Applying Machine Learning to Many-Body Studies of Infinite Nuclear Matter

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Recent Progress in Many-Body Theory XXI

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Introduction

Ingredients for a Many-Body Calculation

Many-Body Calculation = Many-Body Method + System

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Many-Body Perturbation Theory or Coupled-Cluster Theory

Infinite Matter

Many-Body Calculation = Many-Body Method + System

Ingredients for a Many-Body Calculation

Many-Body Perturbation Theory or Coupled-Cluster Theory

Infinite Matter

Many-Body Calculation = Many-Body Method + System + Approximations + Computational Methods

To Be Discussed

Many-Body Methods: Many-Body Perturbation Theory and Coupled-Cluster Theory

Many-Body Perturbation Theory (MBPT)

- Provides a method to systematically add in interaction terms to reduce complexity of calculation
  - MBPT2: one and two body interaction terms
- Terms are simple which reduces the run time of a calculation

Coupled-Cluster Theory (CC)

- Arranges the basis into excitation clusters that provide a favorable truncation scheme
  - CCSD: one-particle one-hole and two-particle two-hole excitation clusters
- Interactions are summed to infinite order which reduces error

G. Baardsen et. al. Physical Review C **88**, 054312 (2013).; Lecture Notes in Physics (LNP) **936**; arXiv 1312.7872

Energy and Correlation Energy from MBPT and CC

$$\Delta E^{(2)} = \frac{1}{4}\sum_{abij}\langle ij|\hat{v}|ab\rangle\frac{\langle ab|\hat{v}|ij\rangle}{\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b}$$

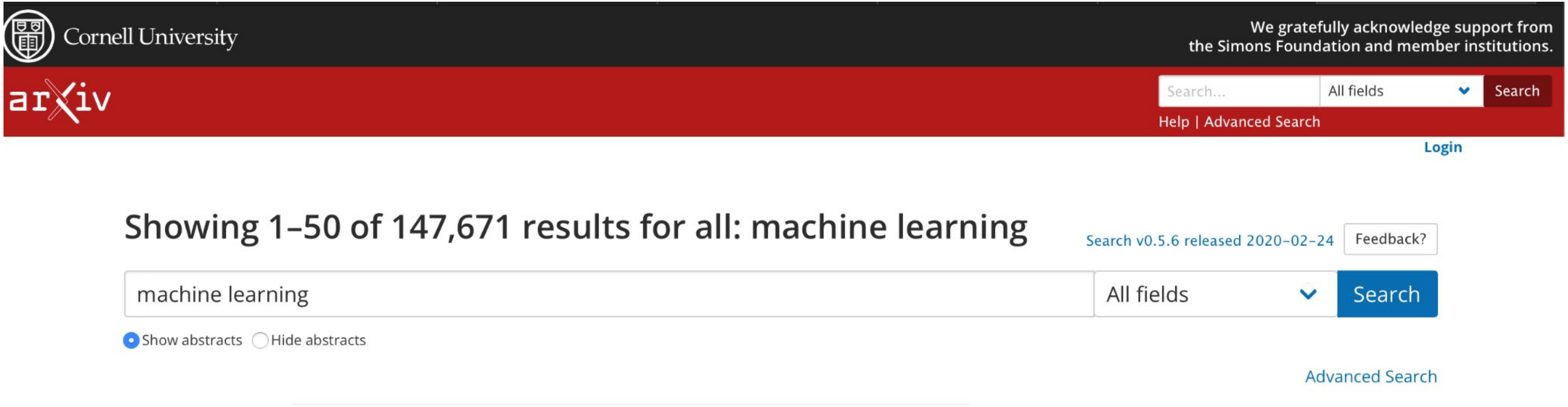
$$E_C = E_{CC} - E_0 = \sum_{ia}\langle i|\hat{f}|a\rangle t_i^a + \frac{1}{4}\sum_{aibj}\langle ij|\hat{v}|ab\rangle t_{ij}^{ab} + \frac{1}{2}\sum_{aibj}\langle ij|\hat{v}|ab\rangle t_i^a t_j^b$$

Correlation Energy:

$\Delta E_X = E_X - E_{ref} \leq 0$, X = CC or MBPT

- Reference energy is typically Hartree-Fock (quick to calculate)

Machine Learning



Machine learning: A set of computer algorithms that learn to accomplish a task by considering examples but without explicitly being told what to do

Examples: neural networks, principal component analysis (PCA), random forest, linear regression

Bayesian Ridge Regression

$$\hat{y}_{Ridge} = X\theta$$

$$J_{Ridge}(\theta) = \lambda\theta^2 + \frac{1}{M}[X\theta - Y][X\theta - Y]$$

$$\theta_{Ridge} = (X^T X + \lambda I)^{-1} X^T y$$

- λ is a **hyperparameter,** its value has to be set by the user and can greatly affect the algorithm
- Bayesian statistics are used to find the optimal value of λ instead of a traditional grid search method

Hands-On Machine Learning by Aurélien Géron and Sci-Kit Learn's website

Sequential Regression Extrapolation (SRE)

- **Traditional**: $f_{RR}(x) = y$, an input value is matched to an output value

- **SRE**: $f_{RR}(y_{k-2}, y_{k-1}) = y_k$, a sequence of output values is matched to the next output

- **Motivation**: Teaching the ridge regression algorithm a sequence of y values should make the algorithm better at predicting the next y value
  - Note that machine learning is typically not used for extrapolation

J. Butler et. al. *Manuscript under preparation.*

Homogeneous Electron Gas: Building the Methodology

The Homogeneous Electron Gas

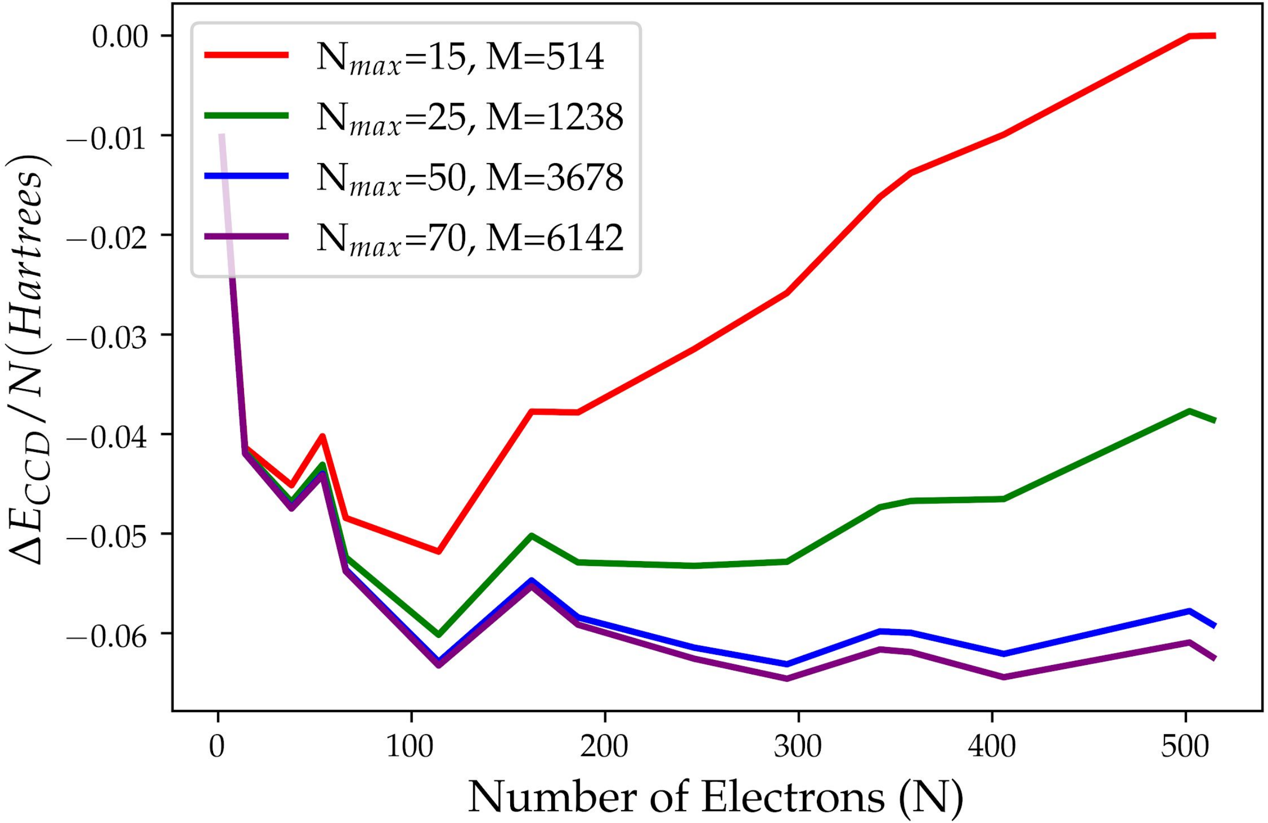
- Infinite matter system containing only electrons (long-range Coulomb force)
- Uniform positive background charge for a total net charge of zero
- Can only simulate a finite system: Plane wave basis and periodic boundary conditions
- Measure of density: Wigner-Seitz Radius

$$r_s = r_0/r_B$$

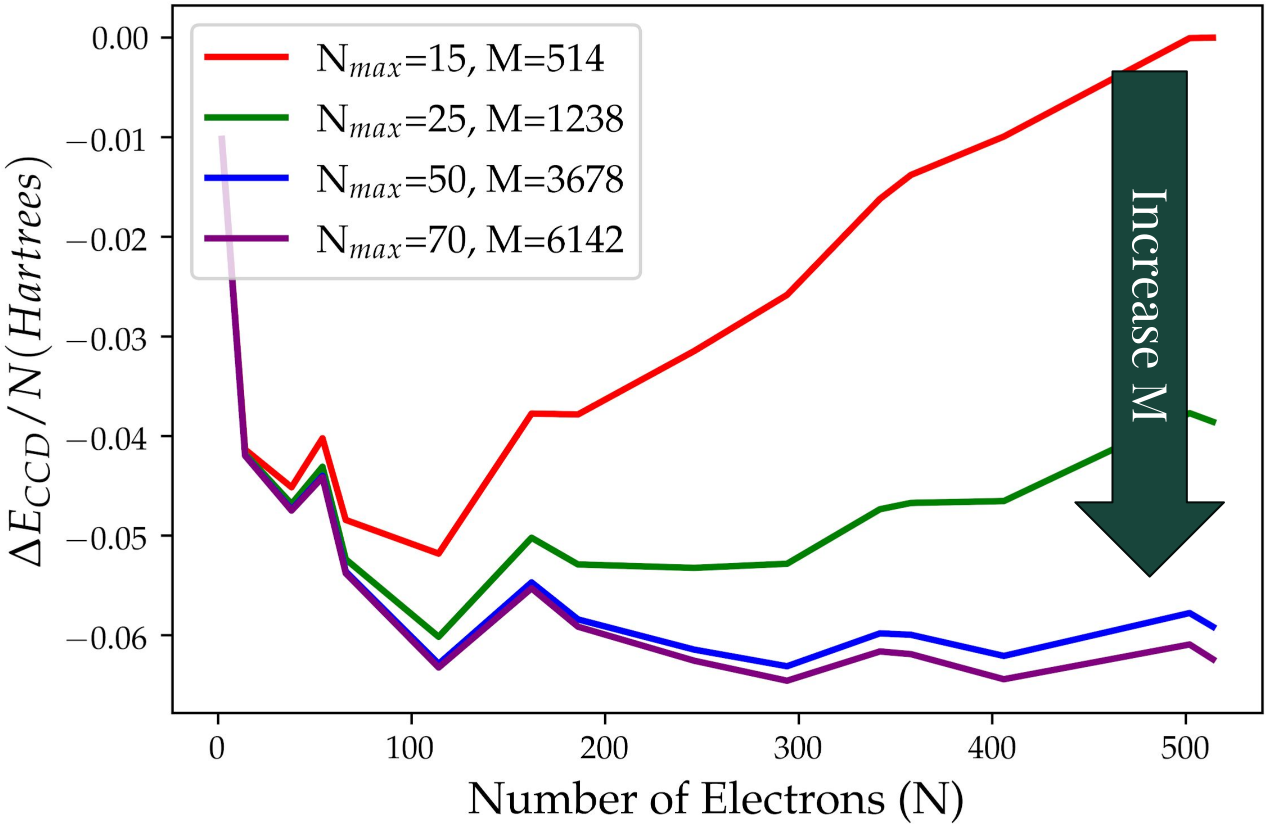
- Calculations are performed at "magic numbers" of electrons

G. Baardsen et. al. Physical Review C **88**, 054312 (2013).; C. Drischler et. al., Annual Review of Nuclear and Particle Science **71**, 403 (2021).; LNP **936**

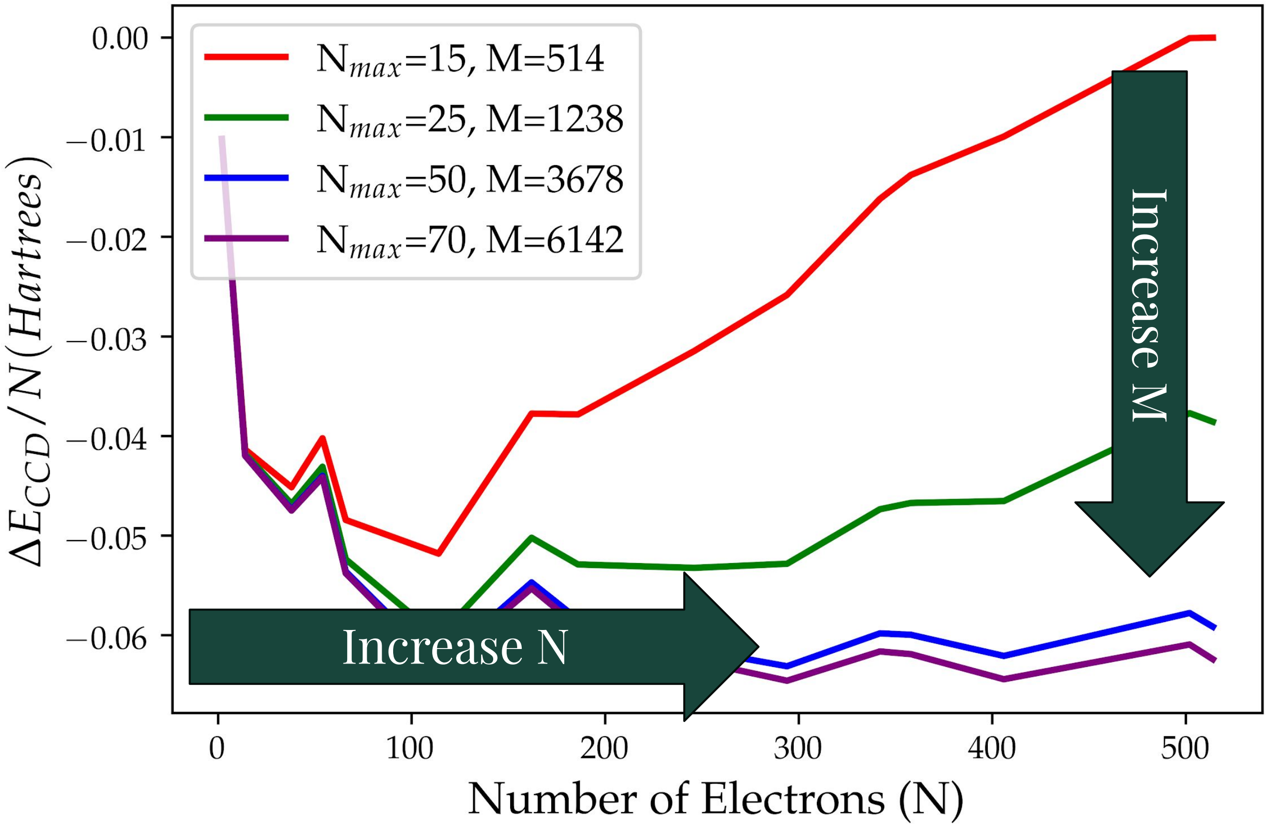
Finite Size Effects: Truncating N and M



Finite Size Effects: Truncating N and M



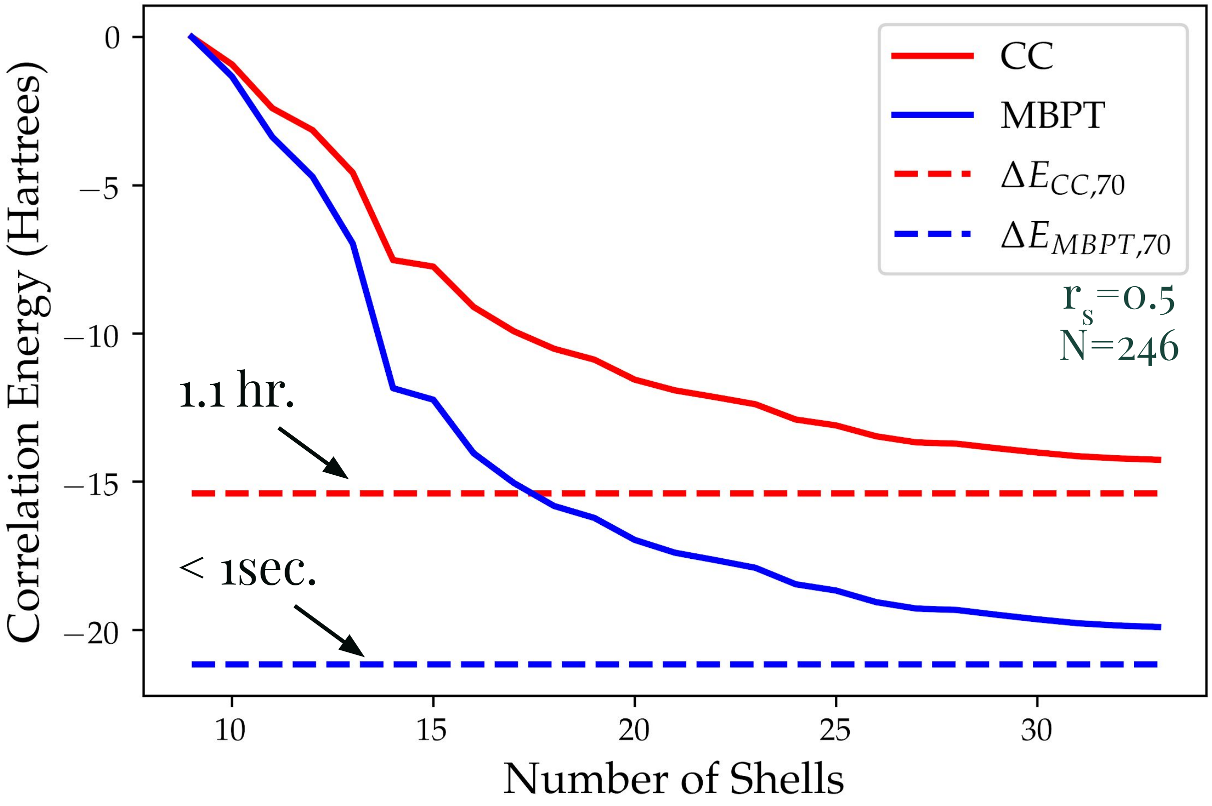
Finite Size Effects: Truncating N and M



Accurate Calculations at the Thermodynamic Limit

N,V→∞, r_s const.

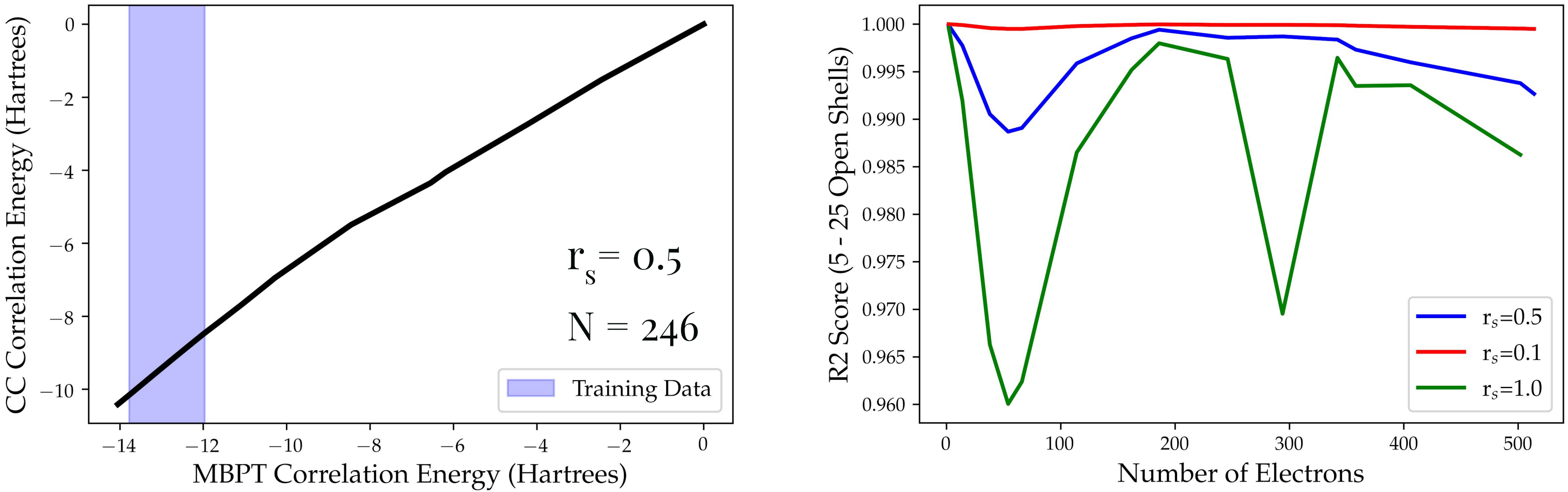
Convergence of MBPT and CC Results



Motivation: Use MBPT2 correlation energies to predict the CCD correlation energy for the same system

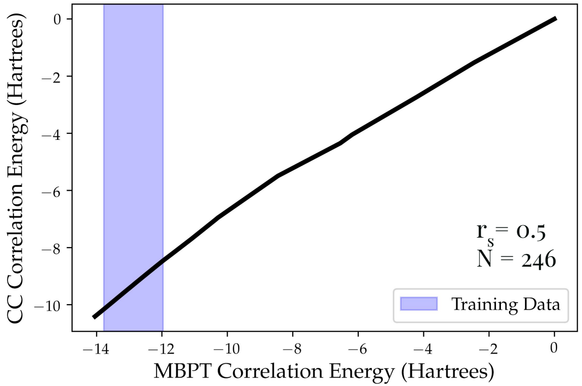
Goal: $f(\Delta E_{MBPT2}) = \Delta E_{CCD}$

MBPT vs CC--A Linear(ish) Relationship



This relationship should become increasingly linear as M increases!

SRE Methodology



J. Butler et. al. *Man under preparation.*

$$\frac{\Delta E_{CC}(M)}{\Delta E_{MBPT}(M)} \longrightarrow constant$$

$$y = \frac{\Delta E_{CC}(M)}{\Delta E_{MBPT}(M)} = \frac{\Delta E_{CC,1}}{\Delta E_{MBPT,1}}, \frac{\Delta E_{CC,2}}{\Delta E_{MBPT,2}}, \frac{\Delta E_{CC,3}}{\Delta E_{MBPT,3}}, \ldots$$

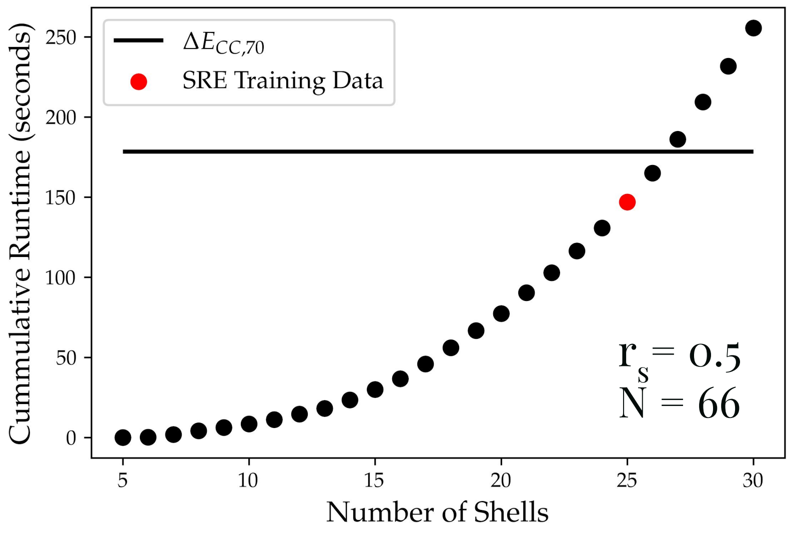
$$f_{Ridge}\left(\frac{\Delta E_{CC,k-3}}{\Delta E_{MBPT,k-3}}, \frac{\Delta E_{CC,k-2}}{\Delta E_{MBPT,k-2}}, \frac{\Delta E_{CC,k-1}}{\Delta E_{MBPT,k-1}}\right) = \frac{\Delta E_{CC,k}}{\Delta E_{MBPT,k}}$$

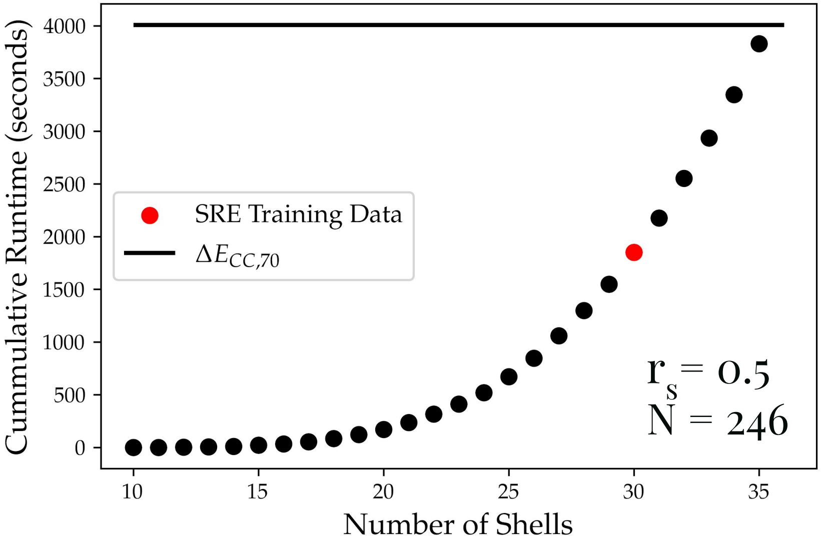
$$\lim_{k\to\infty} \frac{\Delta E_{CC,k}}{\Delta E_{MBPT,k}} = slope = m$$

$$m\Delta E_{MBPT,large\ k} \approx \Delta E_{CC,large\ k}$$

Measurement of Success: SRE Method must be faster than generating the data traditionally and must be fairly accurate.

SRE Prediction for N_{max}=70 using only 5-20 open shells: Time Savings



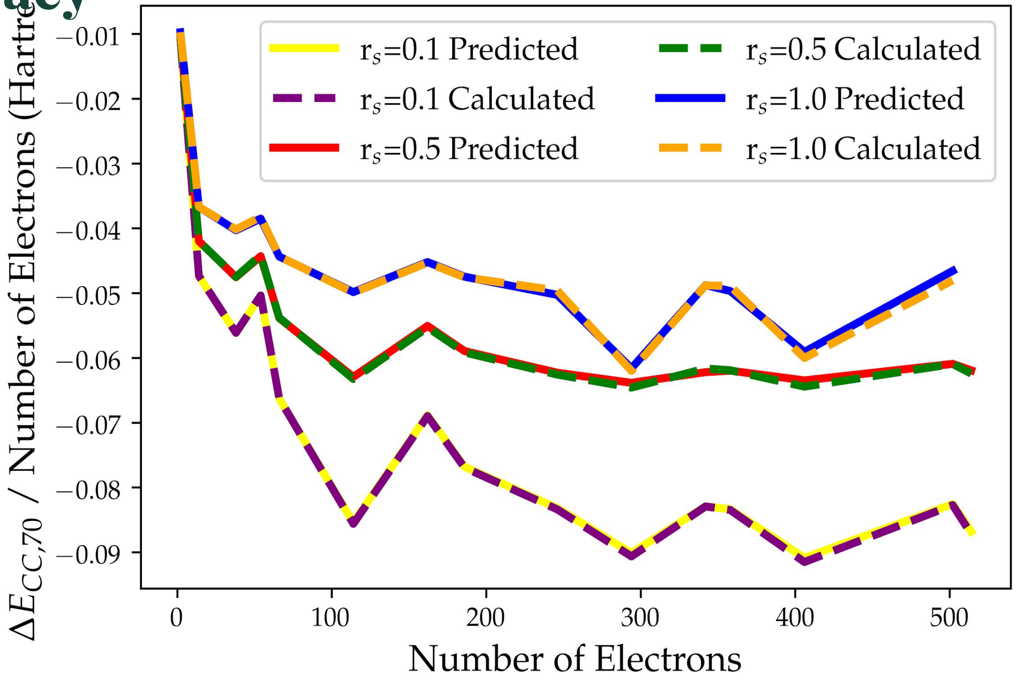


Time Savings: ~32 seconds

Time Savings: ~35 minutes

Note: Comparisons are made to Nmax=70, but predictions should be the fully converged result

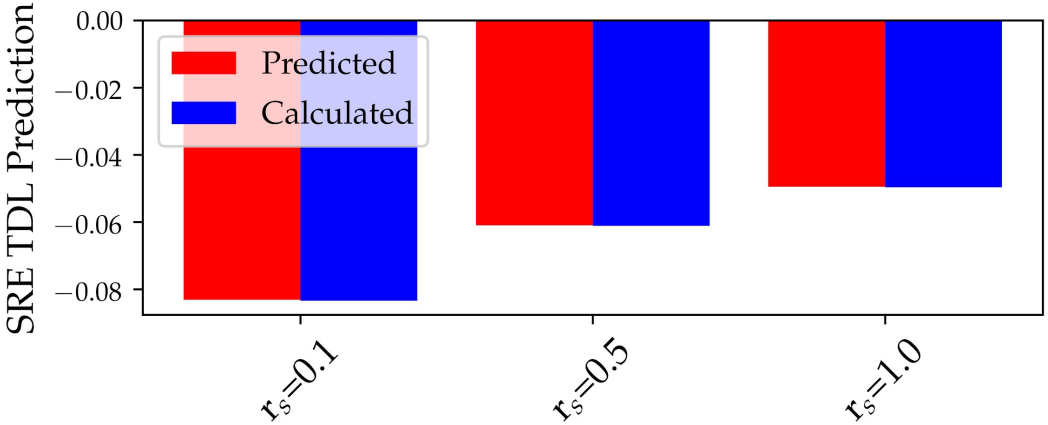
SRE Prediction for N_{max}=70 using only 5-20 open shells: Accuracy



r_s	Average Percent Error
0.1	0.021%
0.5	0.046%
1.0	0.076%

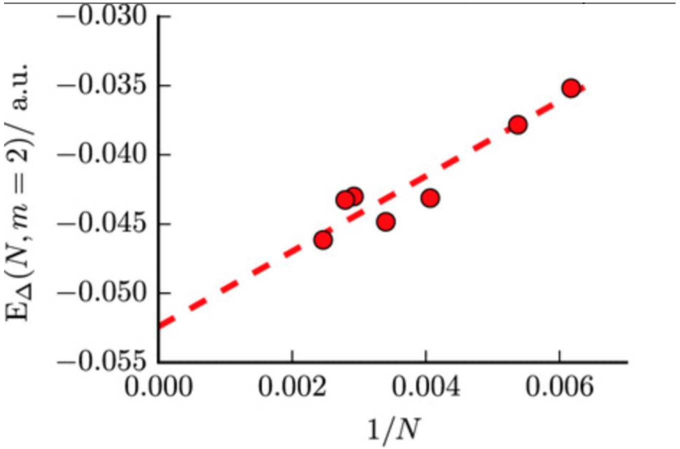
Note: the yellow line is right under the purple one

Extrapolation to the Thermodynamic Limit with SRE



r_s = 1.0: -0.0517 Hartrees

Close to literature values!



J. Chem. Phys. **145**, 031104 (2016)

Pure Neutron Matter and Symmetric Nuclear Matter

Infinite Nuclear Matter

Pure Neutron Matter

- Only contains neutrons (so has no electric charge)

Symmetric Nuclear Matter

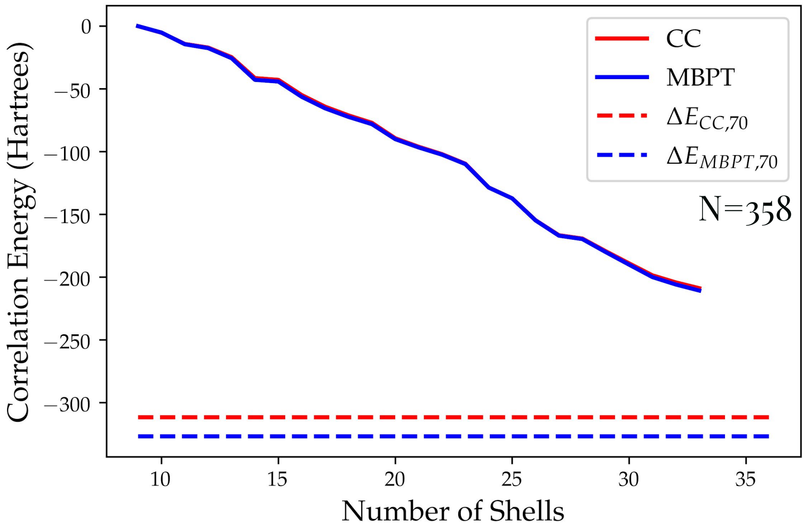
- Matter containing an equal number of protons and neutrons in a negative electric field (so no net charge)

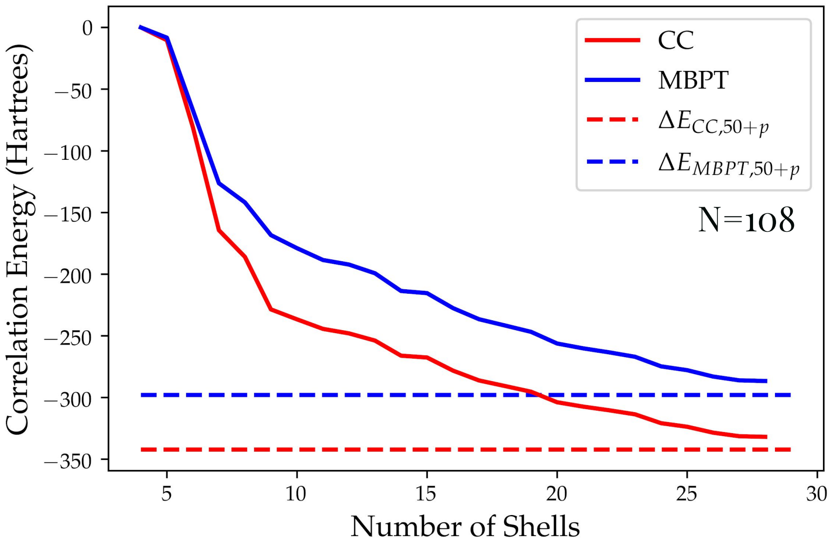
- Calculations are performed at particle numbers that have closed shells, d = 0.16 fm^{-3} (nuclear matter saturation density)
- Periodic boundary conditions, optimized block diagonal structure

Nuclear matter only has short range interactions!

LNP 936; G. Baardsen et. al. Physical Review C **88;** C. Drischler et. al., Annual Review of Nuclear and Particle Science **71**, 403 (2021).

Convergence of Many-Body Methods (Pure Neutron Matter and Symmetric Nuclear Matter)





Ridge Regression Does Not Work Well Here, Use Kernel Ridge Regression Instead

$$\hat{y}_{KRR} = \sum_{i=1}^{N} \theta_i k(x_i, x)$$

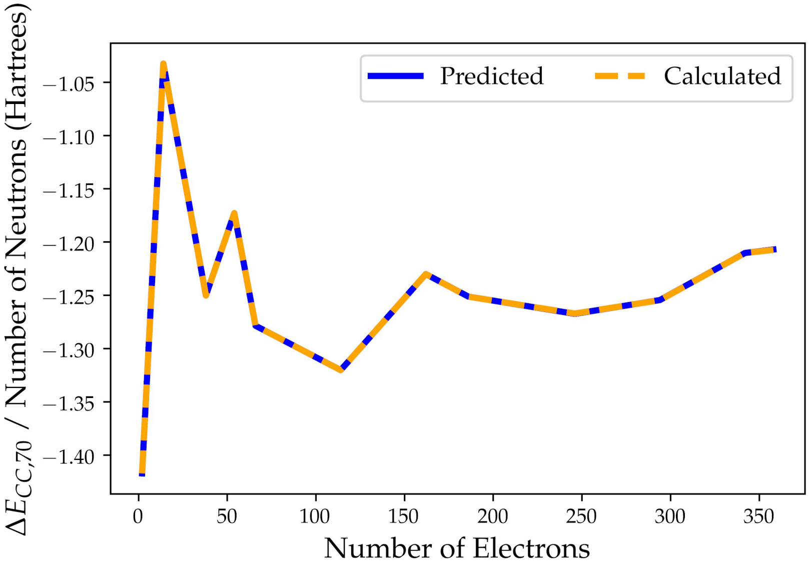
$$J_{KRR}(\theta) = \lambda\theta^2 + \frac{1}{M}[\theta K - Y][\theta K - Y]$$

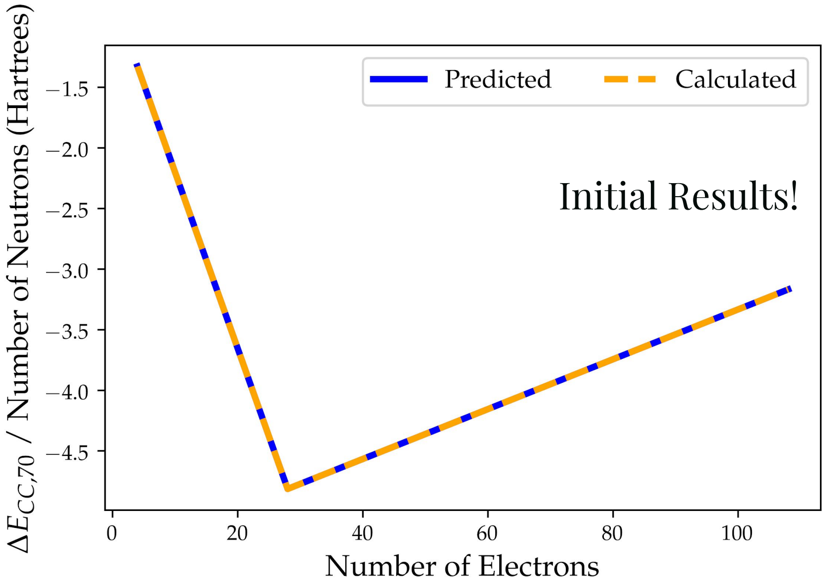
$$\theta_{KRR} = (\mathbf{K} - \lambda\mathbf{I})^{-1}\mathbf{Y}$$

- Output is a linear combination of kernel functions instead of inputs → Can model more complicated data
- **Drawback**: Hyperparameter tuning must be done via brute force/grid search (for now…)

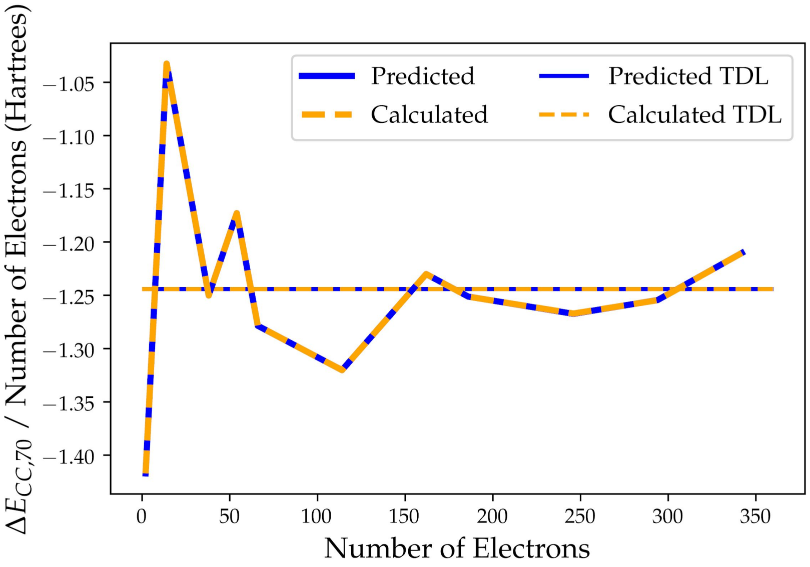
Hands-On Machine Learning by Aurélien Géron and Sci-Kit Learn’s website

SRE Prediction for N_{max}=70 using only 5-25 open shells





Extrapolation to the Thermodynamic Limit



In Progress!!

Conclusions and Future Works

Conclusions and Future Works

Conclusions

- SRE is an excellent tool in many-body theory for extrapolations to reduce finite size effects and to extrapolate to the thermodynamic limit

Future Works

- **Electron Gas:** Extend the calculations to higher values of r_s
- **Nuclear Matter**: Extend the analysis to higher particle numbers, Implement Bayesian hyperparameter tuning for kernel ridge regression
- Change the boundary conditions from periodic to average angles
- Extend this methodology to achieve triples predictions at significantly reduced runtimes

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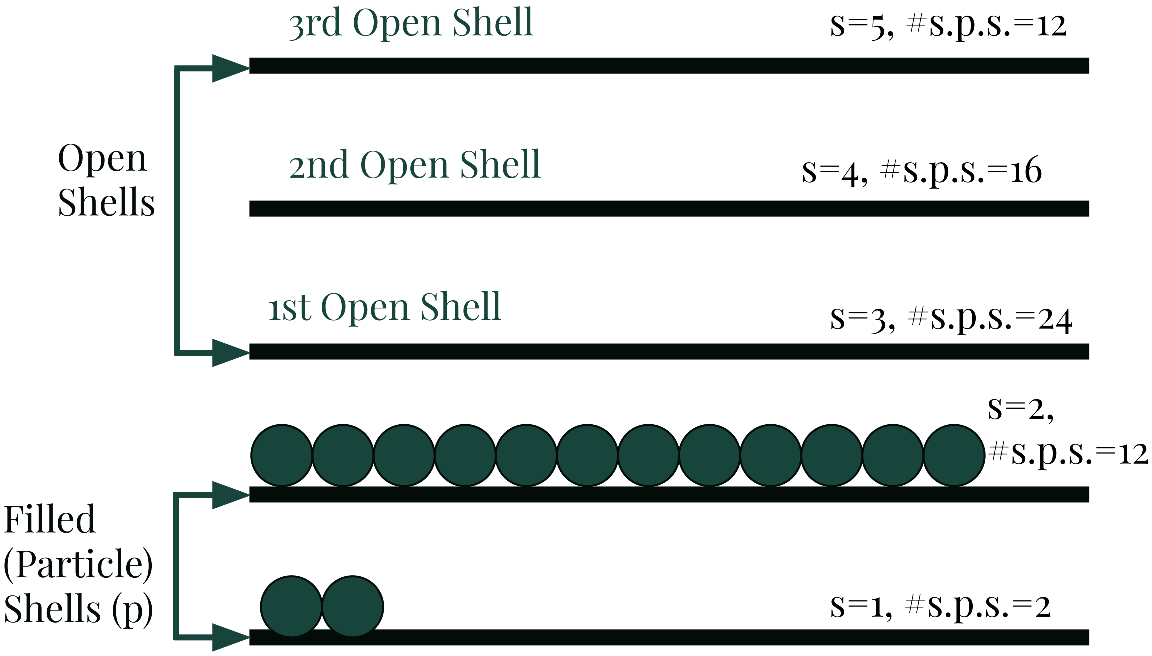
Extra Slides

Shell Structure and Finite Size Effects

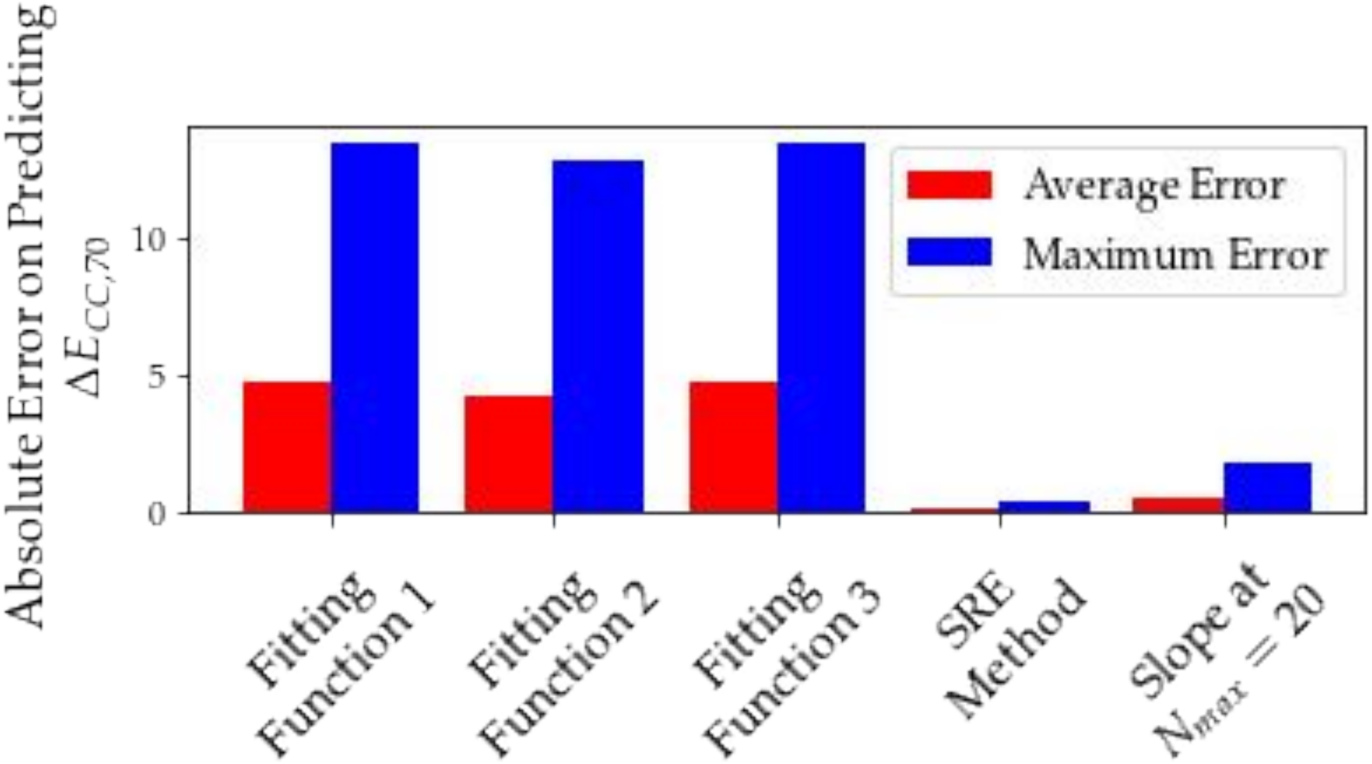
- Truncating the number of open shells introduces an error into the calculations for energy.
- **Magic Number**: The number of particles exactly fills the last particle shell (2,14,38,54,66,...)
- **Notation**: $\Delta E_{X,Y}(N)$
  - X = MBPT or CC, Y = Number of shells. N = Number of particles
  - $\Delta E_{CC,70}$,$\Delta E_{CC,20+p}$

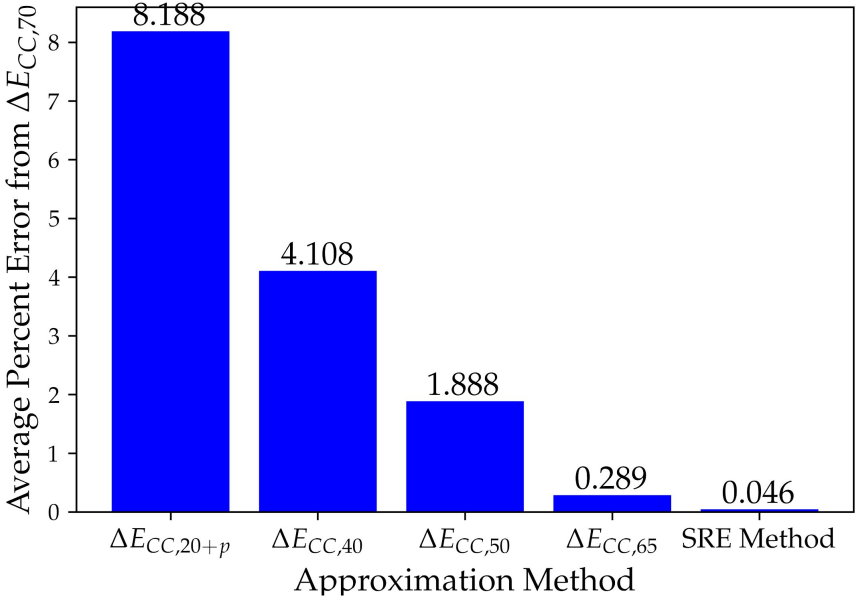


N: Number of Particles, M: Number of Single Particle States

N_{max}: Number of Levels

Comparison to Traditional Fitting Methods (r_s=0.5)




8.188
4.108
1.888
0.289
0.046
Average Percent Error from $\Delta E_{CC,70}$
0
1
2
3
4
5
6
7
8
$\Delta E_{CC,20+p}$
$\Delta E_{CC,40}$
$\Delta E_{CC,50}$
$\Delta E_{CC,65}$
SRE Method
Approximation Method

r_s=0.5