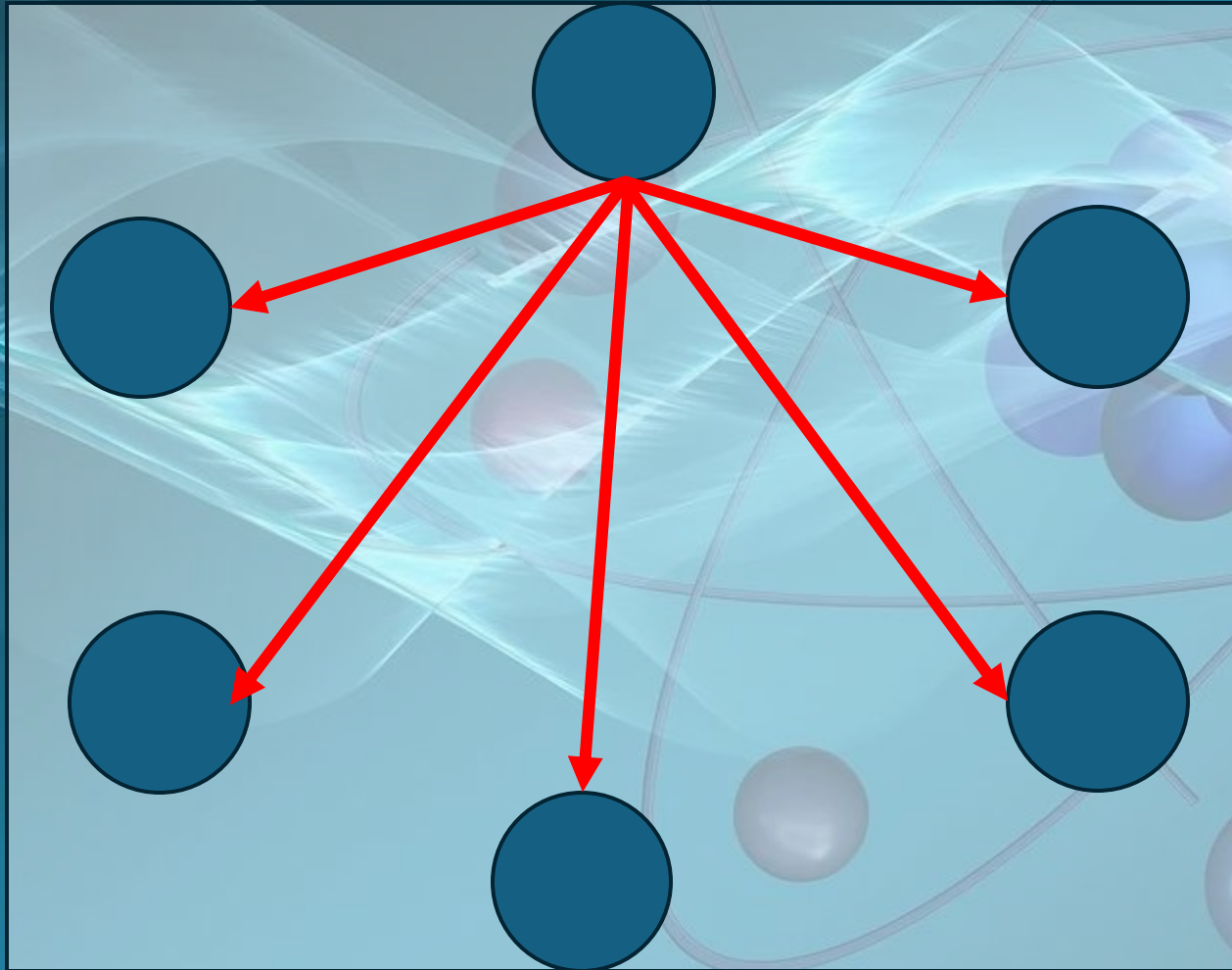
Introduction to Many-Body Physics

Four-Particle Example



How many configurations?
210 configurations

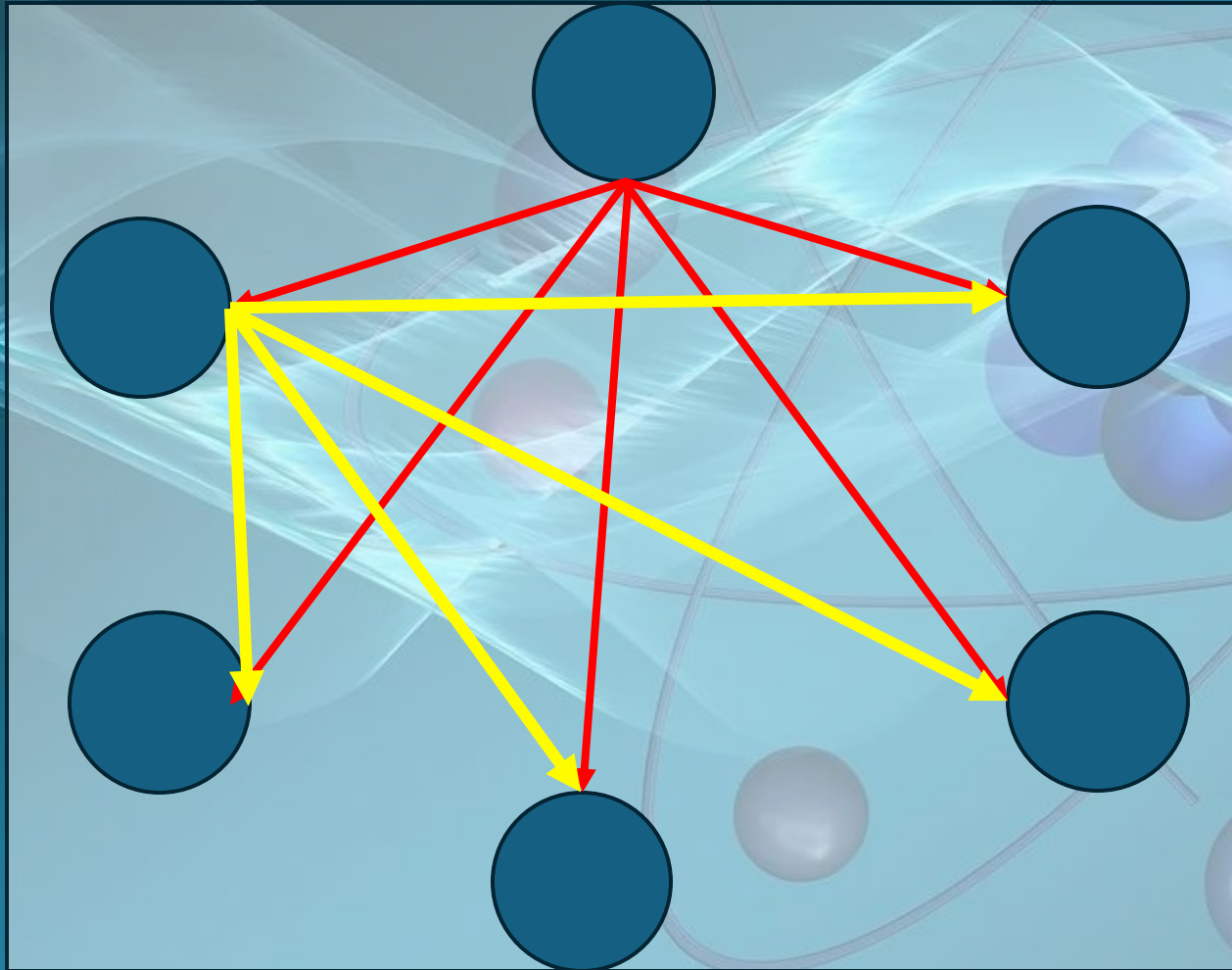
Introduction to Many-Body Physics



Two-Particle Interactions
(Potential)

How many interactions?

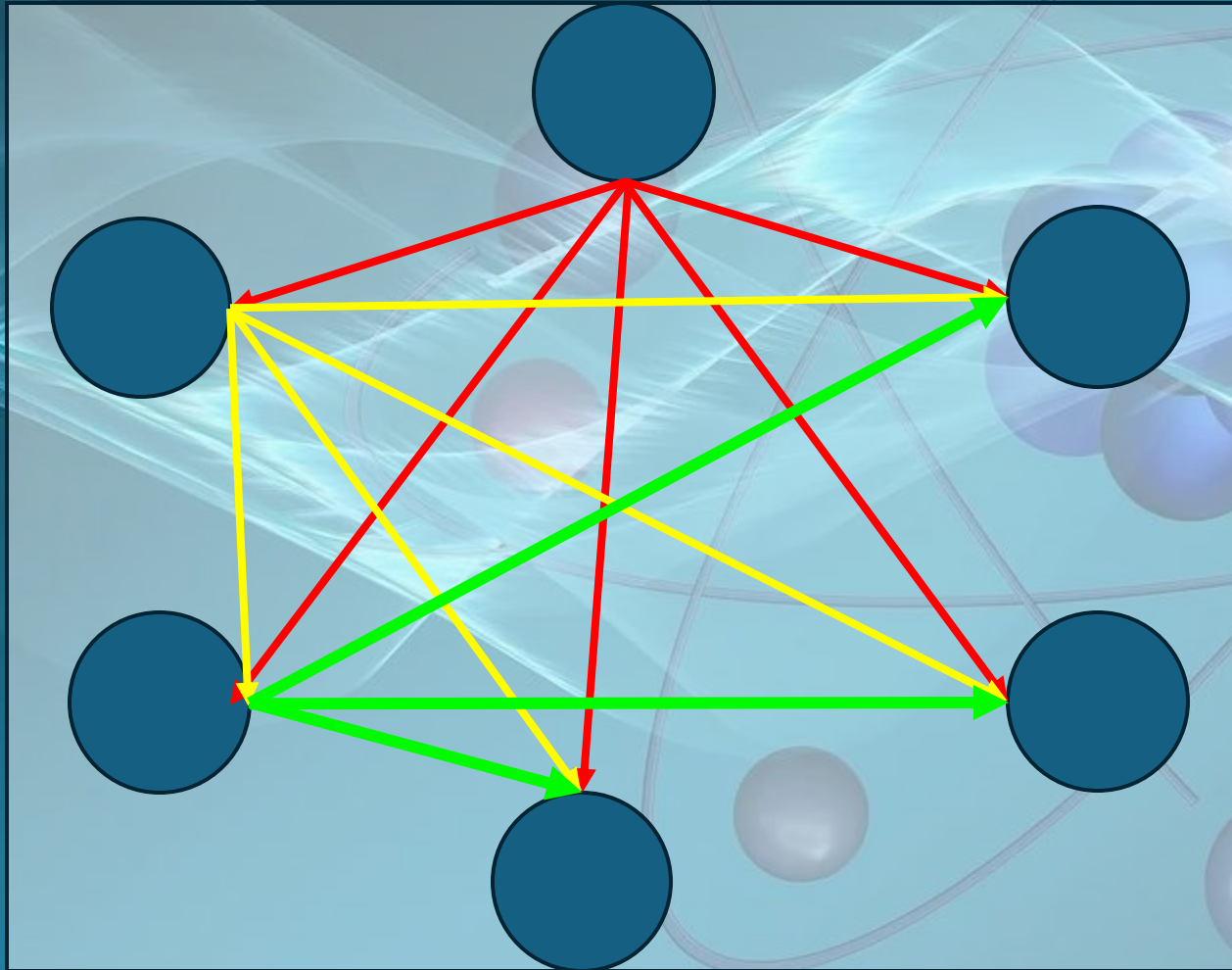
Introduction to Many-Body Physics



Two-Particle Interactions
(Potential)

How many interactions?

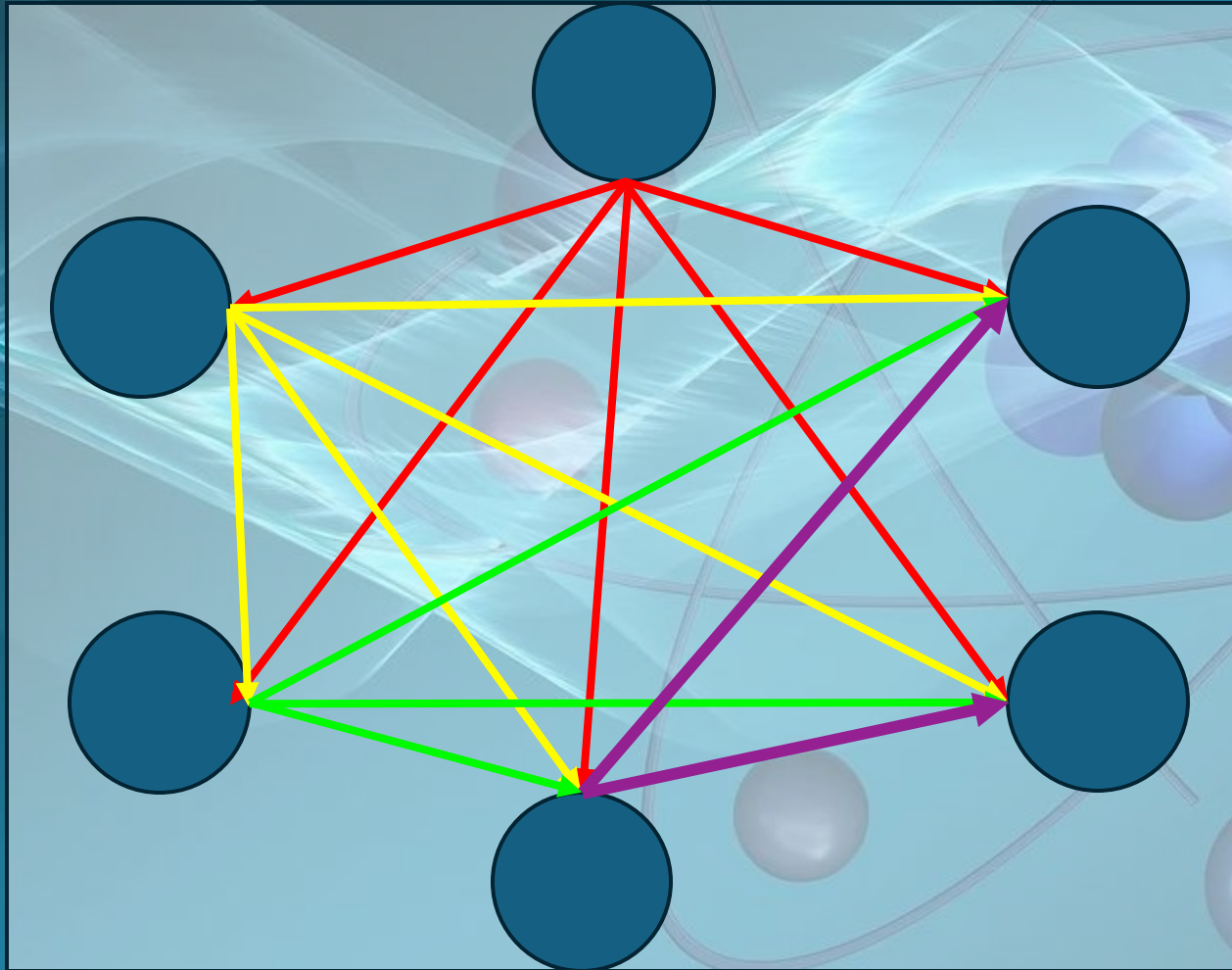
Introduction to Many-Body Physics



Two-Particle Interactions
(Potential)

How many interactions?

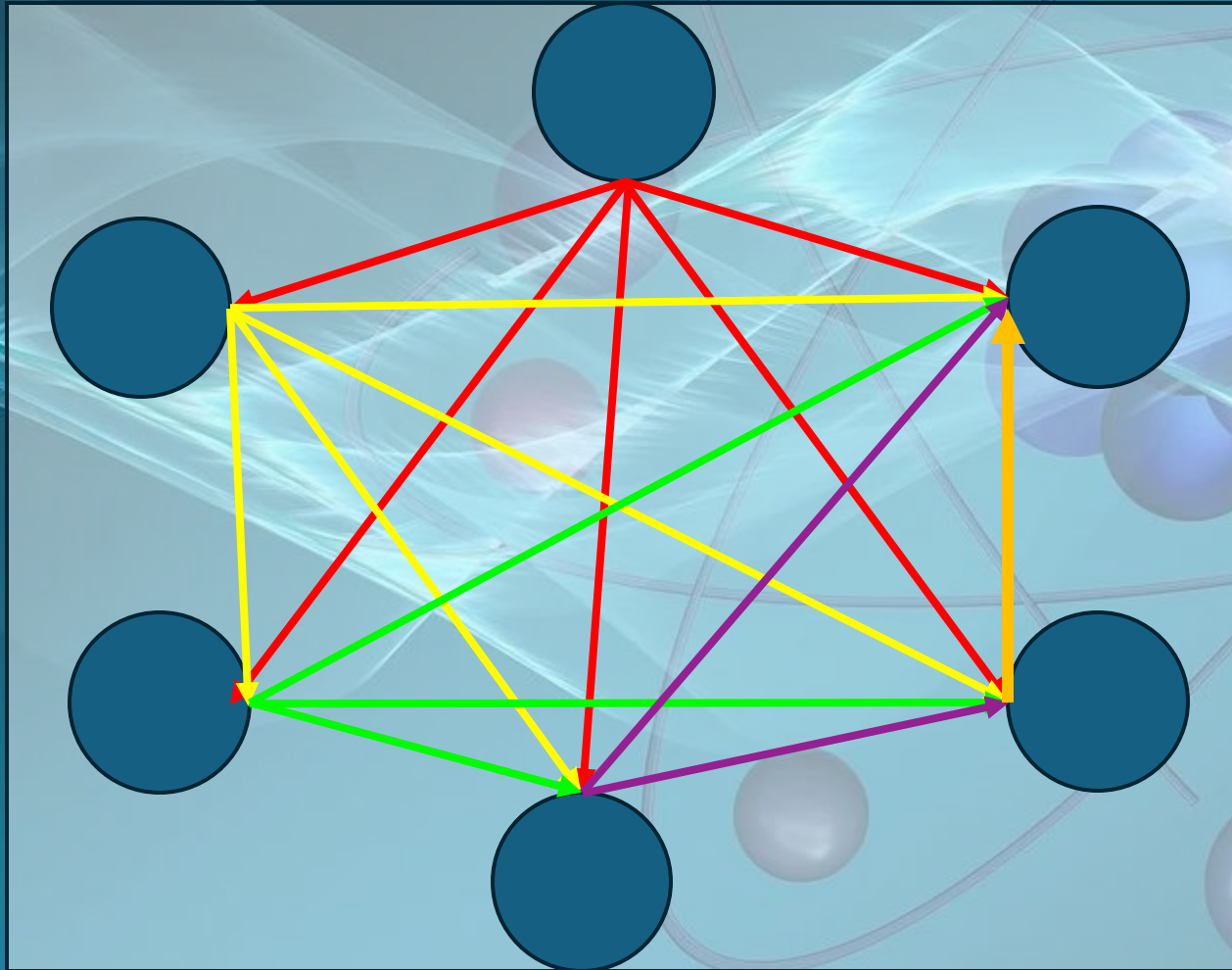
Introduction to Many-Body Physics



Two-Particle Interactions
(Potential)

How many interactions?

Introduction to Many-Body Physics

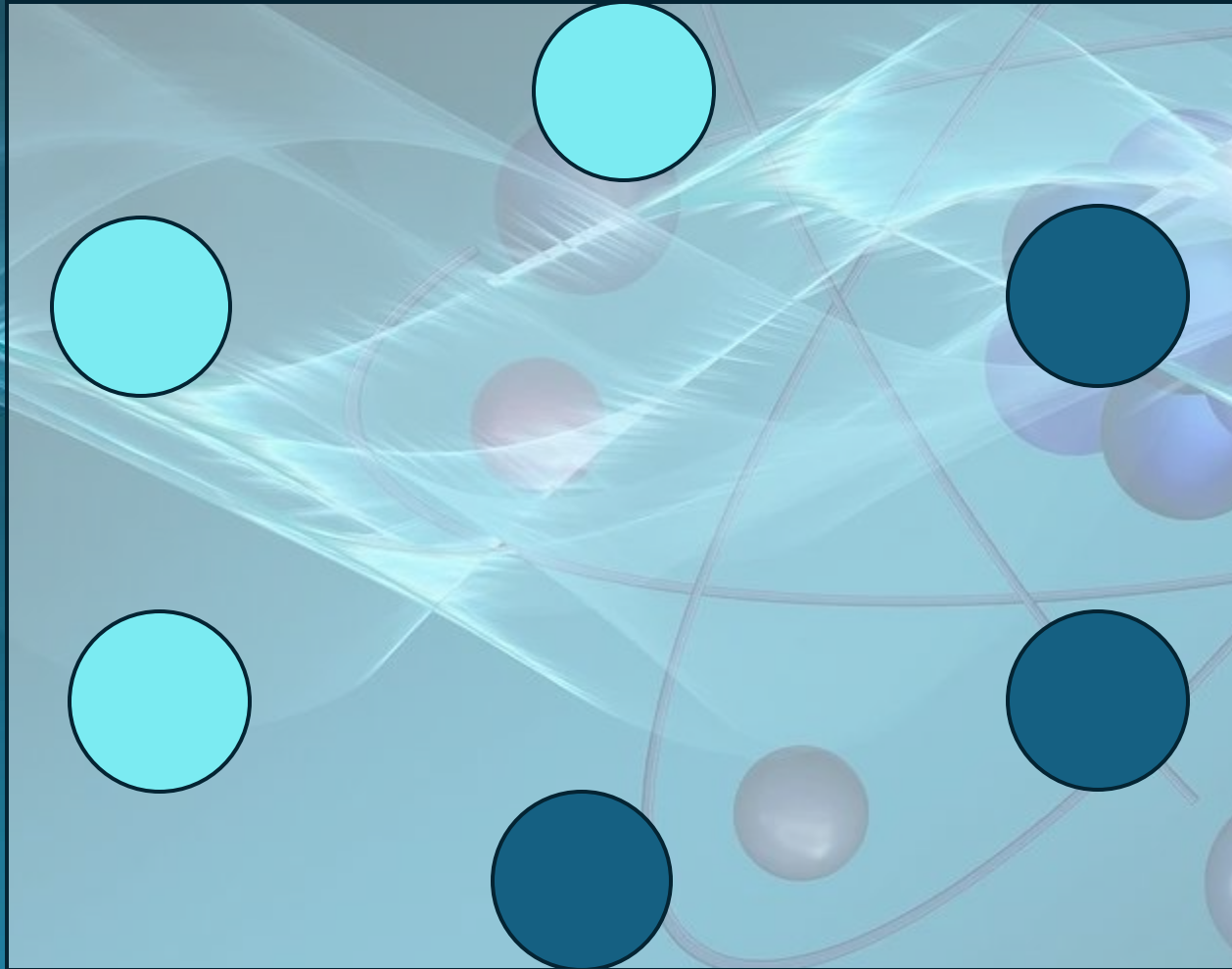


Two-Particle Interactions
(Potential)

How many interactions?

15 two-particle interactions

Introduction to Many-Body Physics



Three-Particle Interactions
(Potential)

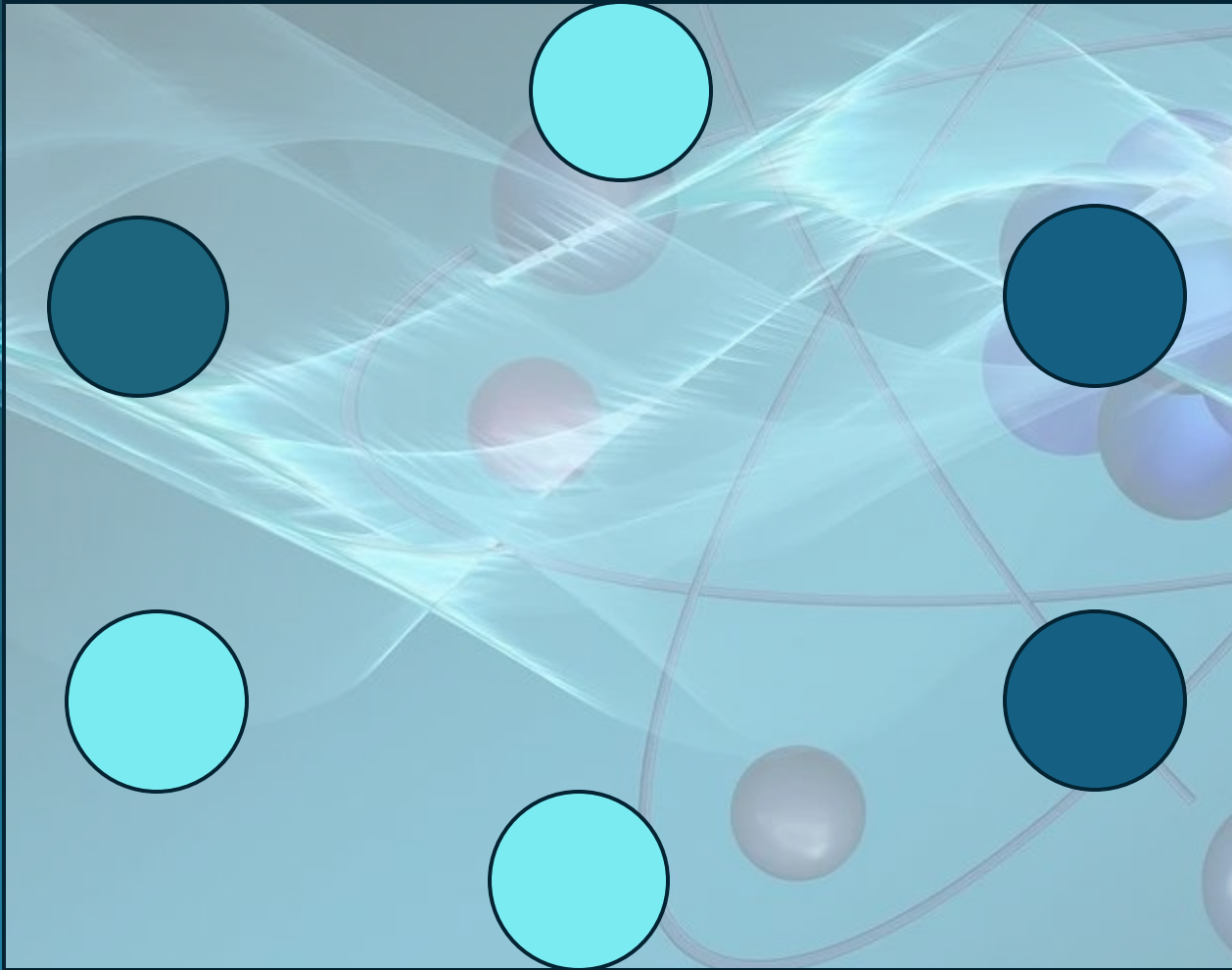
How many interactions?

Introduction to Many-Body Physics

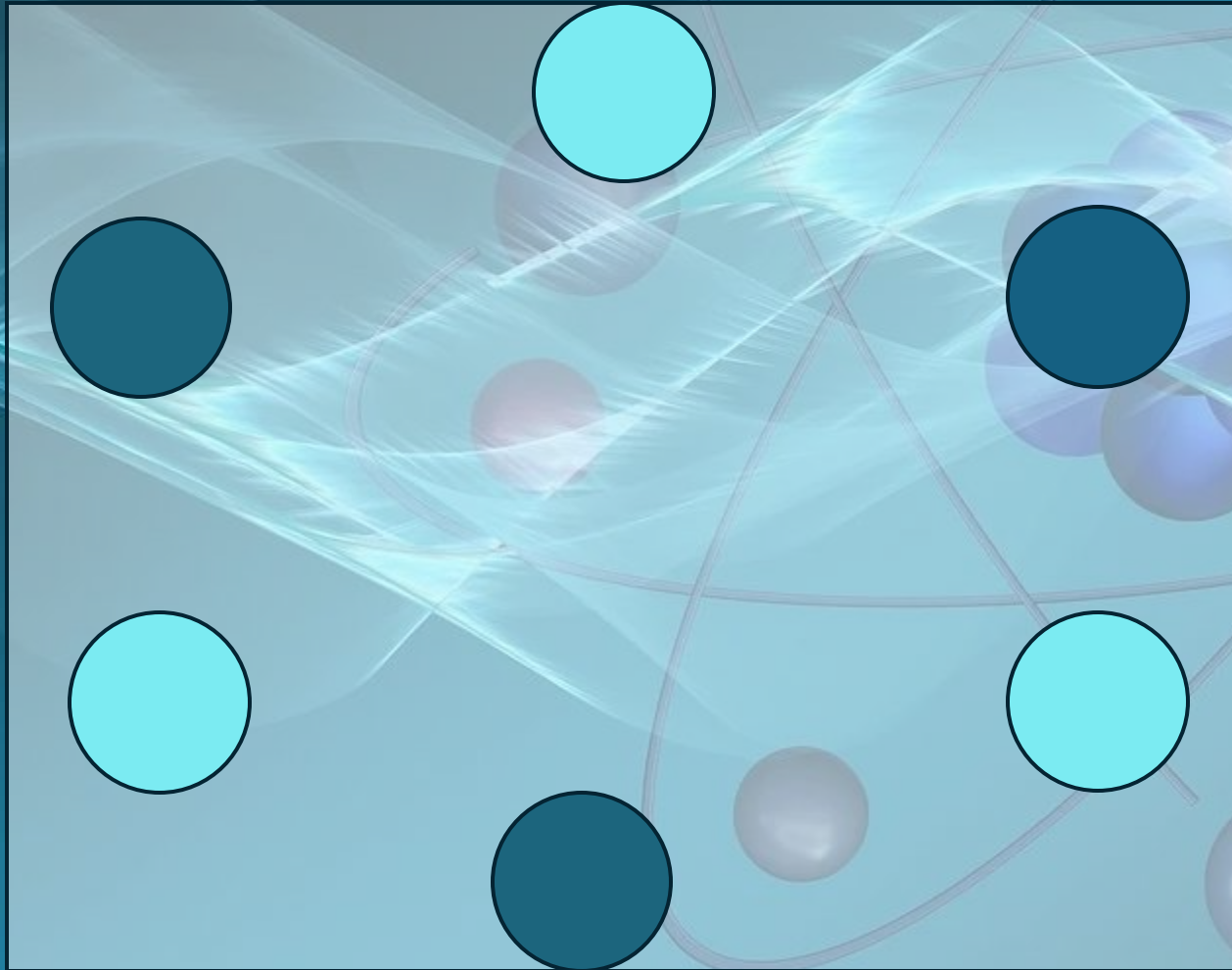


Three-Particle Interactions
(Potential)

How many interactions?



Introduction to Many-Body Physics



Three-Particle Interactions
(Potential)

How many interactions?
20 interactions

Considerations When Performing a Many-Body Calculation

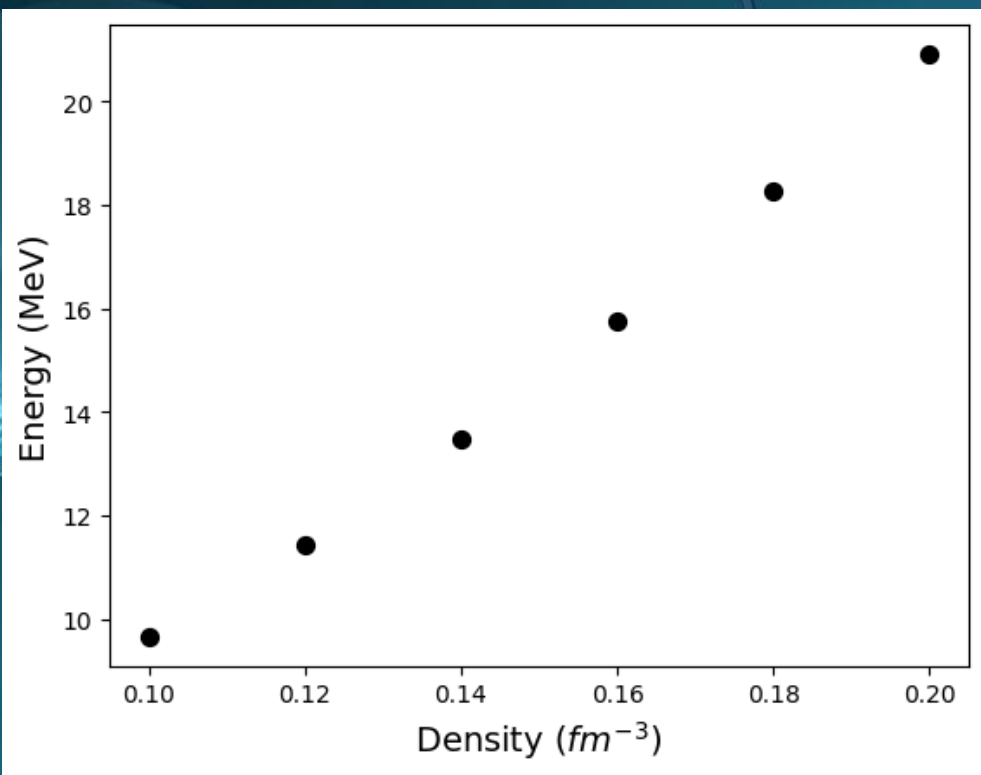
- Number of Single-Particle State and Total Number of Configurations
 - In real systems the number of single particle states is infinite
 - The number of particles is finite
 - Infinite number of configurations
- Number of n-body interactions
 - Two-body interactions
 - Three-body interactions
 - Four body interactions
 - N-body interactions

Typically higher-order interactions are much more complicated than lower-order interactions

Approximations That Have to Be Made

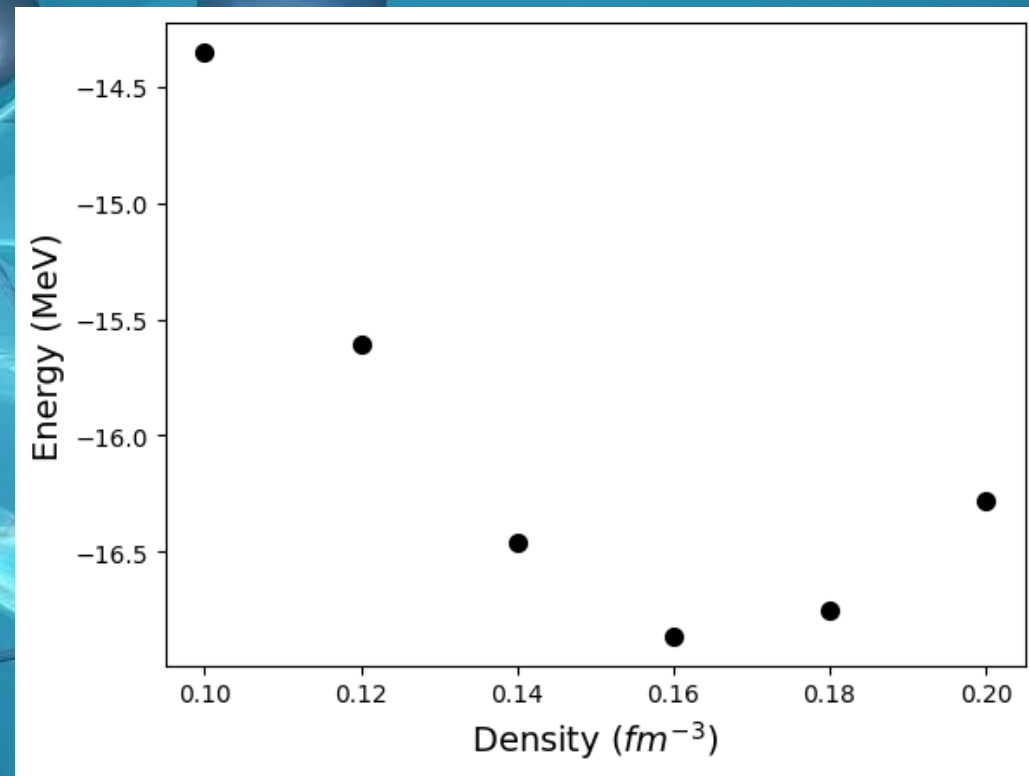
- Not feasible to perform a full calculation
- **Basis Truncation**
 - Reduce the number of single particle states to a finite number
- **Interaction Truncations**
 - Reduce the number of interactions allowed in the calculation
 - Two-body usually include, sometimes three-body, rarely higher
- All approximations and truncations reduce the accuracy of calculations

Example: Infinite Nuclear Matter



Pure Neutron Matter (66 Neutrons)

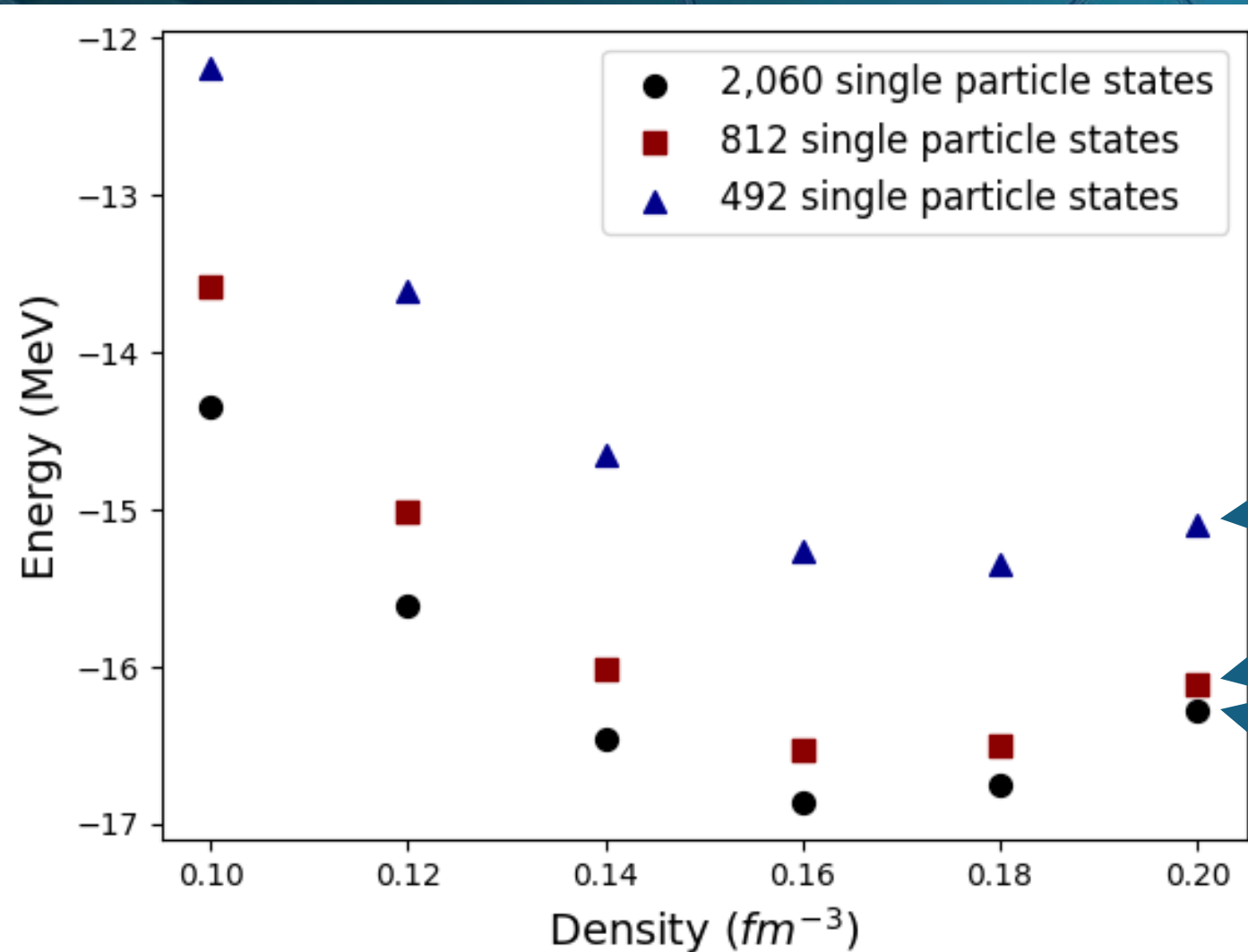
1,478 single particle states
88.25 hours for 6 points



Symmetric Nuclear Matter (66 Neutrons, 66 Protons)

2,060 single particle states
390.1 hours for 6 points

Reducing the Number of Single Particle States Reduces the Accuracy (But Saves Time)



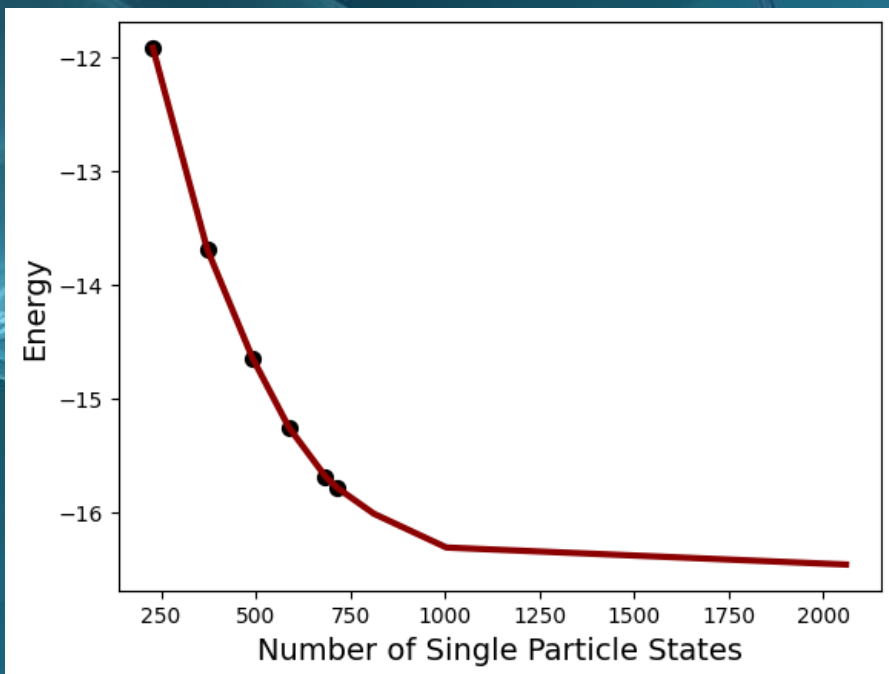
Need to develop a method to extrapolate to a high number of single particle states from data at a low number of single particle states...but the amount of data is limited

7.30 hours

38.4 hours

390.1 hours

Sequential Regression Extrapolation (SRE)



Traditional Methods of Extrapolation Fail

Use Machine Learning?

$$f_{\text{ML}}(\mathbf{M}) = \mathbf{E}$$

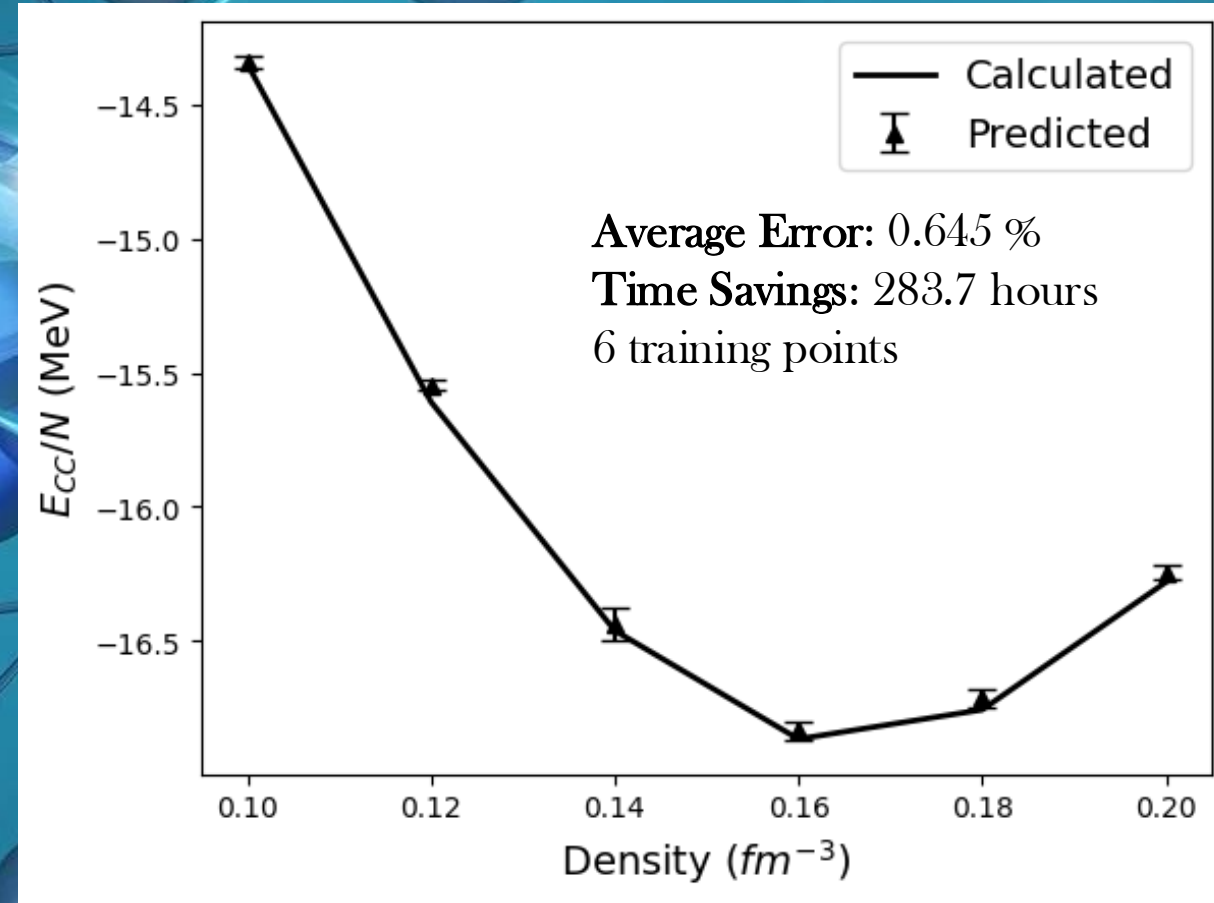
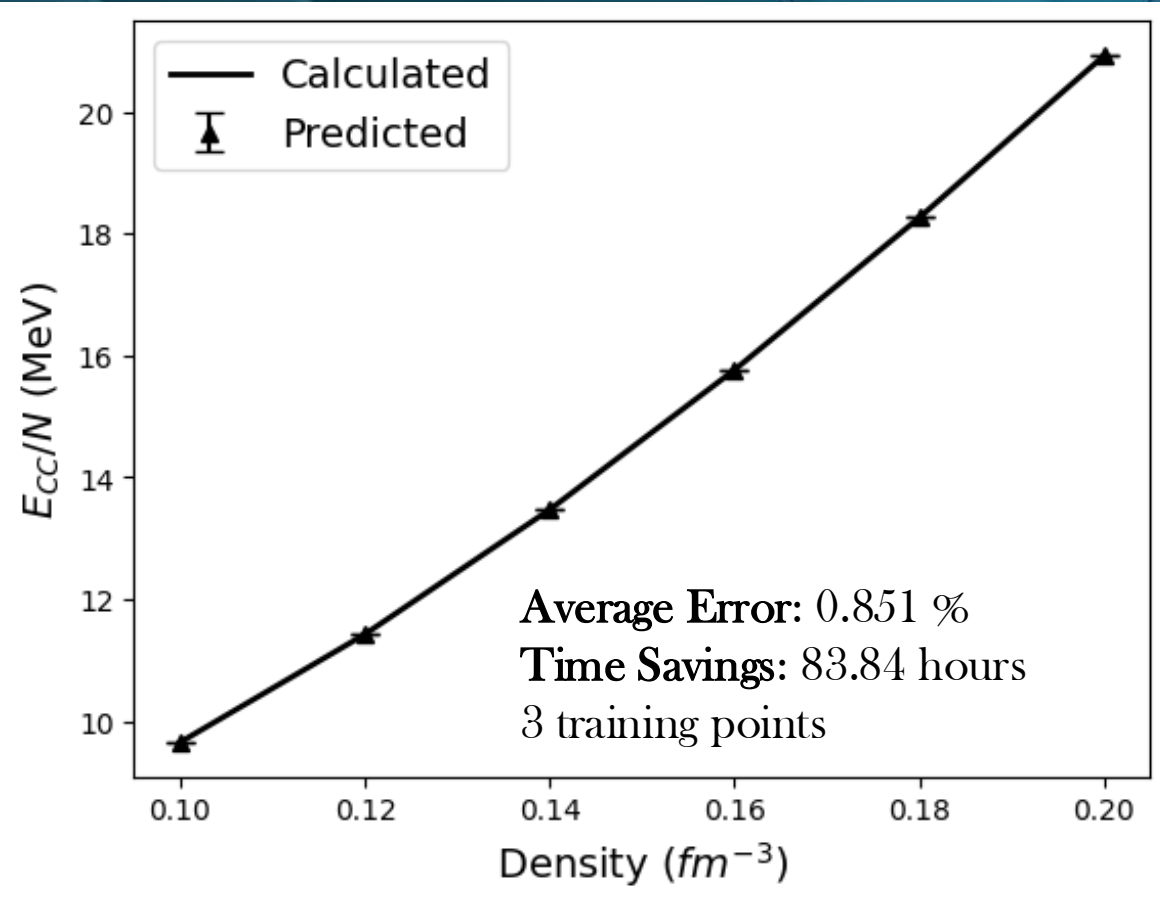
Traditional Extrapolation Fails

Sequential Regression Extrapolation

$$f_{\text{ML}}(\mathbf{E}_{M-1}) = \mathbf{E}_M$$

1, 2, 3, 4, 5, 6, 7, 8, 9, 10

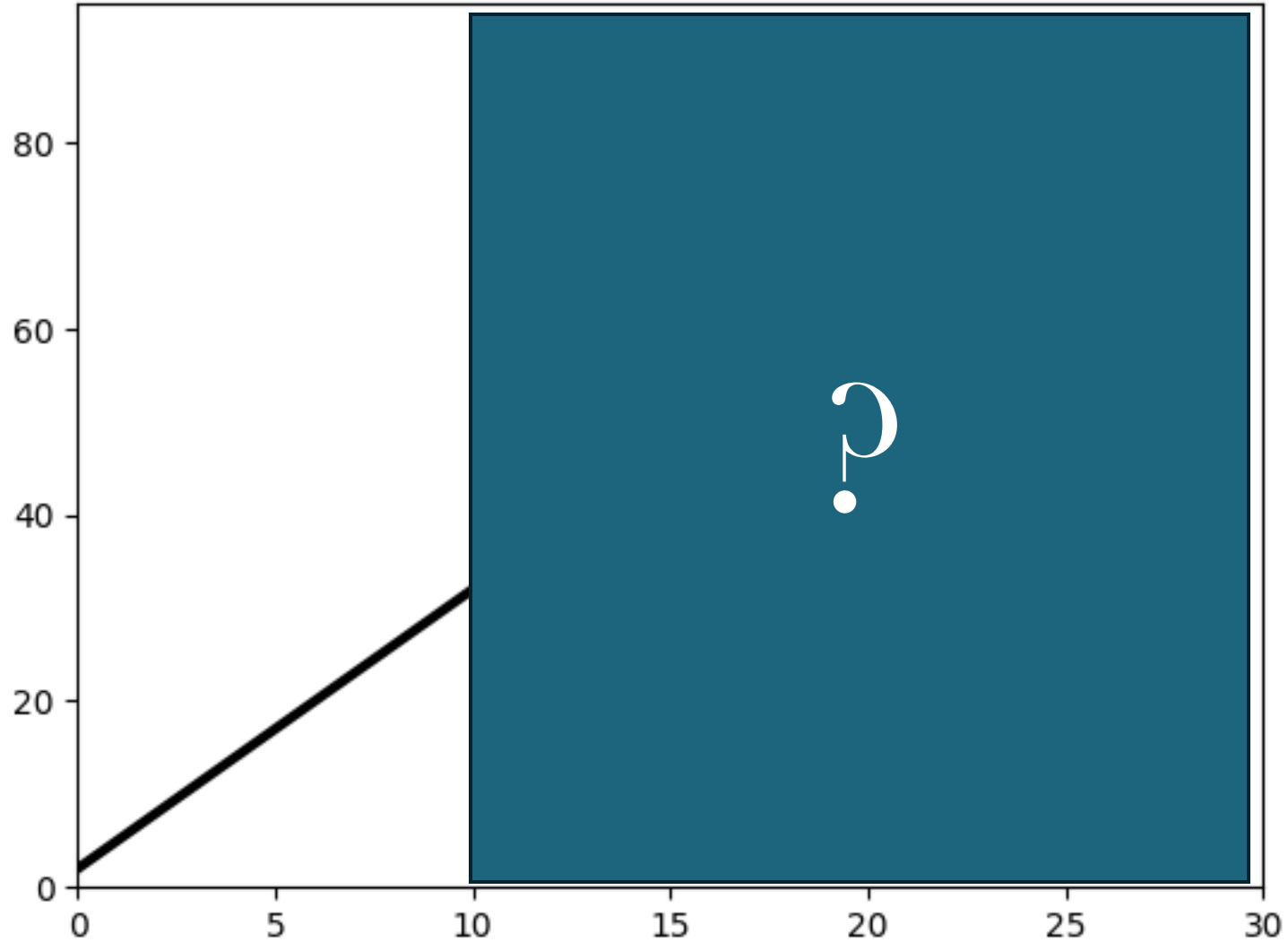
Infinite Nuclear Matter Results \rightarrow SRE Extrapolation



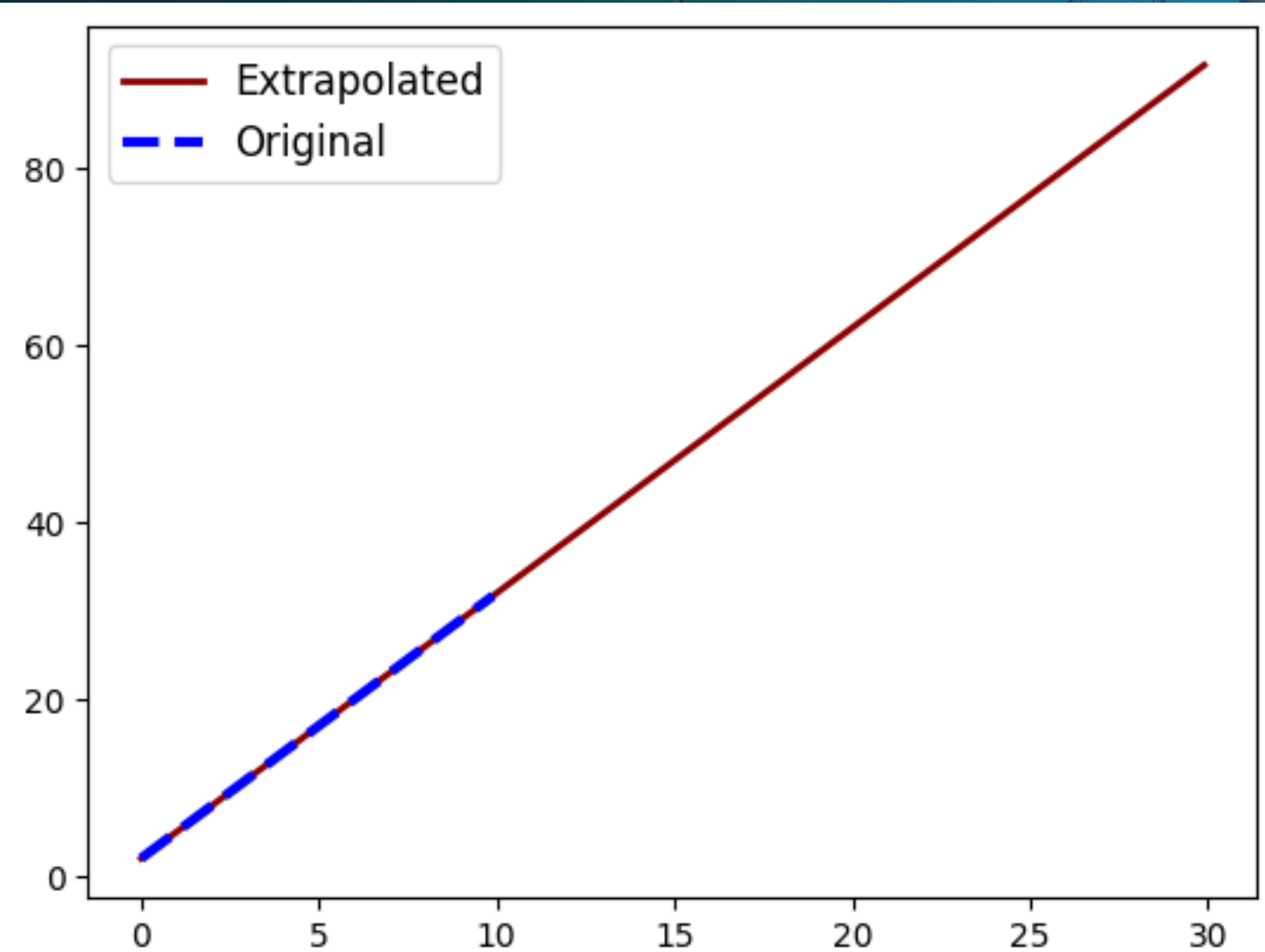
Applications

- Infinite Nuclear Matter
 - Neutron Stars
 - Study of Super Heavy Elements, Creation of New Elements
- Atomic Nuclei
 - Nuclear Fusion and Nuclear Fission (Nuclear Energy)
 - Nuclear Medicine

Extrapolation Example 1



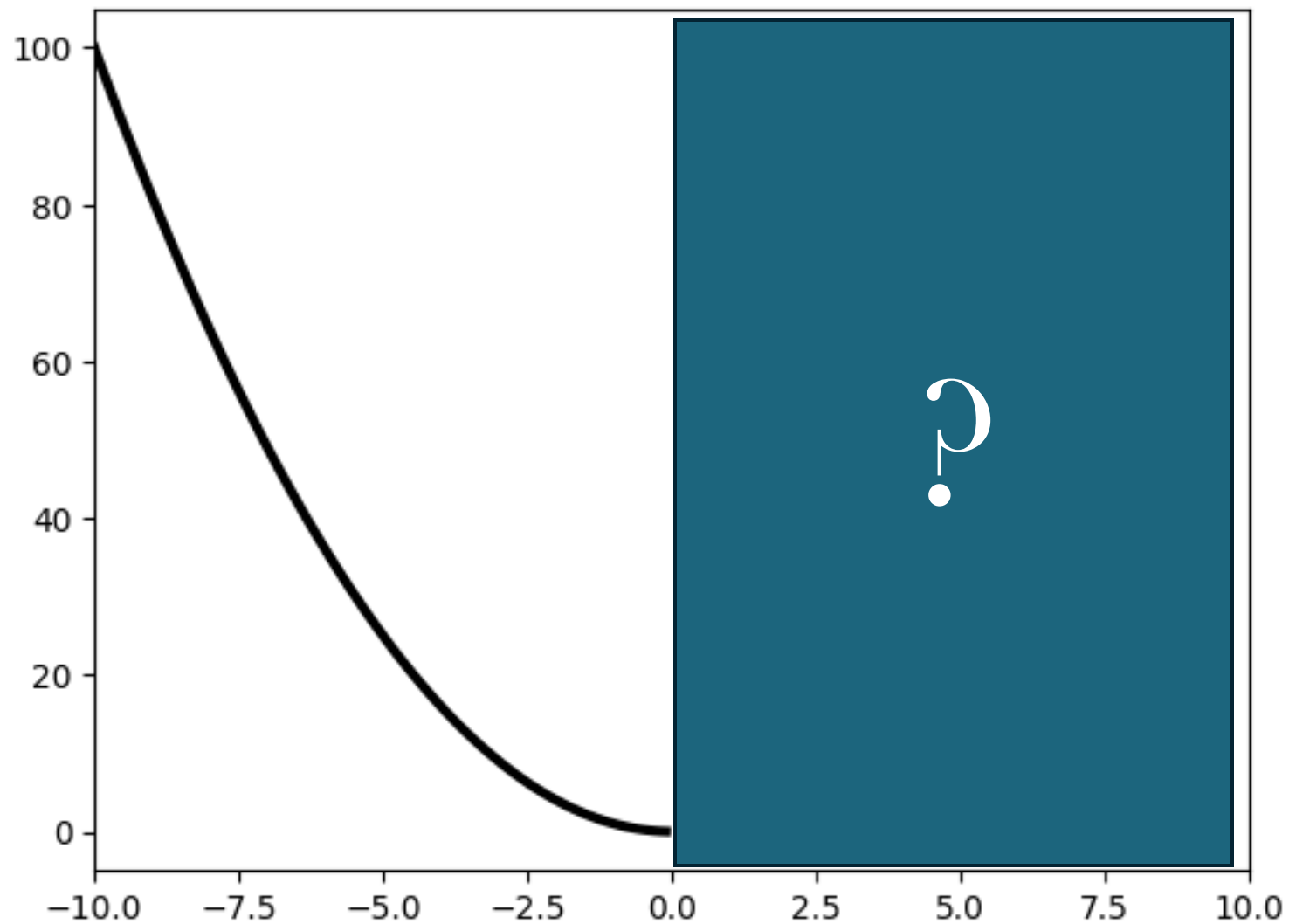
Extrapolation Example 1 \rightarrow SRE Results



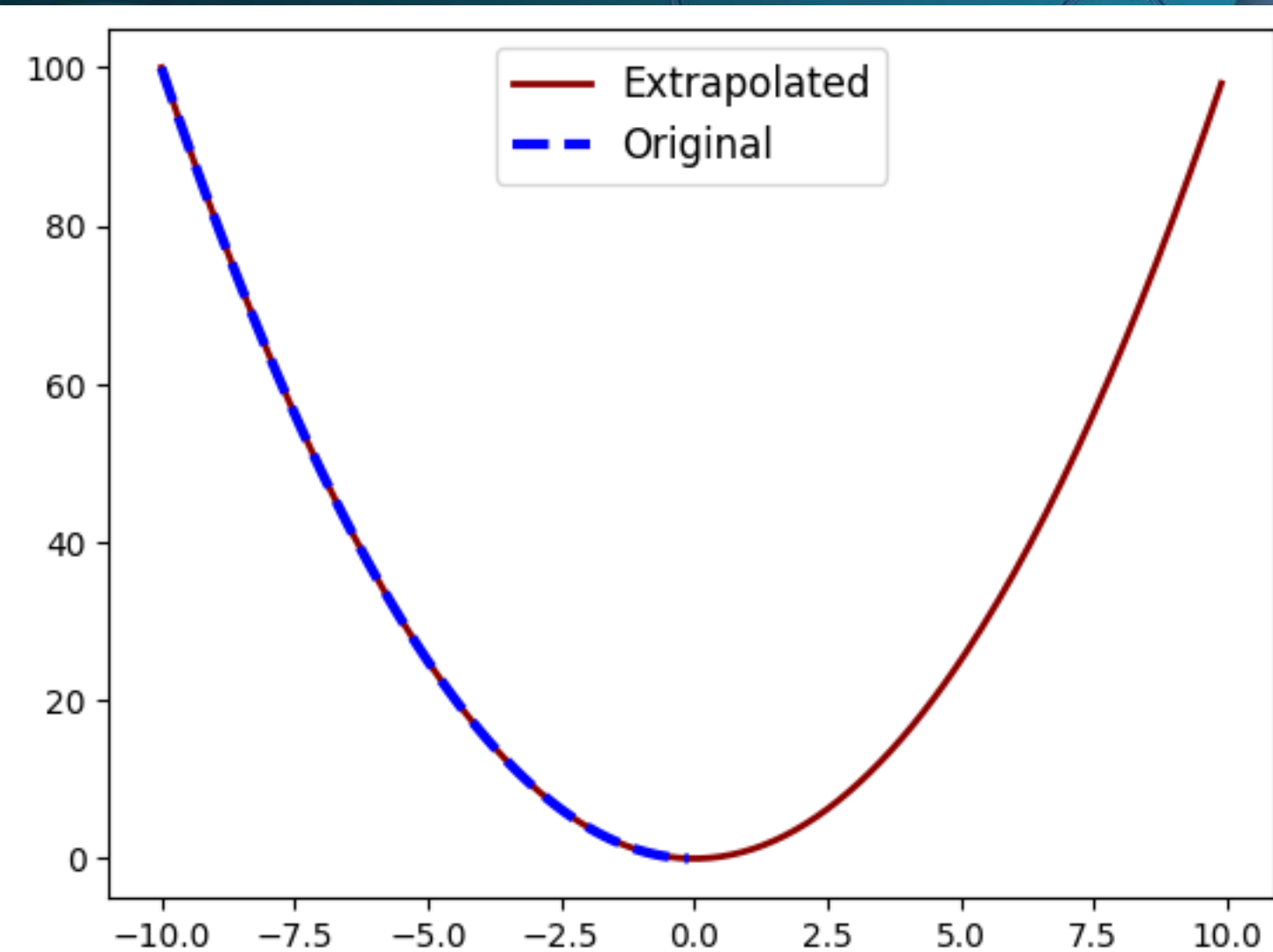
Function: $y=3x+2$

Average Error: 4.54×10^{-9}

Extrapolation Example 2



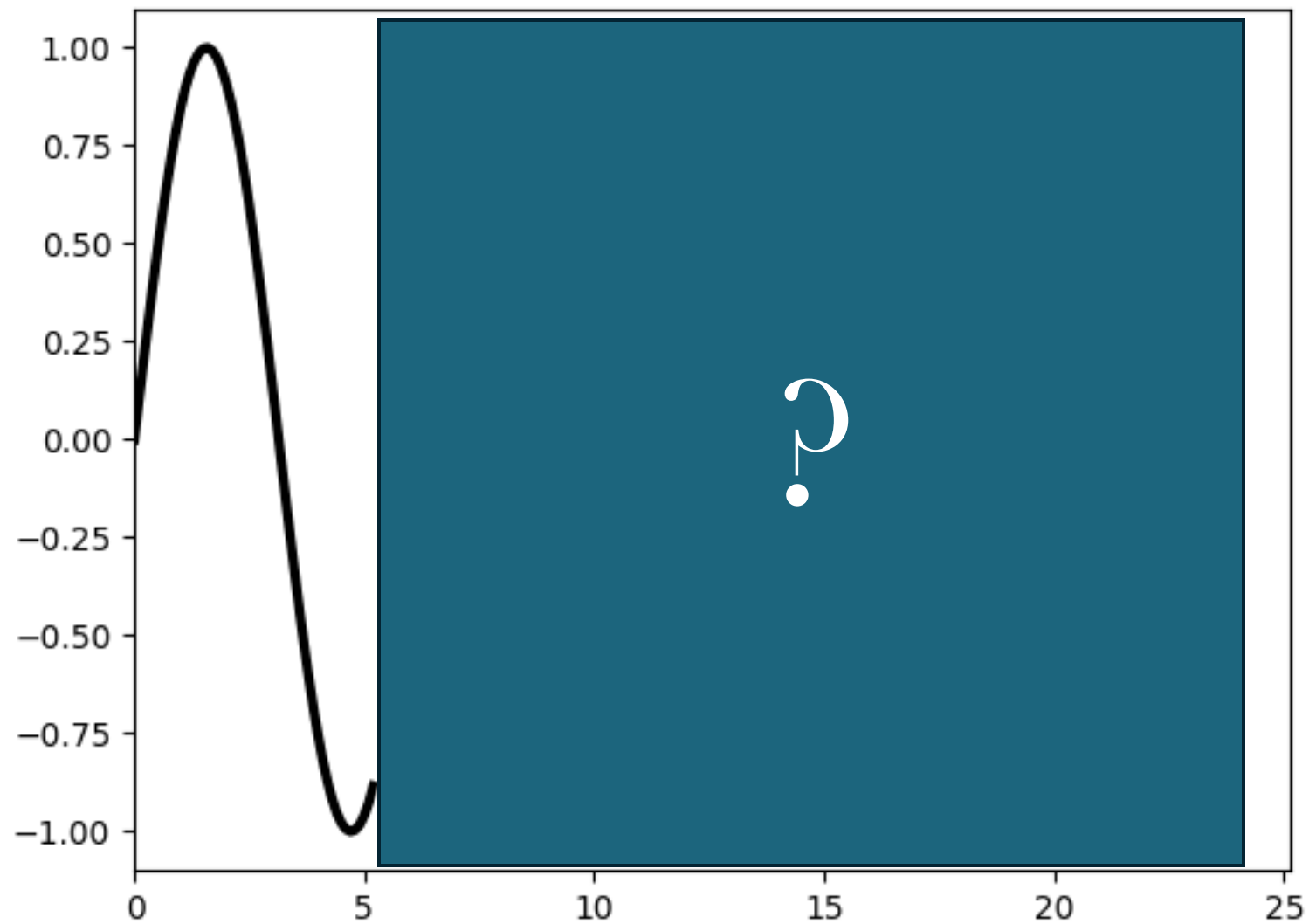
Extrapolation Example 2 → SRE Results



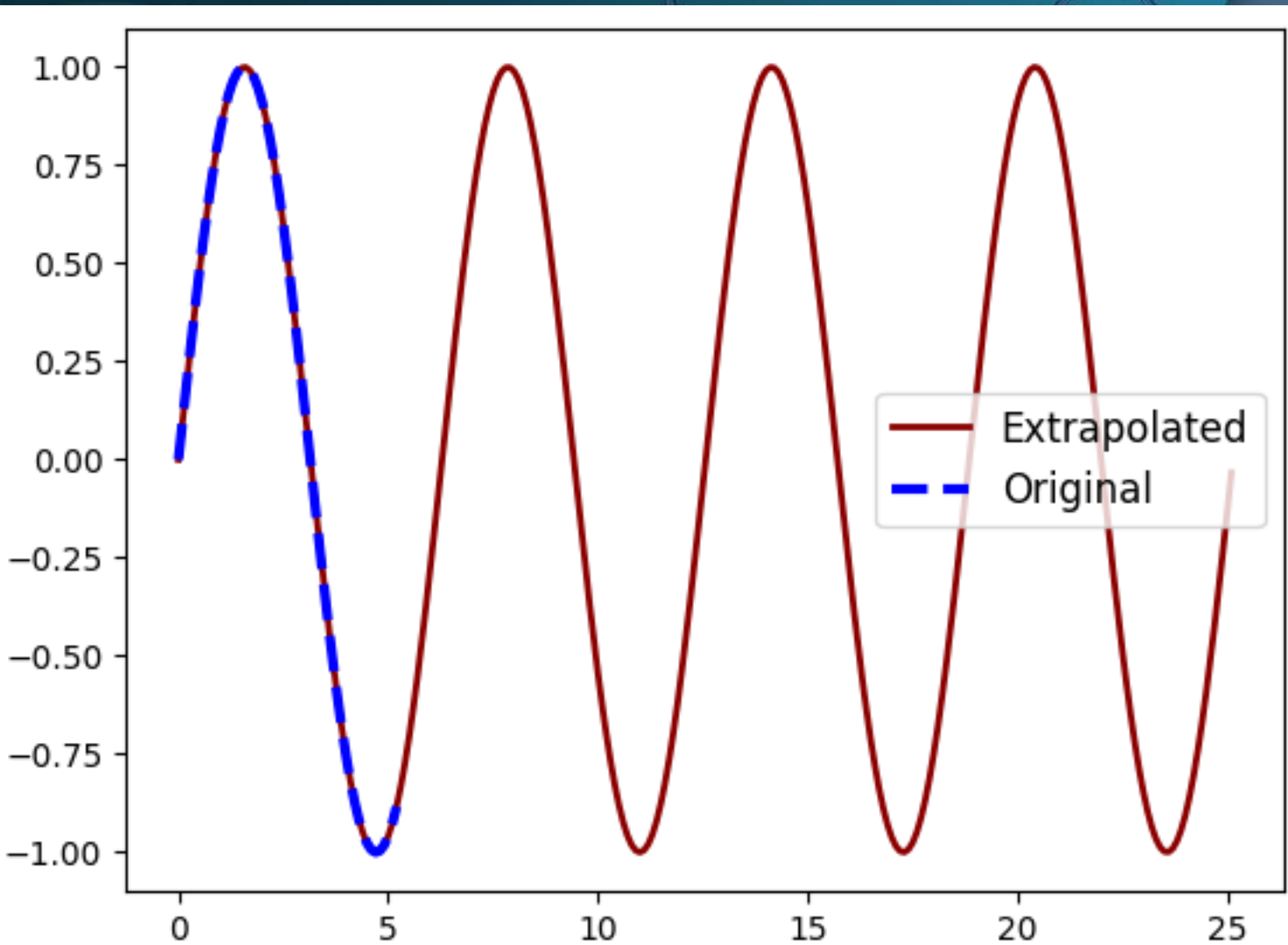
Function: $y=x^2$

Average Error: 6.40×10^{-6}

Extrapolation Example 3



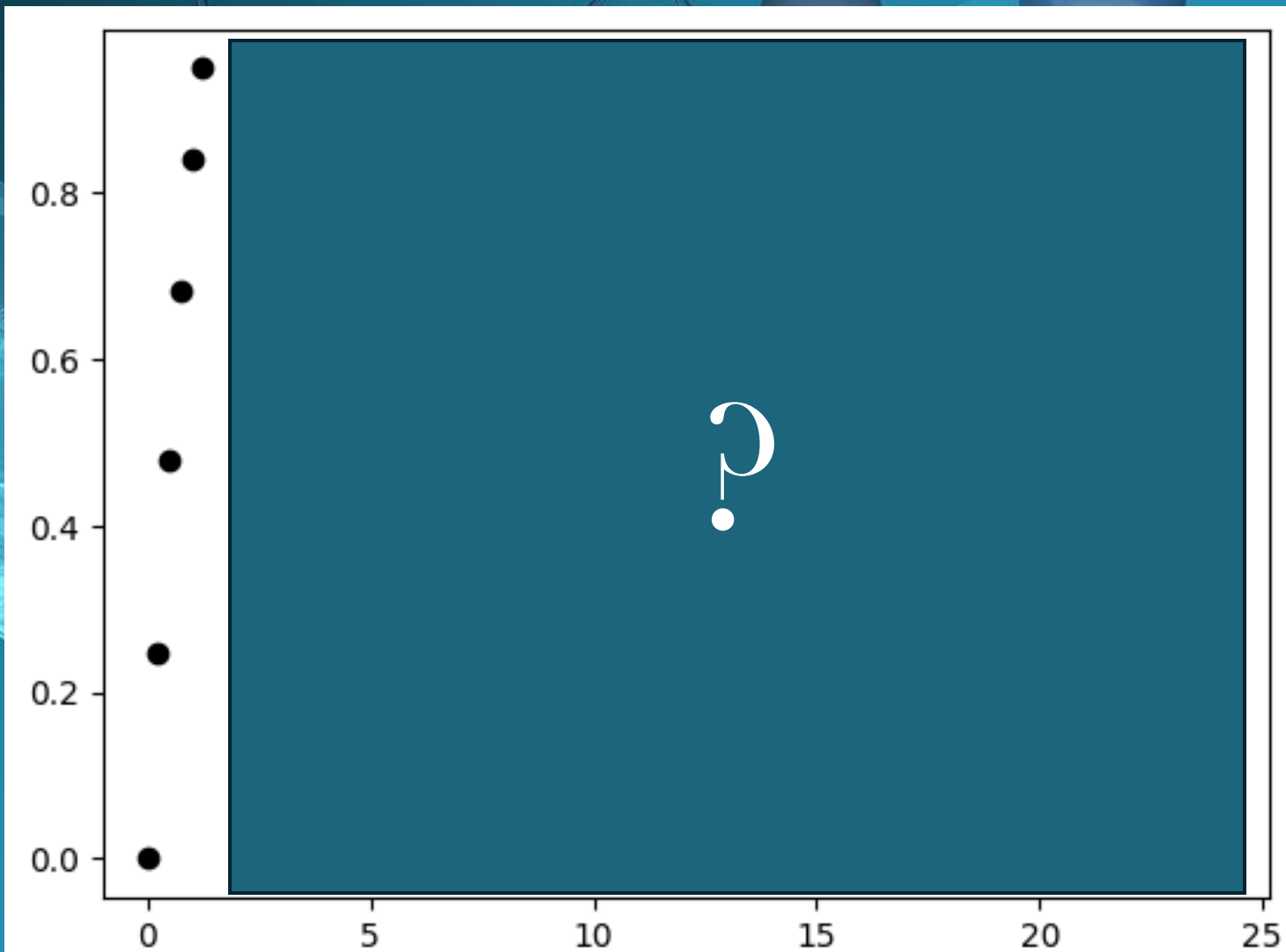
Extrapolation Example 3 \rightarrow SRE Results



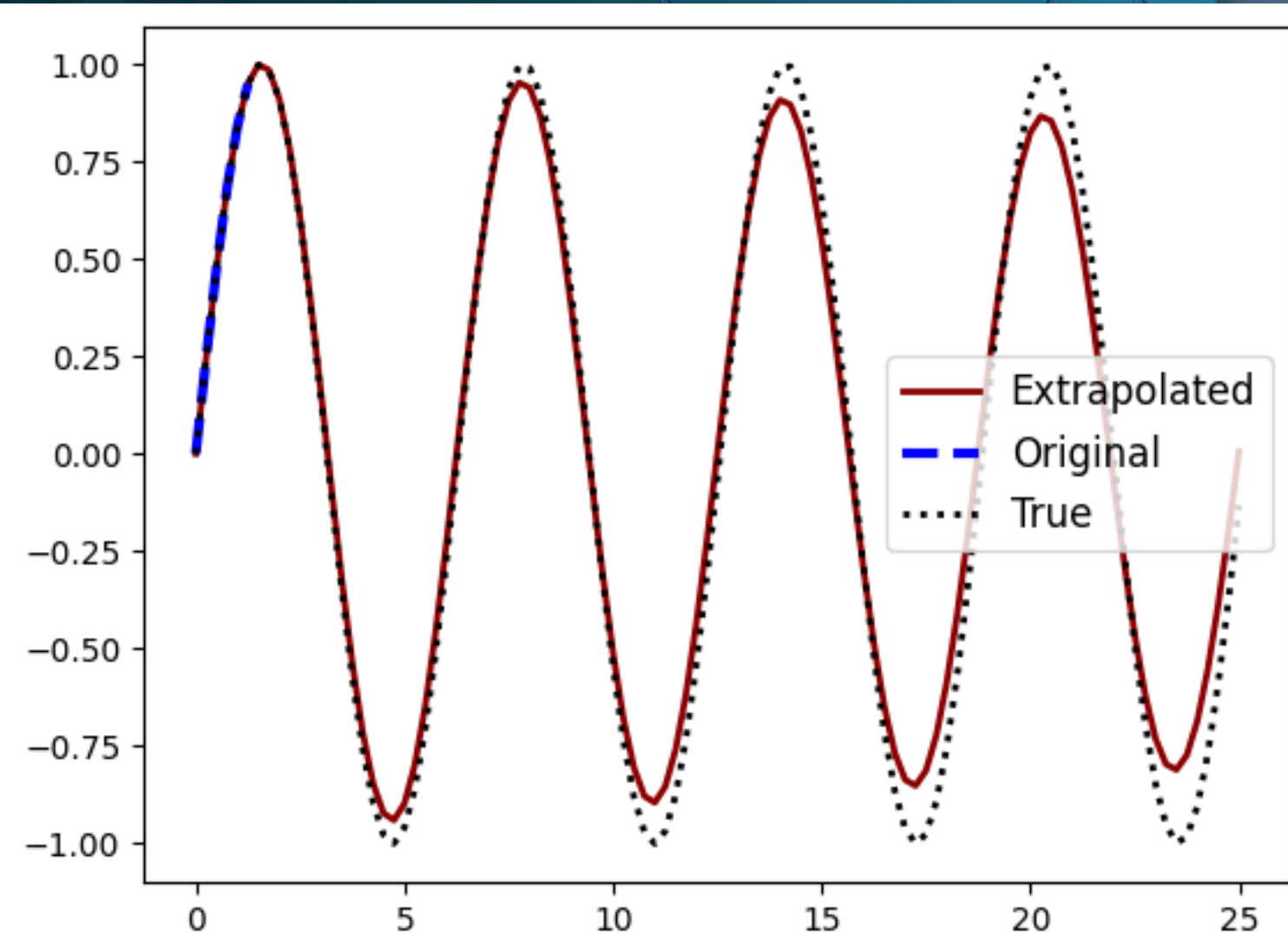
Function: $y = \sin(x)$

Average Error: 2.36×10^{-6}

Example Extrapolation 4



Example Extrapolation 4 \rightarrow SRE Results



Function: $y = \sin(x)$

Average Error: 0.0925

Not perfect, but main
features present
6 Training Points!

Acknowledgements, References, Code, etc.

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Oak Ridge National Laboratory

- Dr. Gustav Jansen

University of Notre Dame

- Dr. Mark Caprio

Nvidia Corporation

- Dr. Justin Leitz

Code

www.github.com/butler-julie/researchsymposium2025

SRE Papers

J. Chem. Phys. 161, 134108 (2024)

[arXiv:2409.18234](https://arxiv.org/abs/2409.18234) [nucl-th]

Questions?