An Efficient Learning Method to Connect Observables

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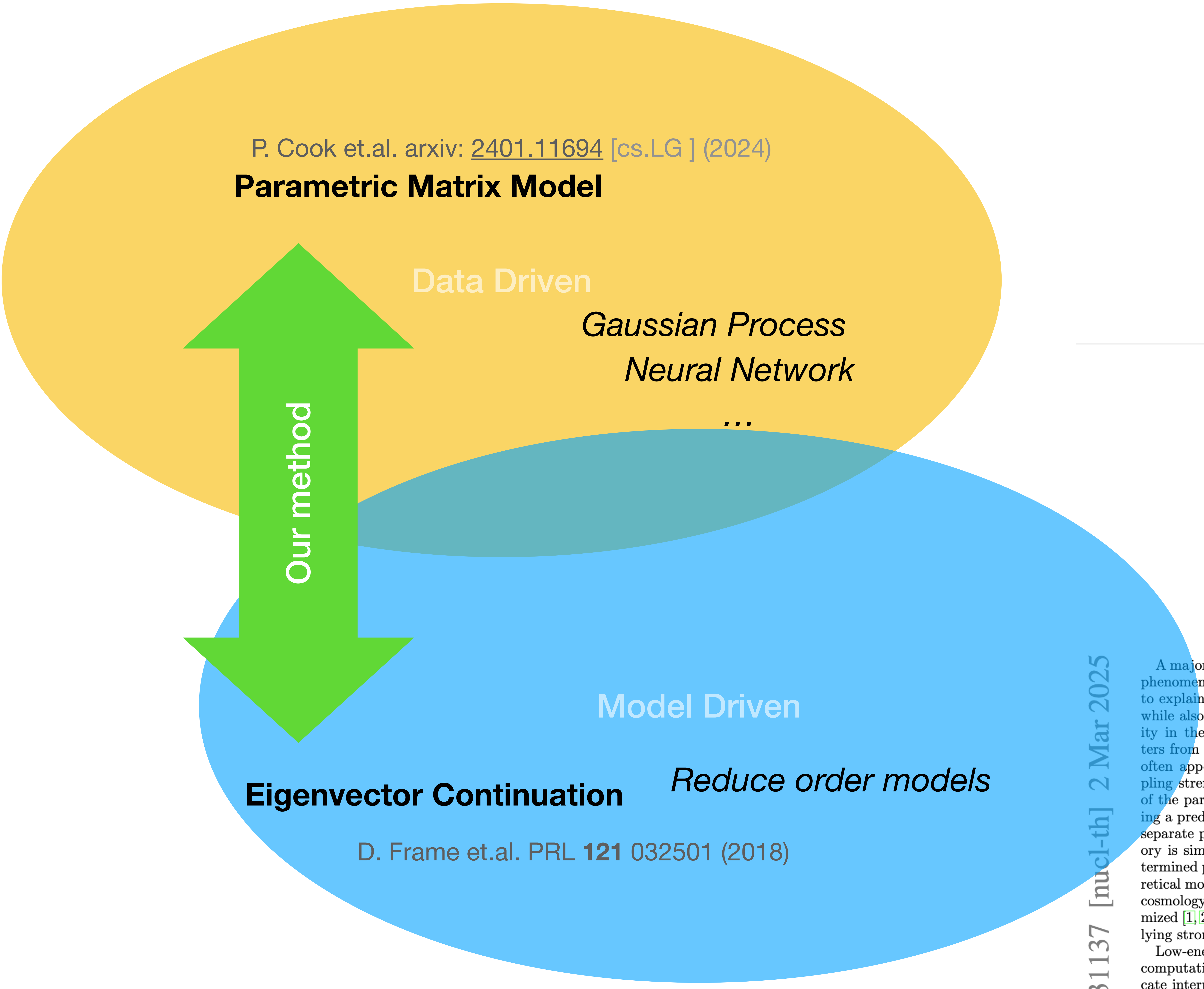
3/3

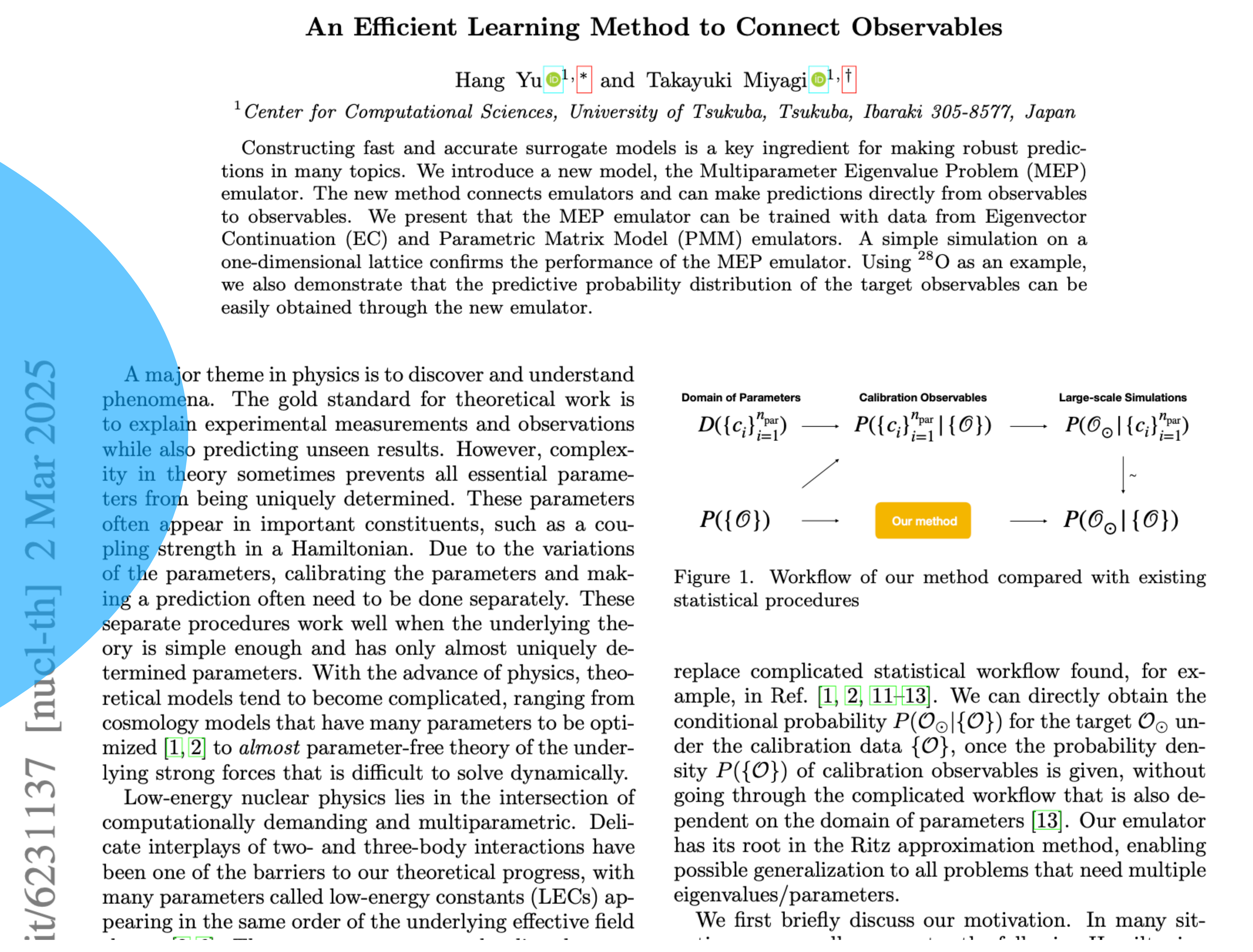
Frontiers in NLEFT, Beihang

ERATO

Collaborator: Takayuki Miyagi



HY and T. Miyagi [soon^{TM}(for real)]



An Efficient Learning Method to Connect Observables

Hang Yu[1,*] and Takayuki Miyagi[1,†]

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Constructing fast and accurate surrogate models is a key ingredient for making robust predictions in many topics. We introduce a new model, the Multiparameter Eigenvalue Problem (MEP) emulator. The new method connects emulators and can make predictions directly from observables to observables. We present that the MEP emulator can be trained with data from Eigenvector Continuation (EC) and Parametric Matrix Model (PMM) emulators. A simple simulation on a one-dimensional lattice confirms the performance of the MEP emulator. Using ^{28}O as an example, we also demonstrate that the predictive probability distribution of the target observables can be easily obtained through the new emulator.

[nucl-th] 2 Mar 2025

A major theme in physics is to discover and understand phenomena. The gold standard for theoretical work is to explain experimental measurements and observations while also predicting unseen results. However, complexity in theory sometimes prevents all essential parameters from being uniquely determined. These parameters often appear in important constituents, such as a coupling strength in a Hamiltonian. Due to the variations of the parameters, calibrating the parameters and making a prediction often need to be done separately. These separate procedures work well when the underlying theory is simple enough and has only almost uniquely determined parameters. With the advance of physics, theoretical models tend to become complicated, ranging from cosmology models that have many parameters to be optimized [1, 2] to *almost* parameter-free theory of the underlying strong forces that is difficult to solve dynamically.

Low-energy nuclear physics lies in the intersection of computationally demanding and multiparametric. Delicate interplays of two- and three-body interactions have been one of the barriers to our theoretical progress, with many parameters called low-energy constants (LECs) appearing in the same order of the underlying effective field

Figure 1. Workflow of our method compared with existing statistical procedures

replace complicated statistical workflow found, for example, in Ref. [1, 2, 11–13]. We can directly obtain the conditional probability $P(\mathcal{O}_\odot|\{\mathcal{O}\})$ for the target $\mathcal{O}_\odot$ under the calibration data $\{\mathcal{O}\}$, once the probability density $P(\{\mathcal{O}\})$ of calibration observables is given, without going through the complicated workflow that is also dependent on the domain of parameters [13]. Our emulator has its root in the Ritz approximation method, enabling possible generalization to all problems that need multiple eigenvalues/parameters.

We first briefly discuss our motivation. In many sit-

A Short Review of EC

When Perturbation Theory met Variational Principle…

$$H(c) = H_0 + cV$$

$$E_{\mathrm{gs}}(c) \leq \frac{\langle \psi | H(c) | \psi \rangle}{\langle \psi | \psi \rangle}$$

$$\psi(c) = \psi_0 + c\psi_1 + c^2\psi_2 + \dots$$

$$S(\psi) = \mathrm{span}(\{\psi_0, \psi_1, \psi_2, \dots\})$$

EC

T. Duguet, et. al.,96 (2024) 3, 031002

EC

Eigenvector Continuation

$$(\mathscr{H}(c) - \tilde{E}\mathscr{N})\tilde{\psi}(c) = 0$$

$$\mathscr{H}(c)_{ij} = \langle \psi(c_i) \,|\, H(c) \,|\, \psi(c_j) \rangle$$

$$\mathscr{N}_{ij} = \langle \psi(c_i) \,|\, \psi(c_j) \rangle$$

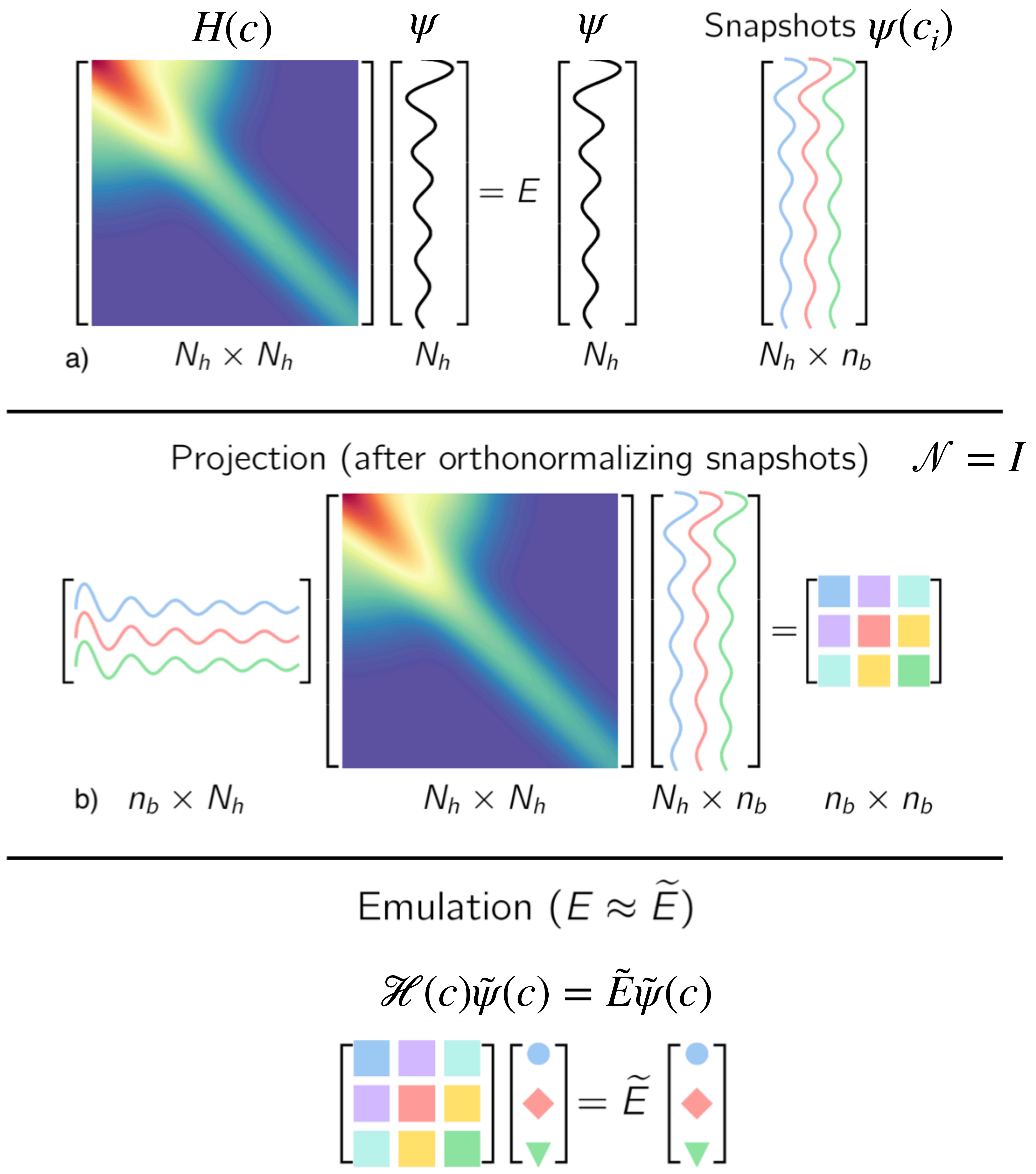
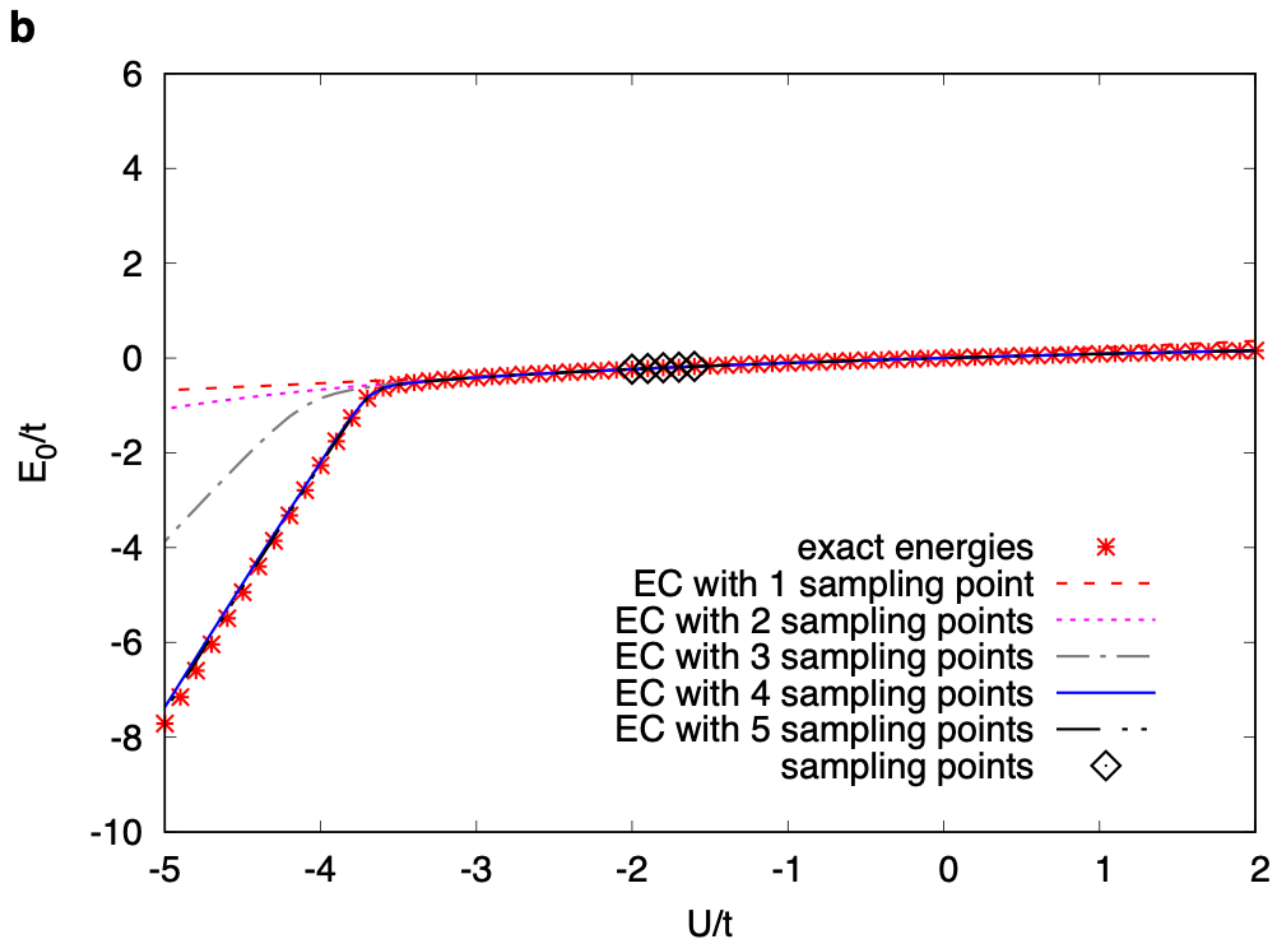


Figure adapted from
T. Duguet, et. al.,96 (2024) 3, 031002

EC

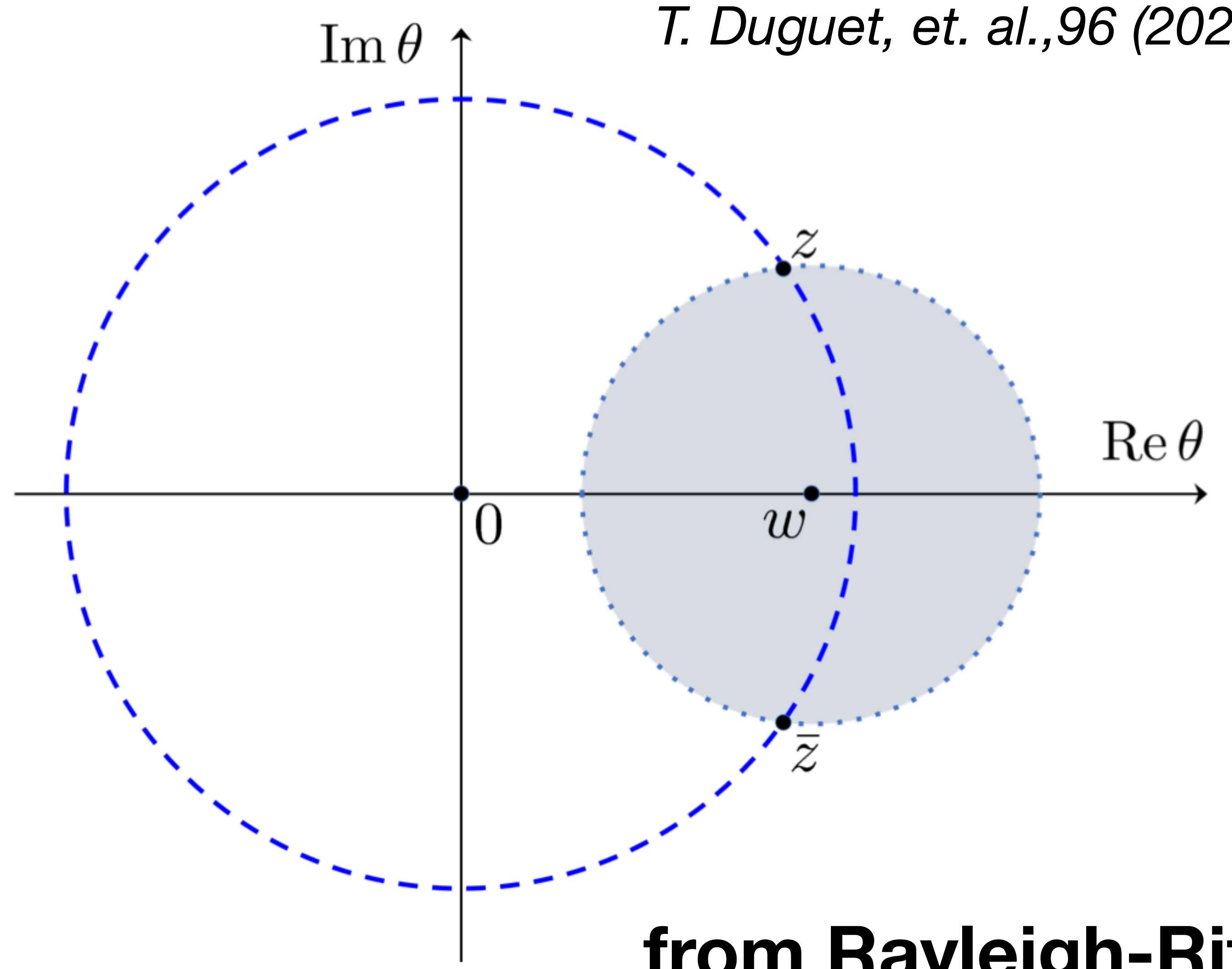
Properties



D. Frame et.al. PRL **121** 032501 (2018)

Bypass convergence radii

T. Duguet, et. al.,96 (2024) 3, 031002



from Rayleigh-Ritz

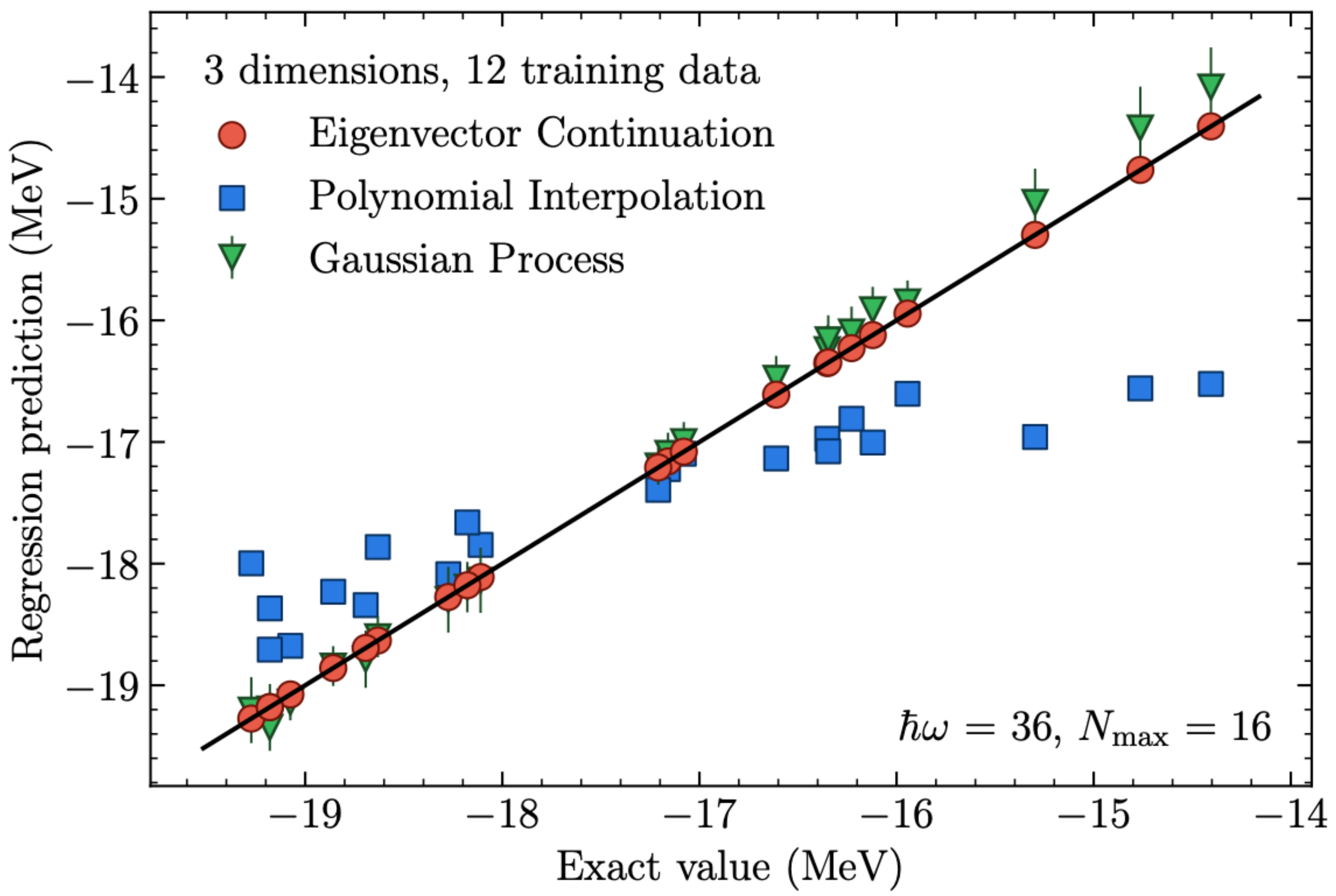
and requires very few snapshots

$$S(\psi) = \mathrm{span}(\{\psi_0, \psi_1, \psi_2, \dots\})$$

from Perturbation Theory

EC

Examples

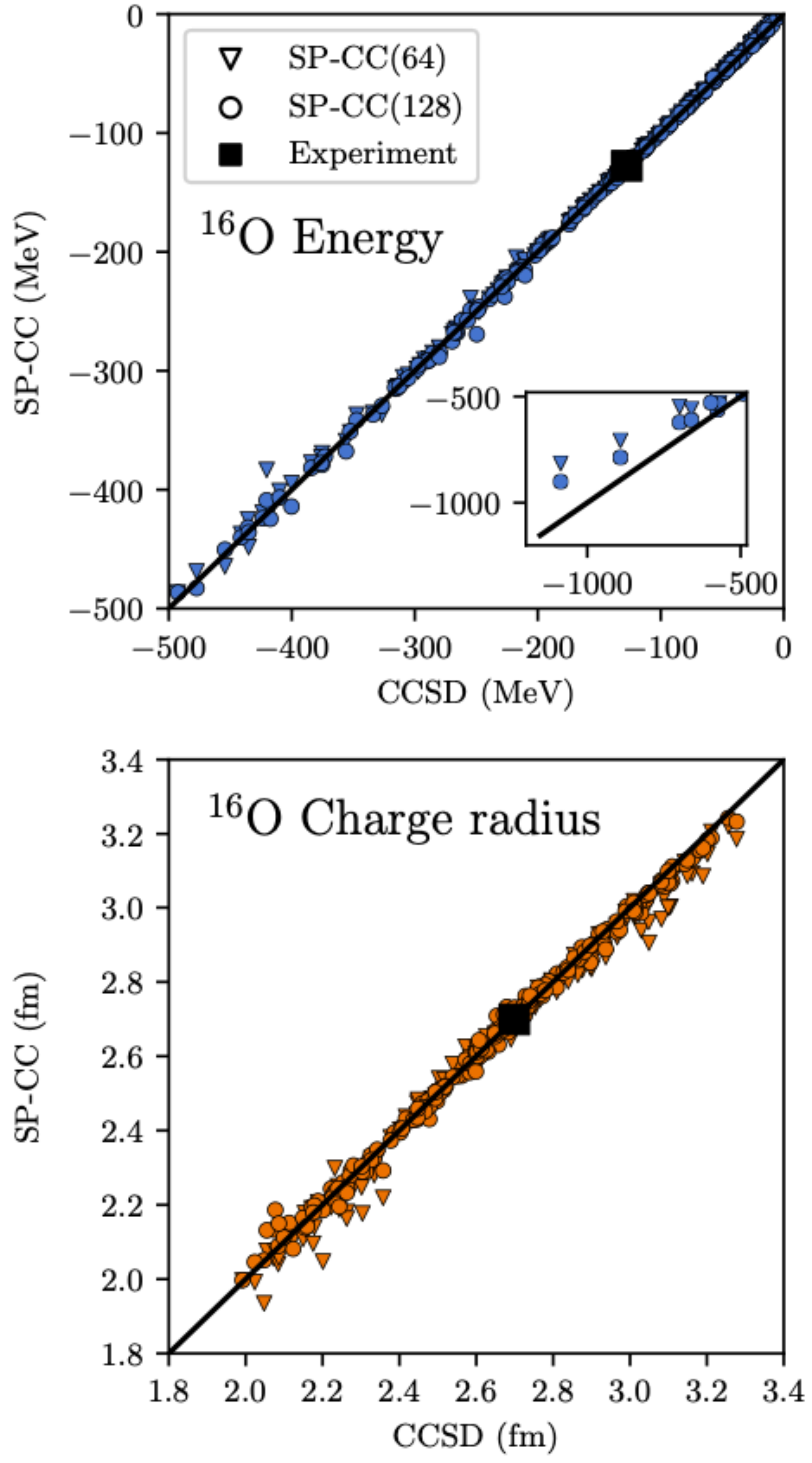


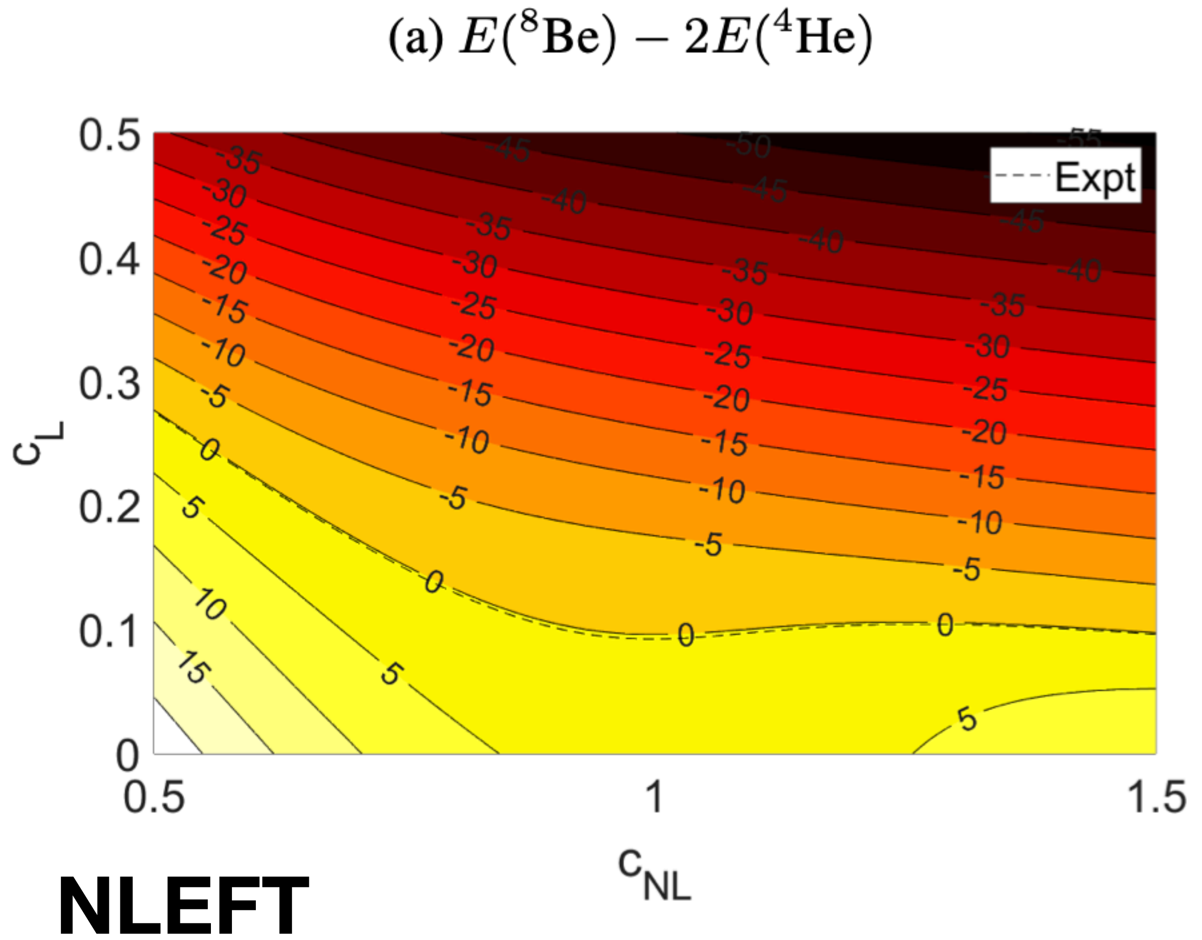
NCSM

S.Koenig et.al. PLB 810 135814 (2019)

Coupled-Cluster

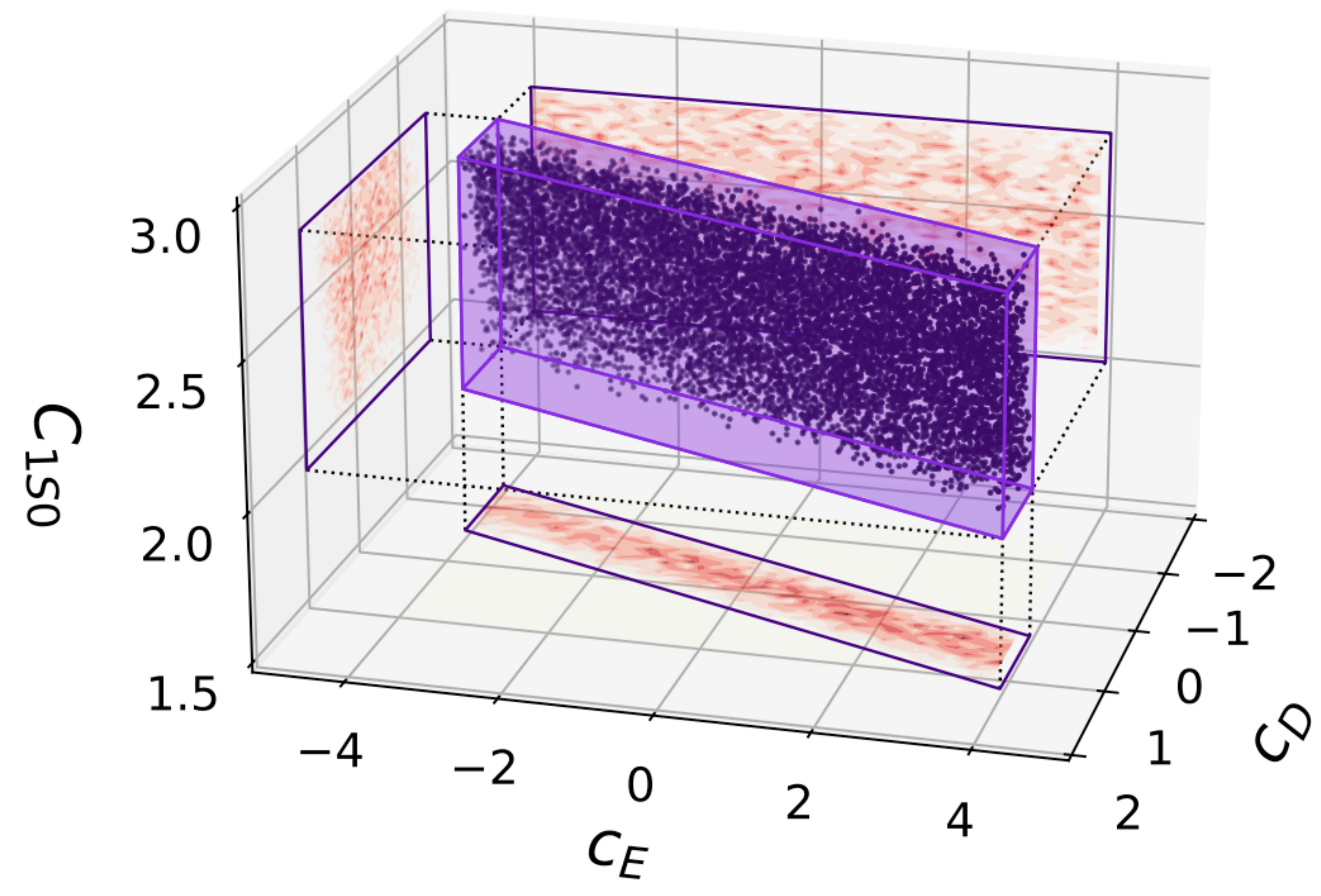
A. Ekstrom, et.al., PRL 123 252501 (2018)





NLEFT

A. Sarkar, et.al., PRL 131 242503 (2023)



Uncertainty Quantificatoin

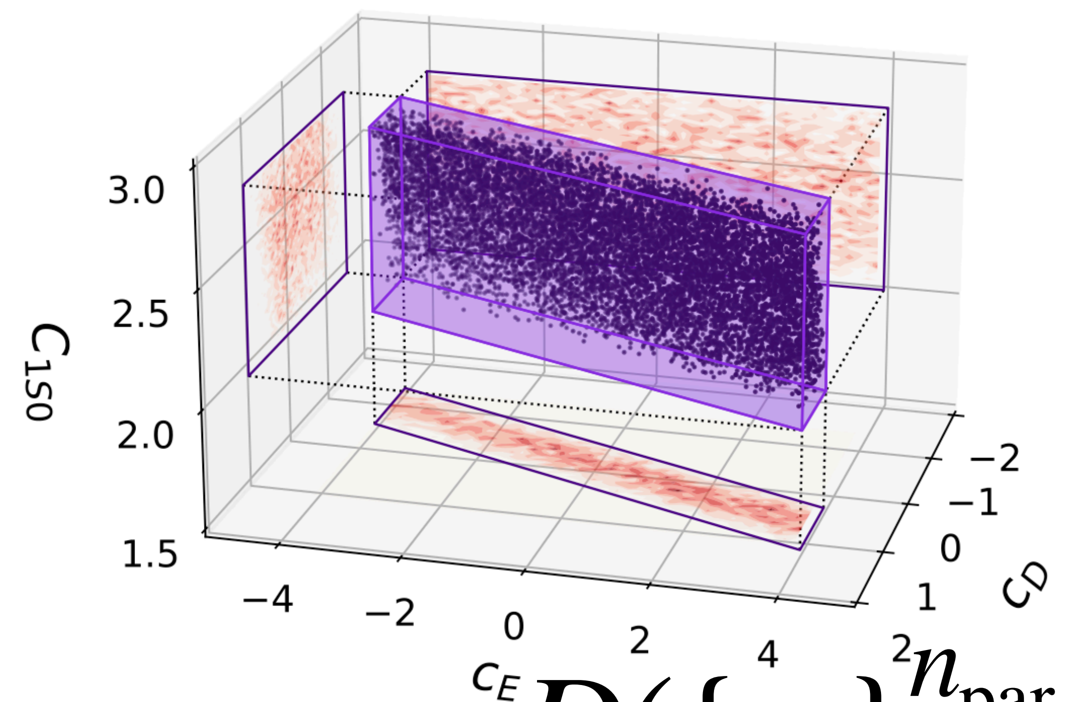
W.G. Jiang et.al., PRC 109 064314 (2024)

8188 ~ 8218 samples of LEC domain

Motivation

Coupling constants (LECs) are not observables…

$P(\mathcal{O}_i) \longrightarrow P(c_j)$



$D(\{c_i\}_{i=1}^{n_{\mathrm{par}}})$

To search for amplified effects

of N(2-4)LO $\chi-\mathrm{EFT}$…

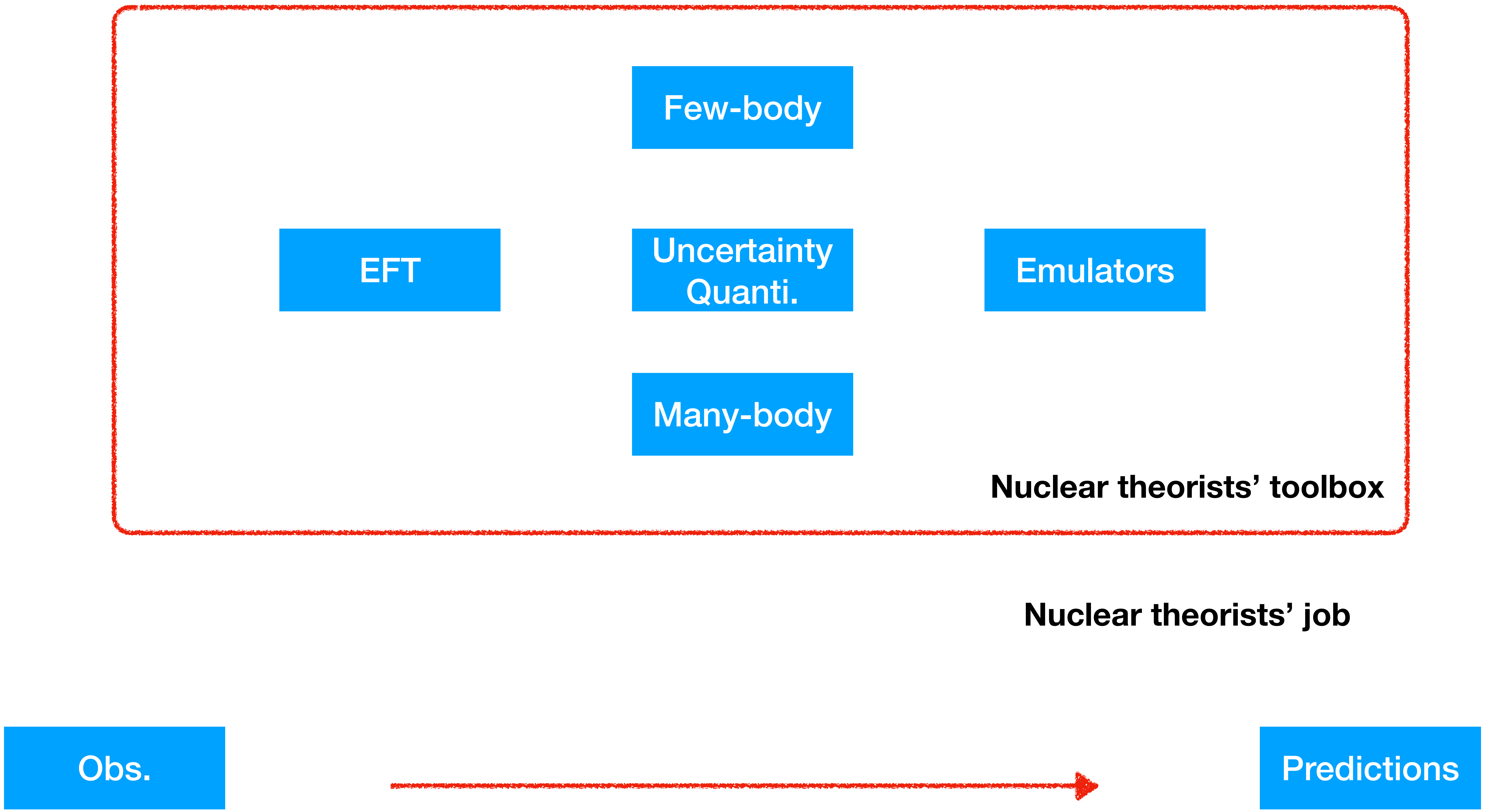
Spin polarized n-d scattering

Obs	EFT	Emulators	Uncertainty Quanti.
RIBF, RCNP, ⋮	RUB		TOMOE

See talk by H. Krebs

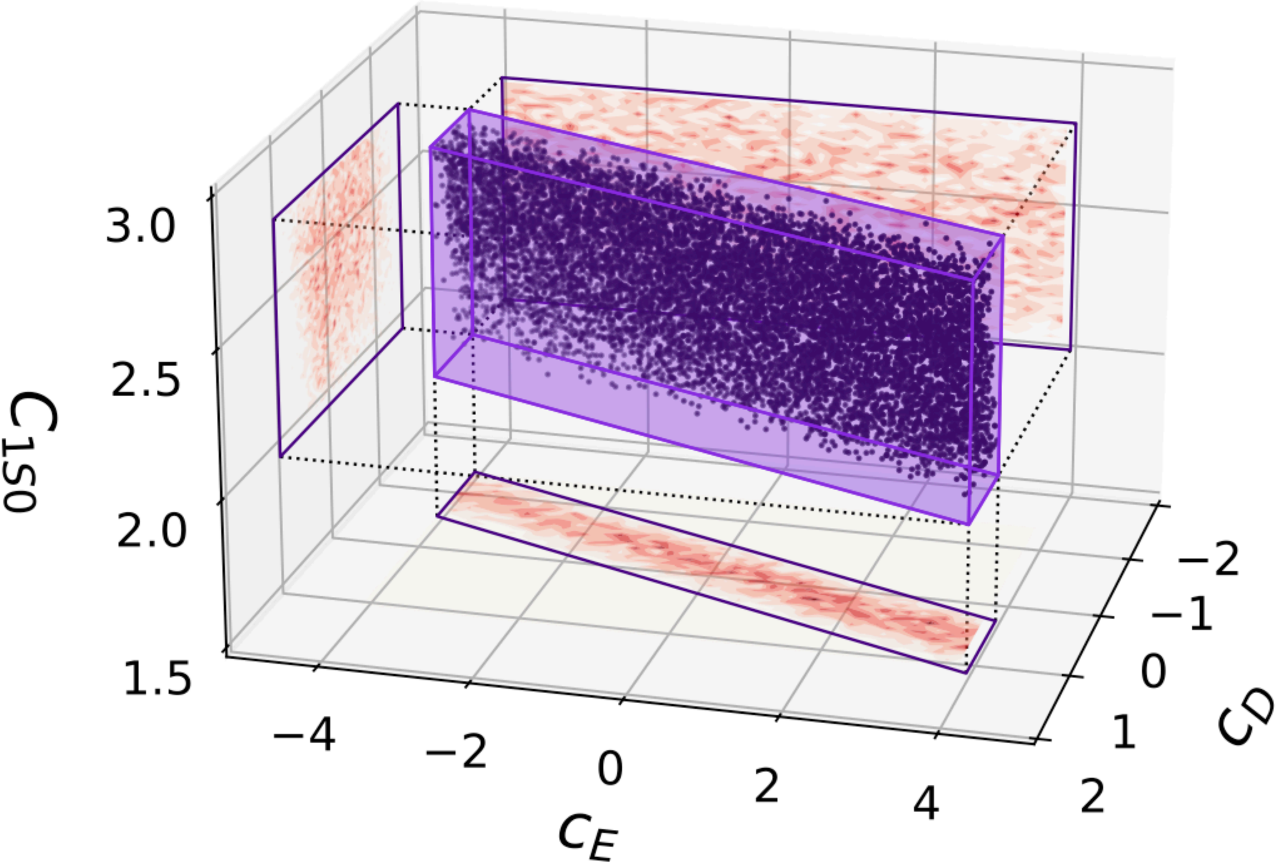
$+10-\mathrm{ish}$ **Threebody LECs**


Nuclear Medecine
RI production
Engineering
Nuclear fusion & fission
Nucleosynthesis
Neutron star
Applied Science
Evolution of Nuclear Data
Polarization Experiment
- Few-Nucleon Systems-
High-Accuracy
Quantum Many-Body
Calculations
Determination of
Three-Nucleon Force
Towards High Precision
Nuclear Force
Ultra Cold Atom
Experiment
Fundamental Science
Descriptions of Nuclei from First Principles
Establishment of Quantum Many-Body Simulation Tool of Nuclear Phenomena
with High-predictive Power



$$P(\mathcal{O}_\odot \,|\, \mathcal{O}_1, \mathcal{O}_2, \ldots)$$

statistically connecting observables…



$$P(\mathcal{O}_\odot \,|\, c_1, c_2, \ldots)$$

$$P(\mathcal{O}_\odot \,|\, \mathcal{O}_1, \mathcal{O}_2, \ldots)$$

Obs

EFT

Few-body

Emulators

Many-body

Uncertainty Quanti.

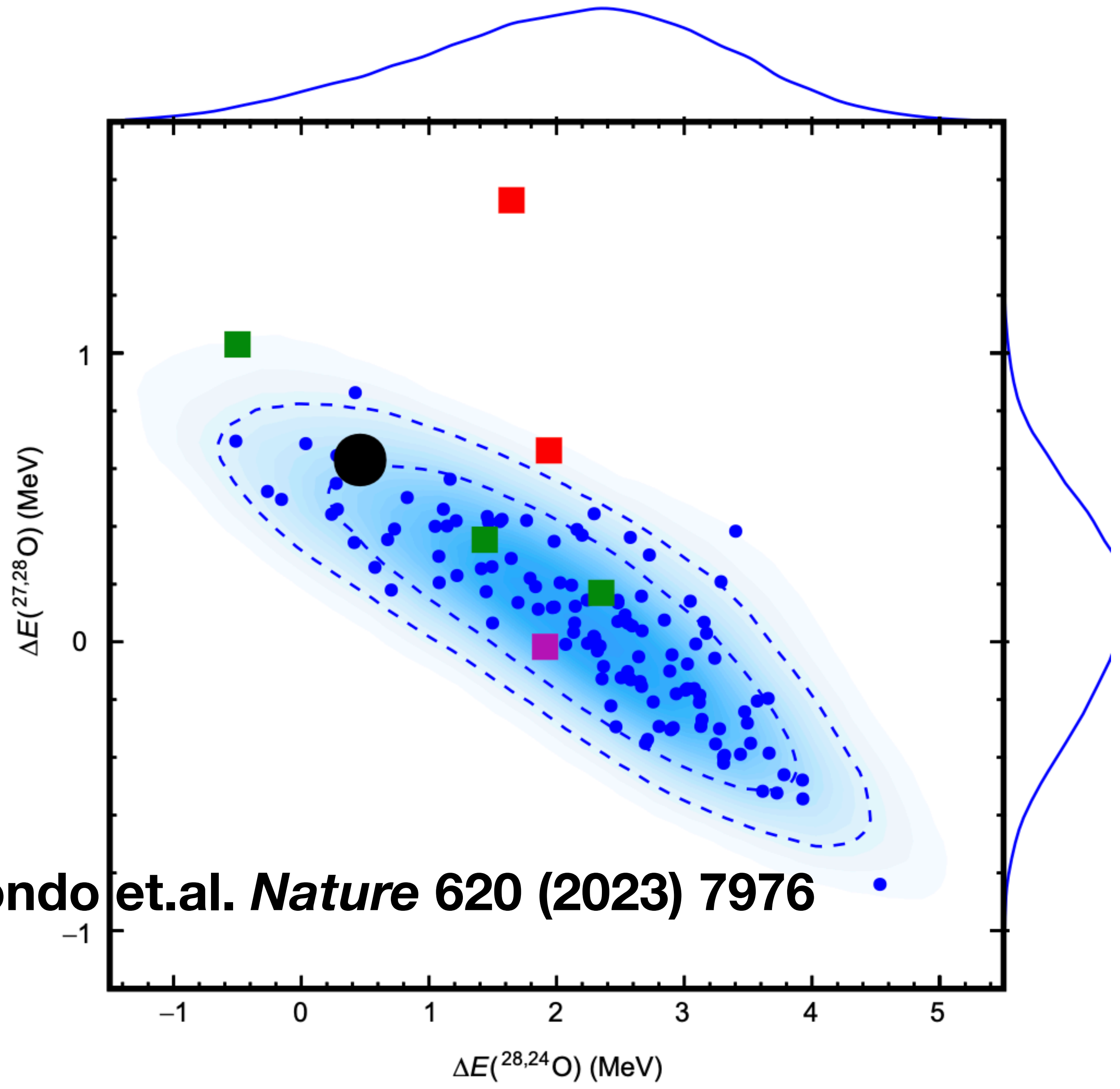
Predictions

$$P(\mathcal{O}_1, \mathcal{O}_2, \ldots)$$

$$P(c_1, c_2, \ldots \,|\, \mathcal{O}_1, \mathcal{O}_2, \ldots)$$

Too complicated

Also could fail where NN..LO contribution is large



Y. Kondo et.al. *Nature* 620 (2023) 7976

Domain of Parameters | **Calibration Observables** | **Large-scale Simulations**

$D(\{c_i\}_{i=1}^{n_{\rm par}}) \longrightarrow P(\{c_i\}_{i=1}^{n_{\rm par}} \,|\, \{\mathcal{O}\}) \longrightarrow P(\mathcal{O}_\odot \,|\, \{c_i\}_{i=1}^{n_{\rm par}})$

$P(\{\mathcal{O}\}) \nearrow$ (to $P(\{c_i\}_{i=1}^{n_{\rm par}} \,|\, \{\mathcal{O}\})$)

$P(\mathcal{O}_\odot \,|\, \{c_i\}_{i=1}^{n_{\rm par}}) \downarrow \sim P(\mathcal{O}_\odot \,|\, \{\mathcal{O}\})$

$P(\{\mathcal{O}\}) \longrightarrow$ **Our method** $\longrightarrow P(\mathcal{O}_\odot \,|\, \{\mathcal{O}\})$

Obs | **Predictions**

A.Zee, QFT in a nutshell

Lets look at the exact math models …

$$\left(H_0^{[a]} + c_1 H_1^{[a]} + c_2 H_2^{[a]} + \ldots + c_{n_{\rm par}} H_{n_{\rm par}}^{[a]} - E^{[a]} N^{[a]}\right) \mathbf{y}^{[a]} = 0$$

Bound

$E^{[a]}$ **are eigenvalues**

$$\left(H_0^{[b]} + c_1 H_1^{[b]} + c_2 H_2^{[b]} + \ldots + c_{n_{\rm par}} H_{n_{\rm par}}^{[b]} - E^{[b]} N^{[b]}\right) \mathbf{y}^{[b]} = 0$$

Continuum

$E^{[b]}$ **are parameters**

$$\left(H_0^{[c]} + c_1 H_1^{[c]} + c_2 H_2^{[c]} + \ldots + c_{n_{\rm par}} H_{n_{\rm par}}^{[c]} - E^{[c]} N^{[c]}\right) \mathbf{y}^{[c]} = 0$$

?

$E^{[b]}$ **are parameters**

$E^{[c]}, c_i$ **are eigenvalues**

$$\vdots$$

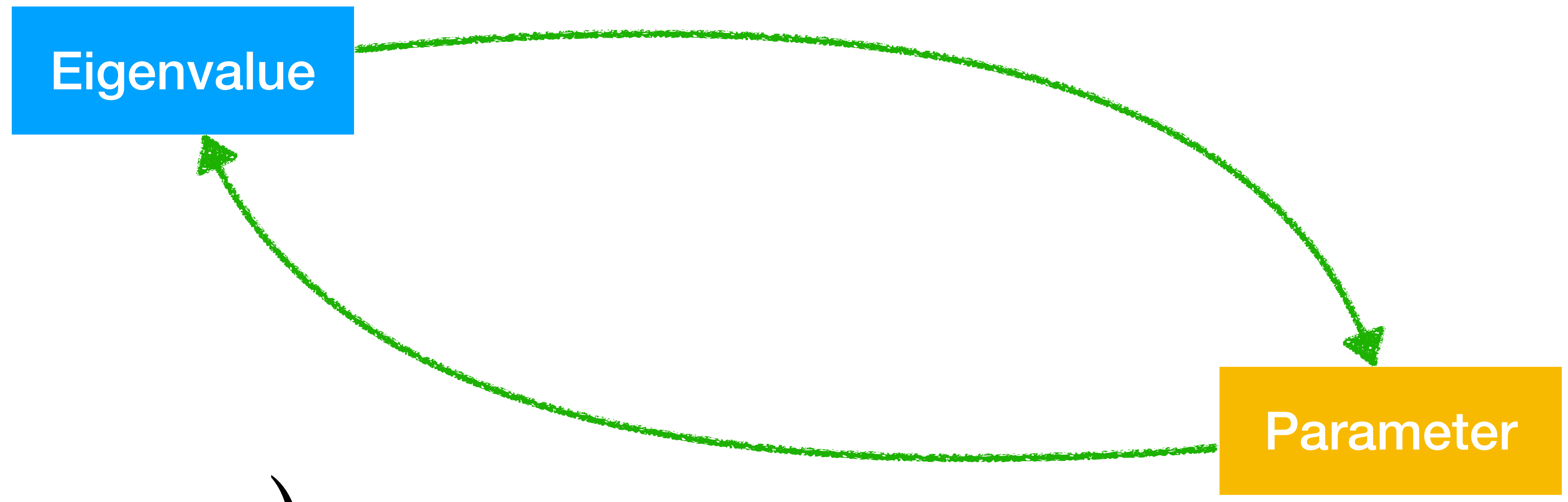
N equations to cancel N non-measurable!

Our Motivation

Our Motivation

N = 1 case

$$\left(H_0 + \sum_{i=1}^{n_{\text{par}}} c_i H_i - EN\right)\mathbf{y} = 0$$



$$H_{n_{\text{par}}}^{-1}\left(H_0 + \sum_{i=1}^{n_{\text{par}}-1} c_i H_i - EN\right)\mathbf{y} + c_{n_{\text{par}}}\mathbf{y} = 0$$

$$\left(H_0' + \sum_{i=1}^{n_{\text{par}}} c_i H_i' - E^{\text{new}}N'\right)\mathbf{y}' = 0$$

General N>1?

MEP Multiparameter Eigenvalue Problem

$$\left(H_0^{[j]} + \sum_{i=1}^{n_{\text{par}}} c_i H_i^{[j]} - E^{[j]} N^{[j]} \right) \mathbf{y}^{[j]} = 0 \qquad 1 \le j \le n_{\text{par}}$$

$$\left(H_0^{[j]} + \sum_{i=1}^{n_{\text{par}}} c_i H_i^{[j]} - E^{[j]} N^{[j]} \right) \mathbf{y}^{[j]} = 0 \qquad j > n_{\text{par}}$$

Method
(Model Driven)

MEP Math

$$\left(H_0^{[j]} + \sum_{i=1}^{n_{\text{par}}} c_i H_i^{[j]} - E^{[j]} N^{[j]} \right) \mathbf{y}^{[j]} = 0$$

The *Multiparameter* in MEP

means

Multiparametric Eigenvalues

$$\left(O_j + \sum_{i=1}^{m} \alpha_i A_{ij} \right) \mathbf{y}_j = 0 \,, \quad 1 \leq j \leq m$$

Inputs **Outputs**

F. V. Atkinson and A. B.Mingarelli
Multiparameter eigenvalue problems:
Sturm-Liouville theory
(2010)

$$(K_i - \alpha_i K_0)\mathbf{y}_{\otimes} = 0 \,, \quad 1 \leq i \leq m$$

$$\mathbf{y}_{\otimes} = \bigotimes_{j=1}^{m} y_j$$

MEP

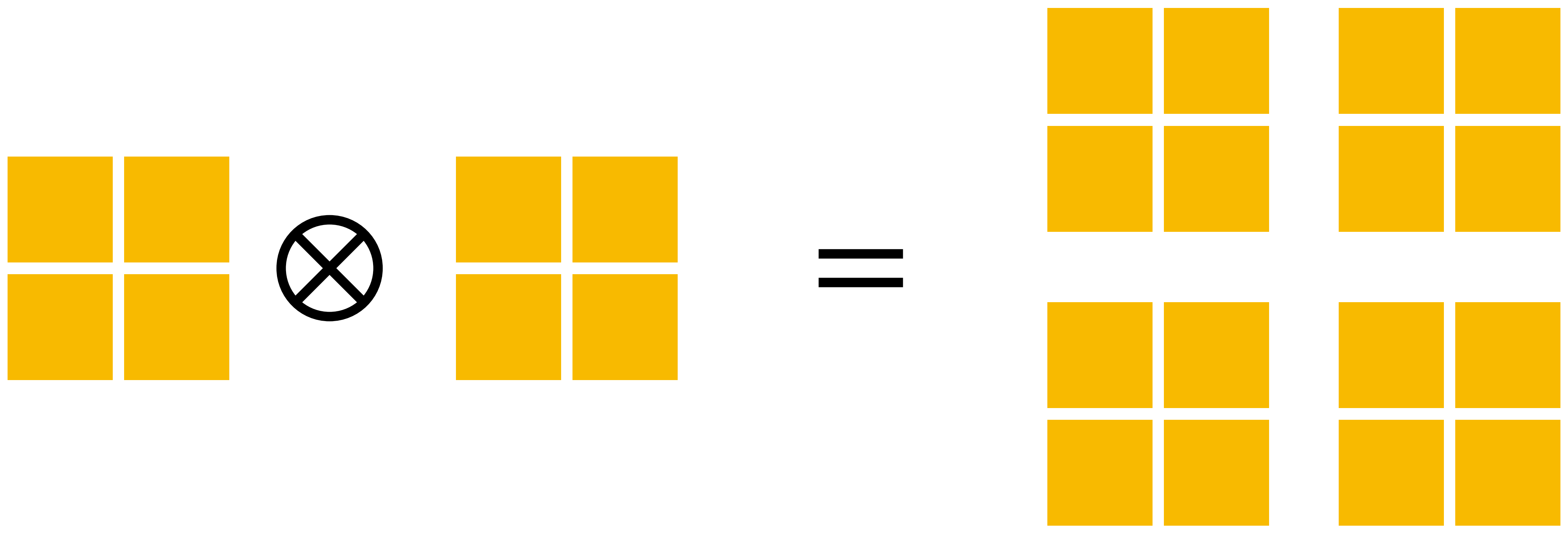
Kronecker Determinant

$$K_0 = \begin{vmatrix} A_{11} & \cdots & A_{1m} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mm} \end{vmatrix}_{\otimes}$$

$$\begin{vmatrix} G_{11} & \cdots & G_{1m} \\ \vdots & \ddots & \vdots \\ G_{m1} & \cdots & G_{mm} \end{vmatrix}_{\otimes} \equiv \sum_{\sigma \in S_m} \operatorname{sgn}(\sigma) G_{1\sigma(1)} \otimes G_{2\sigma(2)} \cdots \otimes G_{m\sigma(m)}$$

$$K_i = \begin{vmatrix} A_{11} & \cdots & A_{1(i-1)} & O_1 & A_{1(i+1)} & \cdots & A_{1m} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{m1} & \cdots & A_{m(i-1)} & O_m & A_{m(i+1)} & \cdots & A_{mm} \end{vmatrix}_{\otimes}$$

Kronecker Product



$$M \times M \qquad\qquad M^m \times M^m$$

***can be different sizes**

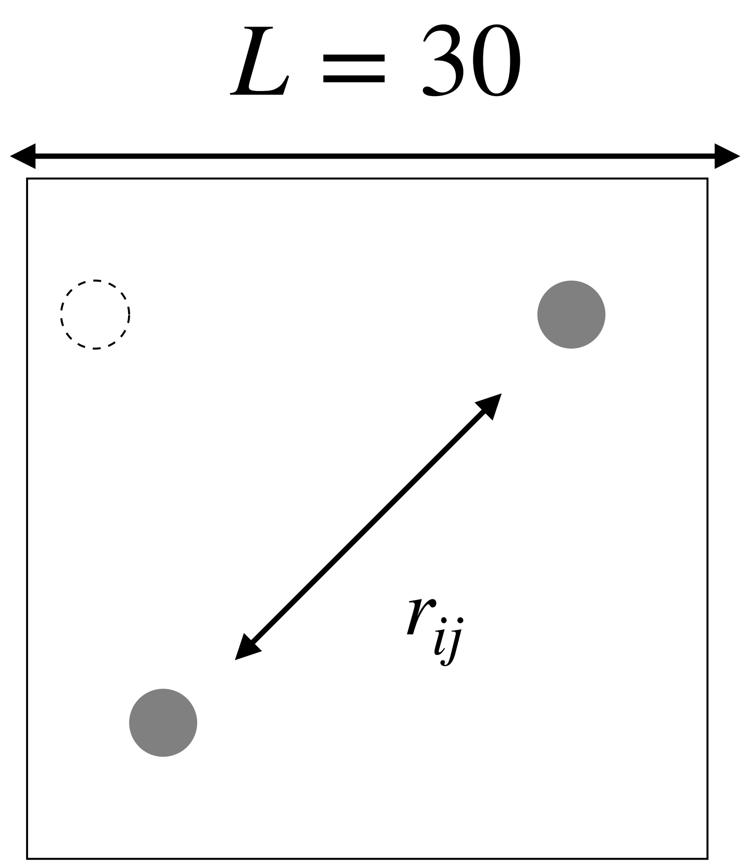
MEP

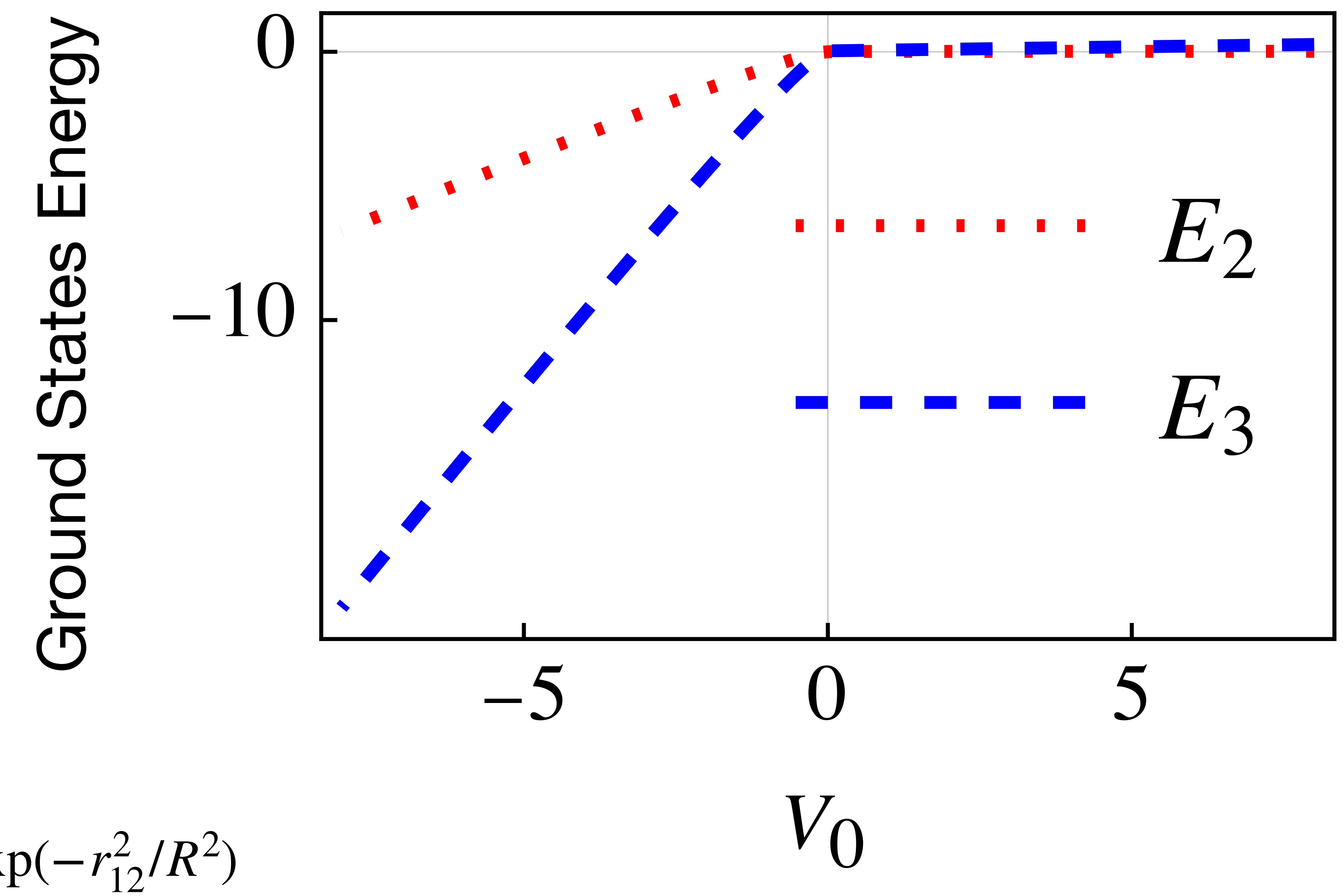
A toy model

$$\left(H_0^{[3]} + V_0 \exp(-r_{12}^2/R^2) + V_0 \exp(-r_{13}^2/R^2) + V_0 \exp(-r_{23}^2/R^2) - E_3 N^{[3]}\right) \mathbf{y}^{[3]} = 0$$

$$H_1^{[3]} \leftarrow \exp(-r_{12}^2/R^2) + \exp(-r_{13}^2/R^2) + \exp(-r_{23}^2/R^2)$$

$m = \hbar = c = 1$





$V_{ij} = V_0 \exp(-r_{ij}^2/R^2)$ $\quad R = 2.0$

$$H_1^{[2]} \leftarrow \exp(-r_{12}^2/R^2)$$

$$\left(H_0^{[2]} + V_0 \exp(-r_{12}^2/R^2) - E_2 N^{[2]}\right) \mathbf{y}^{[2]} = 0$$

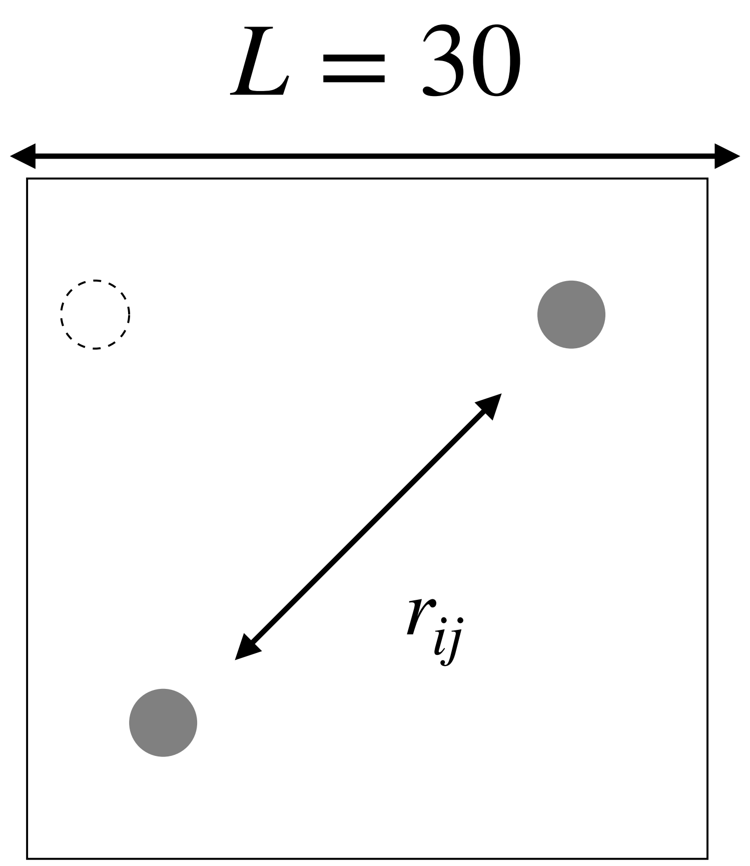
MEP

A toy model

$$\left(H_0^{[3]} + V_0 \exp(-r_{12}^2/R^2) + V_0 \exp(-r_{13}^2/R^2) + V_0 \exp(-r_{23}^2/R^2) - E_3 N^{[3]}\right) \mathbf{y}^{[3]} = 0$$

$m = \hbar = c = 1$

$$H_1^{[3]} \leftarrow \exp(-r_{12}^2/R^2) + \exp(-r_{13}^2/R^2) + \exp(-r_{23}^2/R^2)$$



$V_{ij} = V_0 \exp(-r_{ij}^2/R^2)$ $\quad R = 2.0$

$$O_1 = H_0^{[2]} + V_0 H_1^{[2]}$$

$$O_2 = H_0^{[3]} + V_0 H_1^{[3]}$$

$$\left(O_j + \sum_{i=1}^{2} \alpha_i A_{ij}\right) \mathbf{y}_j = 0\,, \quad 1 \le j \le 2$$

$A_{11} = -N^{[2]}$ $\quad A_{21} = 0$

$A_{12} = 0$ $\quad A_{22} = -N^{[3]}$

$$H_1^{[2]} \leftarrow \exp(-r_{12}^2/R^2)$$

$$\left(H_0^{[2]} + V_0 \exp(-r_{12}^2/R^2) - E_2 N^{[2]}\right) \mathbf{y}^{[2]} = 0$$

Diagonal MEP

$\alpha_1 = E_2$ $\quad \alpha_2 = E_3$

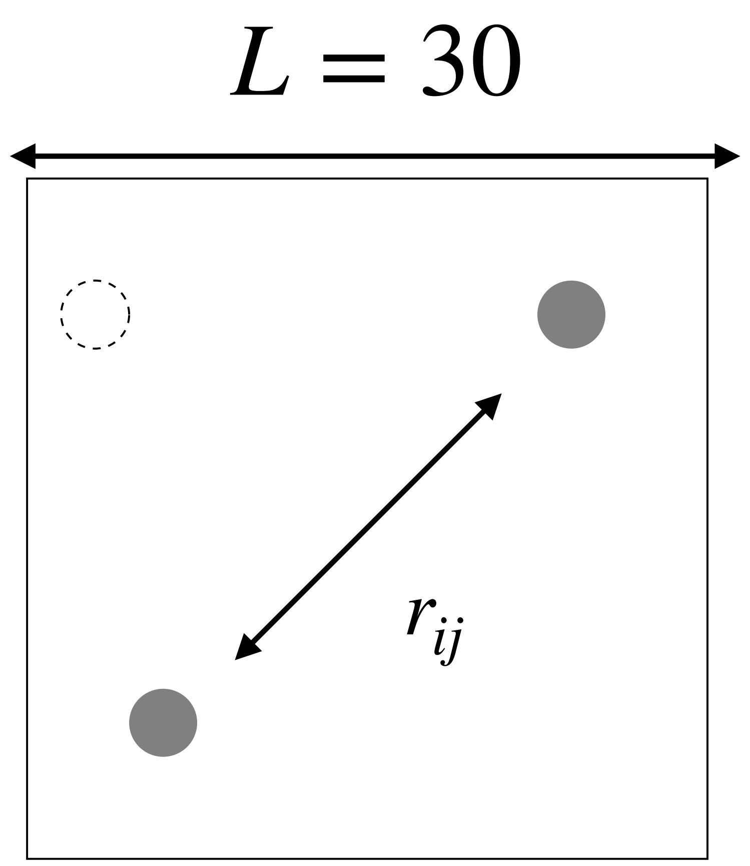
MEP

A toy model

$$\left(H_0^{[3]} + V_0 \exp(-r_{12}^2/R^2) + V_0 \exp(-r_{13}^2/R^2) + V_0 \exp(-r_{23}^2/R^2) - E_3 N^{[3]}\right) \mathbf{y}^{[3]} = 0$$

$$m = \hbar = c = 1$$

$$H_1^{[3]} \leftarrow \exp(-r_{12}^2/R^2) + \exp(-r_{13}^2/R^2) + \exp(-r_{23}^2/R^2)$$



$$O_1 = H_0^{[2]} - E_2 N^{[2]}$$

$$O_2 = H_0^{[3]}$$

$$\left(O_j + \sum_{i=1}^{2} \alpha_i A_{ij}\right) \mathbf{y}_j = 0\,, \quad 1 \le j \le 2$$

$$A_{11} = H_1^{[2]} \qquad A_{21} = 0$$

$$A_{12} = H_1^{[3]} \qquad A_{22} = -N^{[3]}$$

$$V_{ij} = V_0 \exp(-r_{ij}^2/R^2) \qquad R = 2.0$$

$$H_1^{[2]} \leftarrow \exp(-r_{12}^2/R^2)$$

$$\left(H_0^{[2]} + V_0 \exp(-r_{12}^2/R^2) - E_2 N^{[2]}\right) \mathbf{y}^{[2]} = 0$$

$$\alpha_1 = V_0 \qquad \alpha_2 = E_3$$

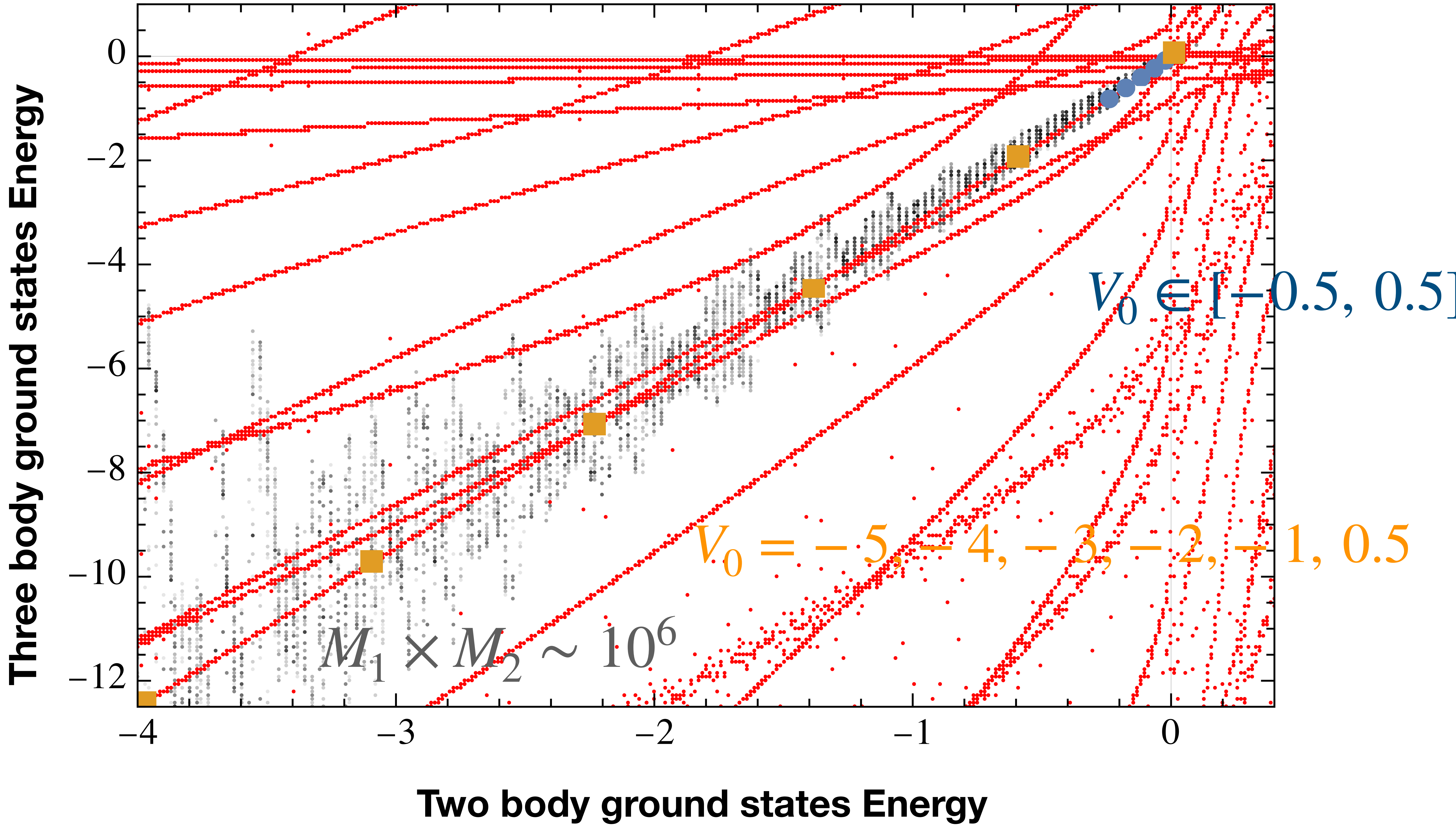
MEP

$$K_2 = \begin{vmatrix} H_1^{[2]} & H_0^{[2]} - E_2 N^{[2]} \\ H_1^{[3]} & H_0^{[3]} \end{vmatrix}_\otimes$$

$$K_0 = \begin{vmatrix} H_1^{[2]} & 0 \\ H_1^{[3]} & -N^{[3]} \end{vmatrix}_\otimes$$

$$M^m = 6^2$$

$$[K_2(E_2) + E_3 K_0]\mathbf{y} = 0$$



Contamination from G.S. ⊗ Fake (Excited)

Kronecker Determinant

$$K_0 = \begin{vmatrix} A_{11} & \cdots & A_{1m} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mm} \end{vmatrix}_\otimes$$

$$(K_i - \alpha_i K_0)\mathbf{y}_\otimes = 0 \qquad M^m \times M^m$$

$$(\mathscr{K}_0)_{kl} = (\mathbf{y}_{\otimes,k})^* \cdot K_0 \cdot \mathbf{y}_{\otimes,l} = \begin{vmatrix} (A_{11})_{kl} & \cdots & (A_{1m})_{kl} \\ \vdots & \ddots & \vdots \\ (A_{m1})_{kl} & \cdots & (A_{mm})_{kl} \end{vmatrix}$$

$$(\mathscr{K}_i - \alpha_i \mathscr{K}_0)\mathbf{y} = 0 \qquad M \times M$$

Matrix Determinant!

MEP | EC

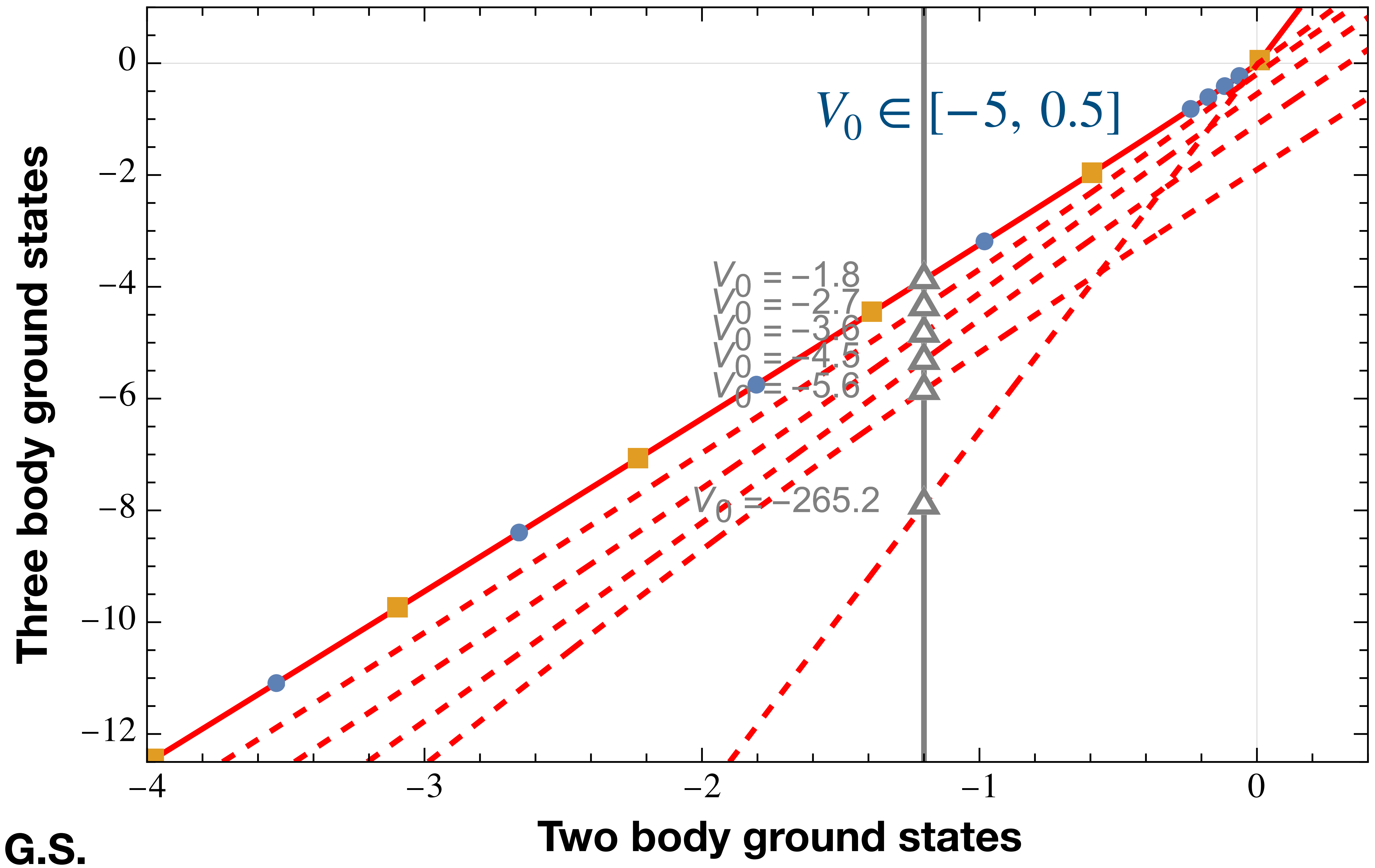
$$(\mathscr{K}_2)_{kl} = -(H_0^{[2]} - E_2 N^{[2]})_{kl}(H_1^{[3]})_{kl} + (H_1^{[2]})_{kl}(H_0^{[3]})_{kl}$$

$$(\mathscr{K}_0)_{kl} = (H_1^{[2]})_{kl}(-N^{[3]})_{kl}$$

$$[\mathscr{K}_2(E_2) + E_3\mathscr{K}_0]\tilde{\mathbf{y}} = 0$$

Only G.S. ⊗ G.S.

$V_0 = -5, -4, -3, -2, -1, 0.5$



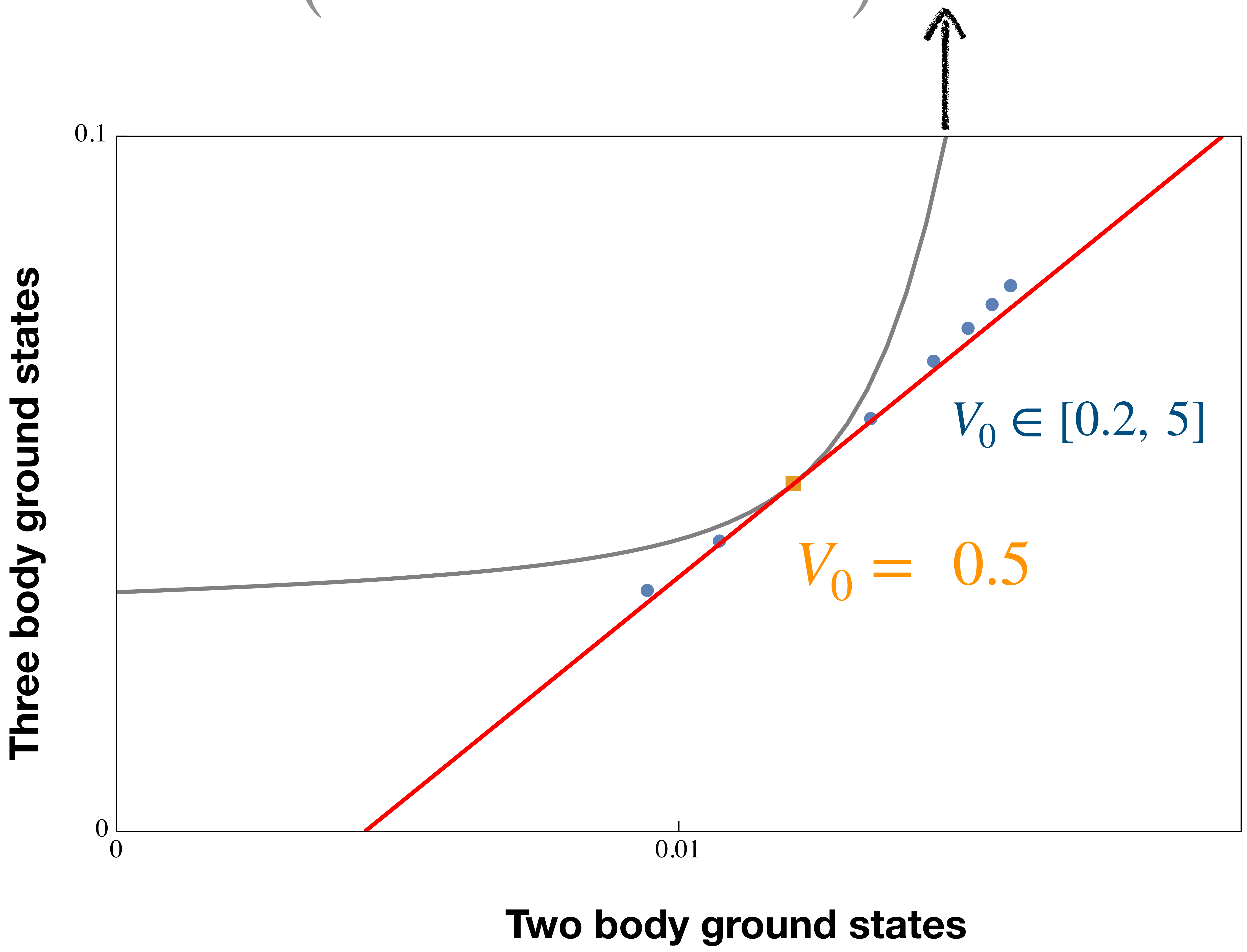
Zooming In

$$H_{n_{\text{par}}}^{-1}\left(H_0 + \sum_{i=1}^{n_{\text{par}}-1} c_i H_i - EN\right)\mathbf{y} + c_{n_{\text{par}}}\mathbf{y} = 0$$

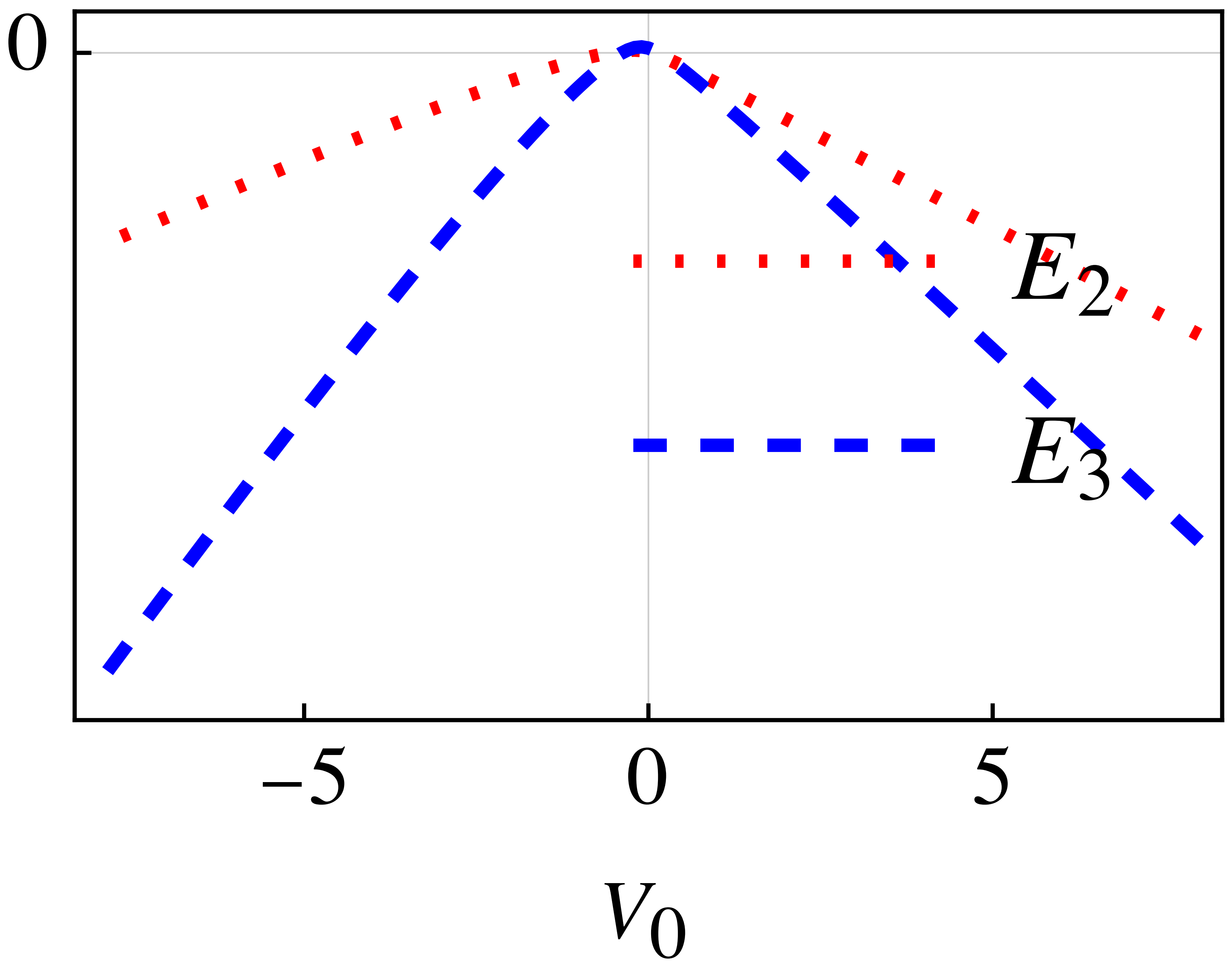
$$(\mathscr{K}_2)_{kl} = -(H_0^{[2]} - E_2 N^{[2]})_{kl}(H_1^{[3]})_{kl} + (H_1^{[2]})_{kl}(H_0^{[3]})_{kl}$$

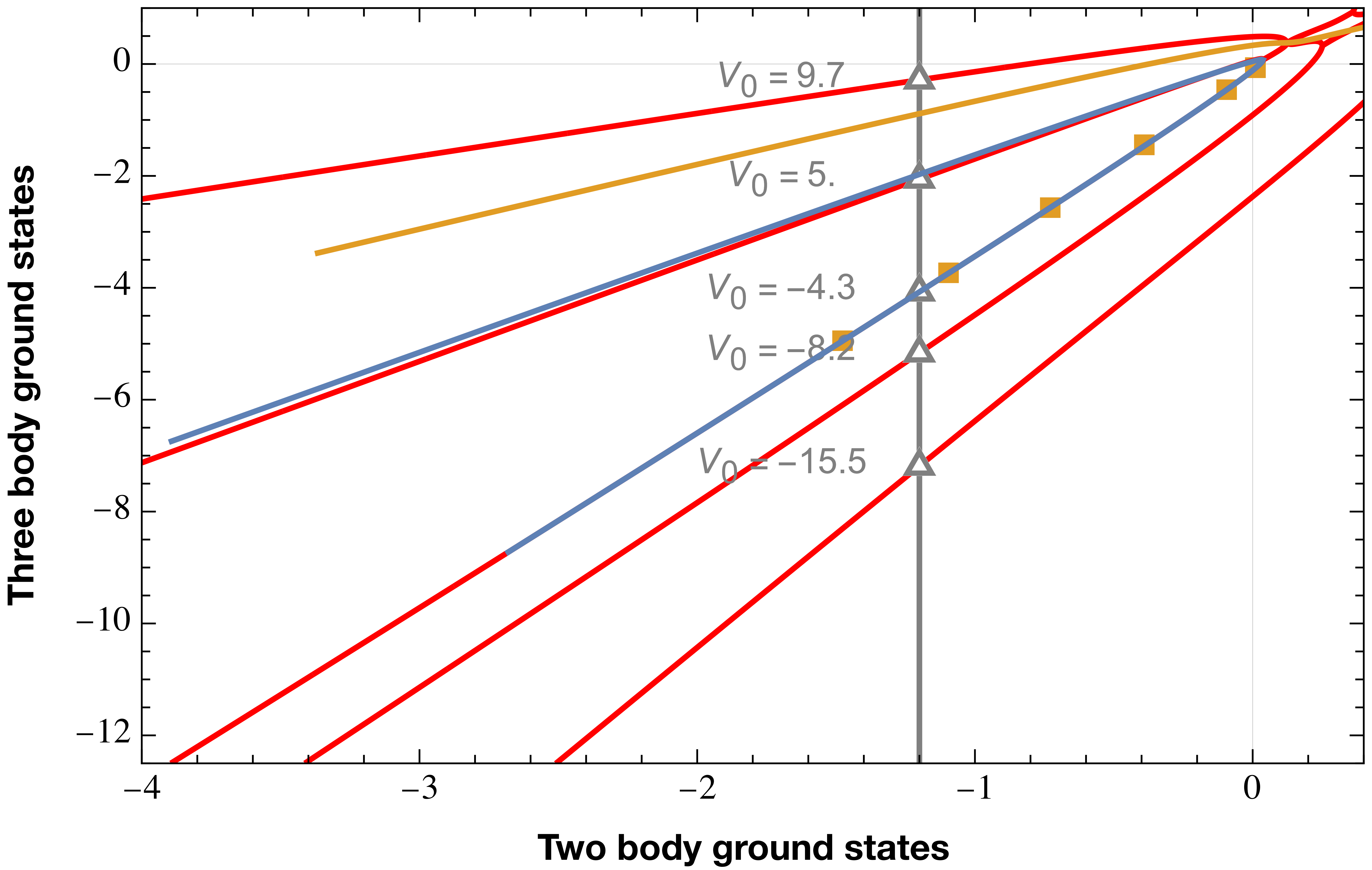
$$(\mathscr{K}_0)_{kl} = (H_1^{[2]})_{kl}(-N^{[3]})_{kl}$$

$$[\mathscr{K}_2(E_2) + E_3\mathscr{K}_0]\tilde{\mathbf{y}} = 0$$



MEP can be Multi(Nil)-Valued





Data-Driven

PMM

Parametric Matrix Model

It could be difficult to access wavefunctions

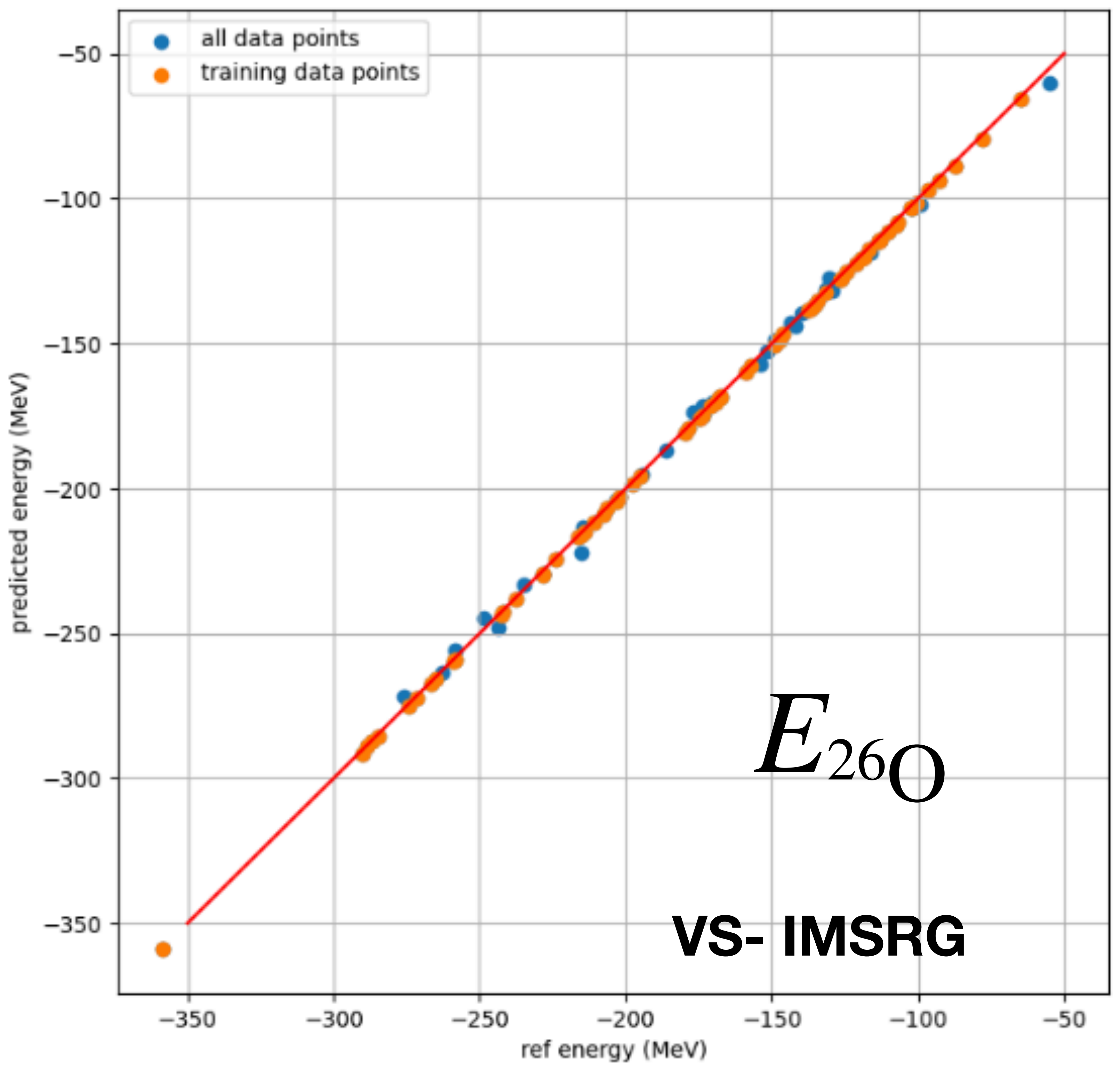
IMSRG
NLEFT
...

EC

$$\left(H_0 + c_1 H_1 + c_2 H_2 + \ldots + c_{n_{\text{par}}} H_{n_{\text{par}}} - EN\right) \mathbf{y} = 0$$

$$H_i^{[a]} \sim [M \times M]$$

~ 1000 parameters



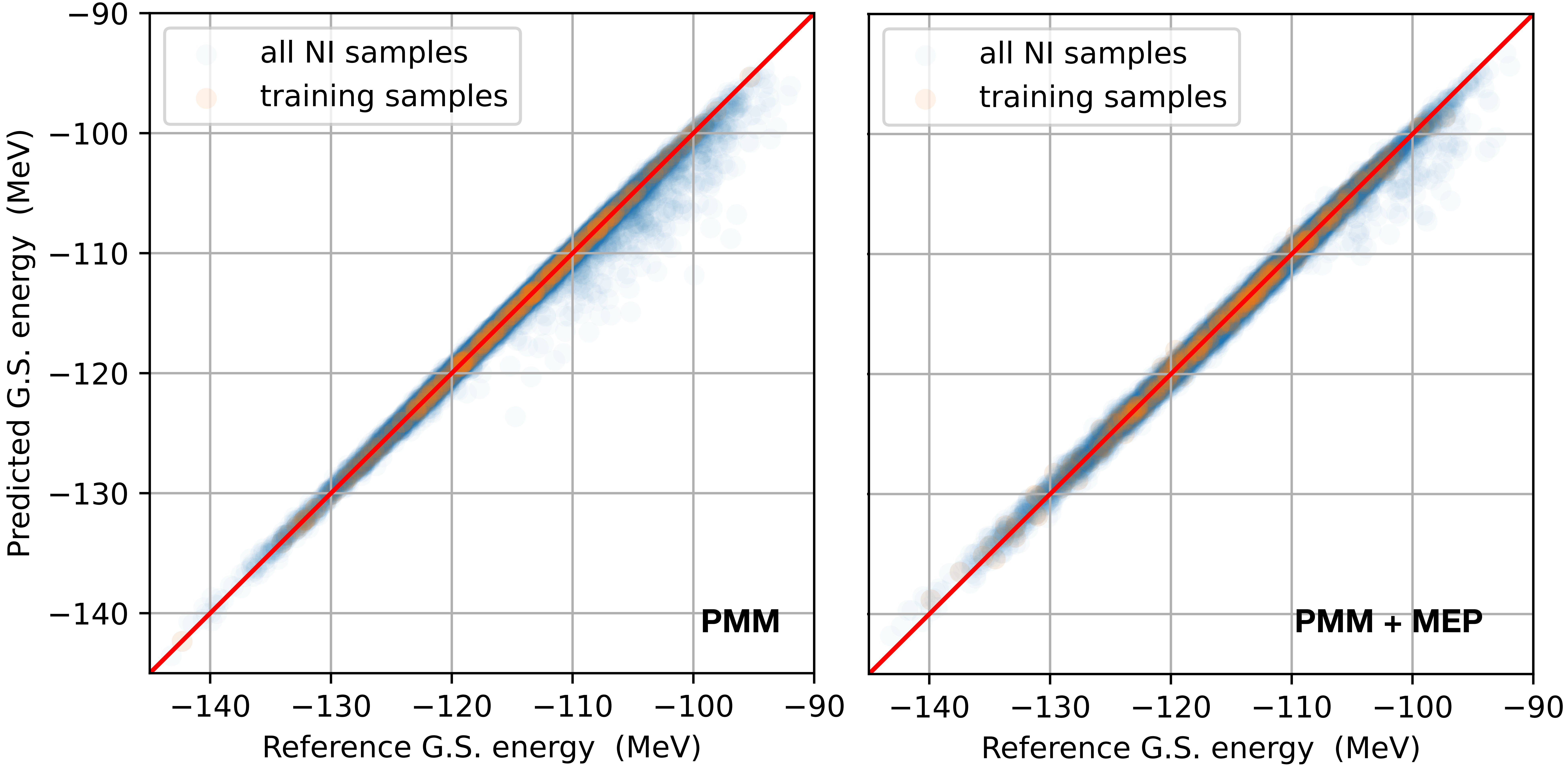
We just need to be lucky 1000 times!

Or Gradient Descent (Adam)

P. Cook et.al. arxiv: 2401.11694 [cs.LG]

$$(\mathscr{K}_i - \alpha_i \mathscr{K}_0)\mathbf{y} = (\mathscr{K}_{i0} + E^{[1]}\mathscr{K}_{i1} + E^{[2]}\mathscr{K}_{i2} + \ldots + E^{[n]}\mathscr{K}_{in} - \alpha_i \mathscr{K}_0)\mathbf{y} = 0$$

MEP PMM



8188 ~ 8218 samples of O16

data from W.G. Jiang et.al., PRC 109 064314 (2024)

Applications

MEP PMM **Application**

$n-p$ **Phase Shifts at Lab Energies 5 MeV and 50 MeV:**

$^1S_0, ^3S_1, ^1P_1, ^3P_0, ^3P_1, ^3P_2$

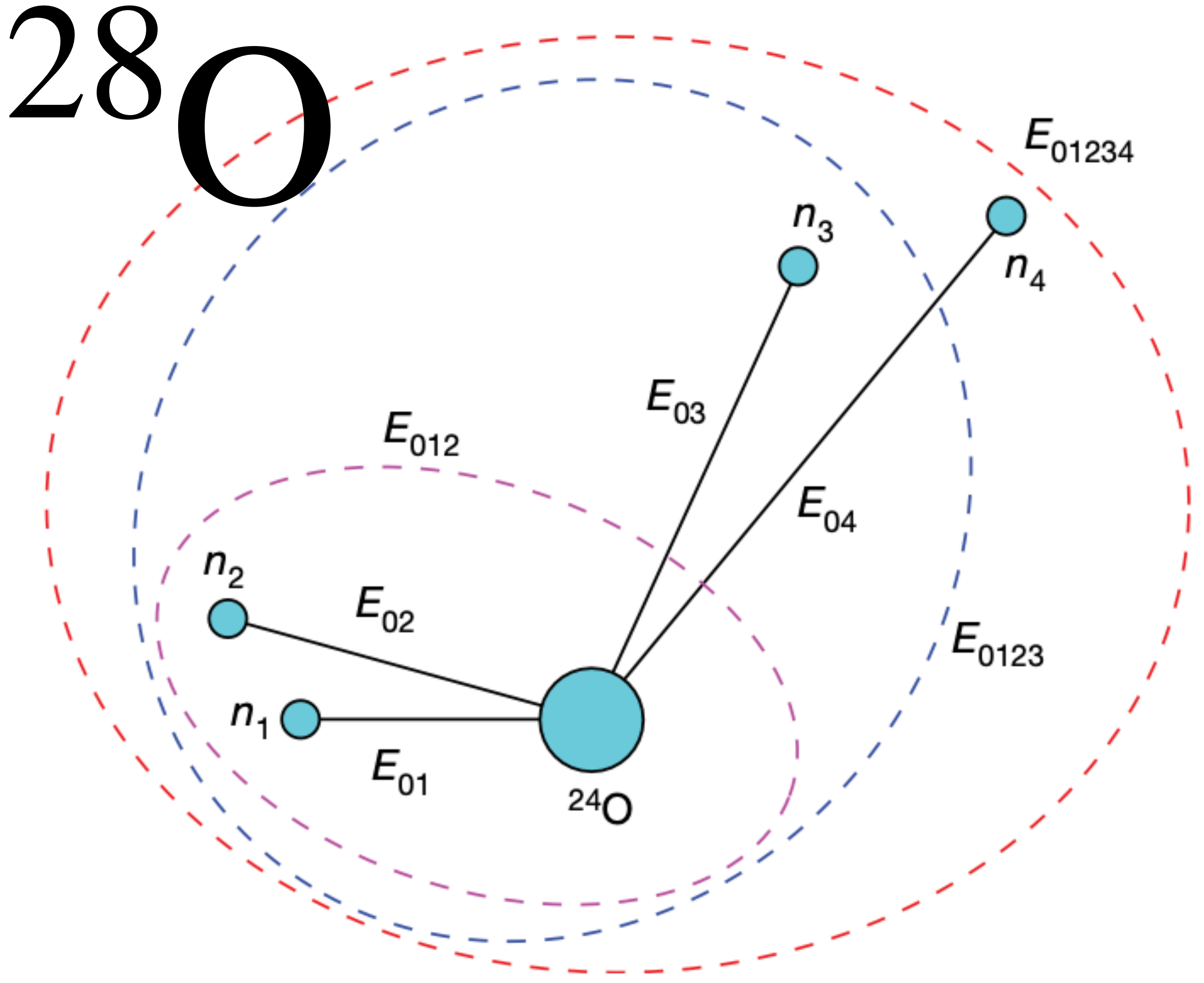
A = 2 ~ 24 Observables

G.S. Energies: $^2\mathrm{H}, ^3\mathrm{H}, ^4\mathrm{He}, ^6\mathrm{Li}, ^{16}\mathrm{O}, ^{24}\mathrm{O}$

W.G. Jiang et.al. PRC 109 (2024) 064314
Supplemental materials

MEP

$^{28}\mathrm{O}$

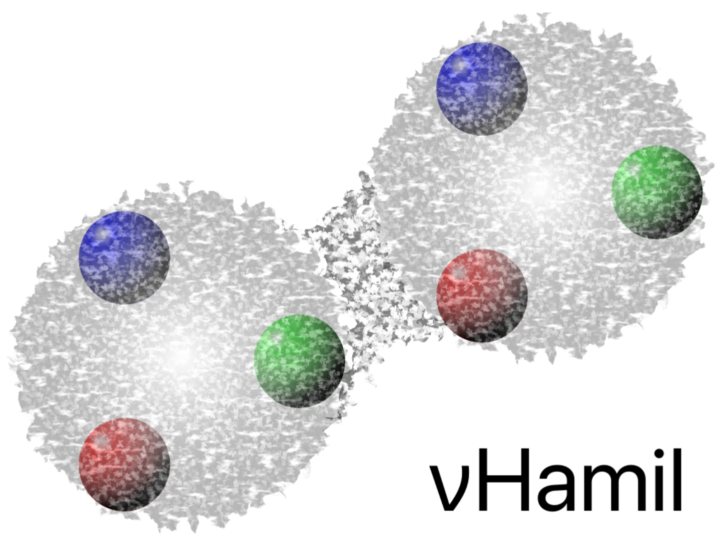


Y. Kondo et.al. *Nature* 620 (2023) 7976

$\Delta-\mathrm{full}\,\chi$- EFT at NNLO

W. G. Jiang, et.al. PRC 102, 054301 (2020)

17 LECs

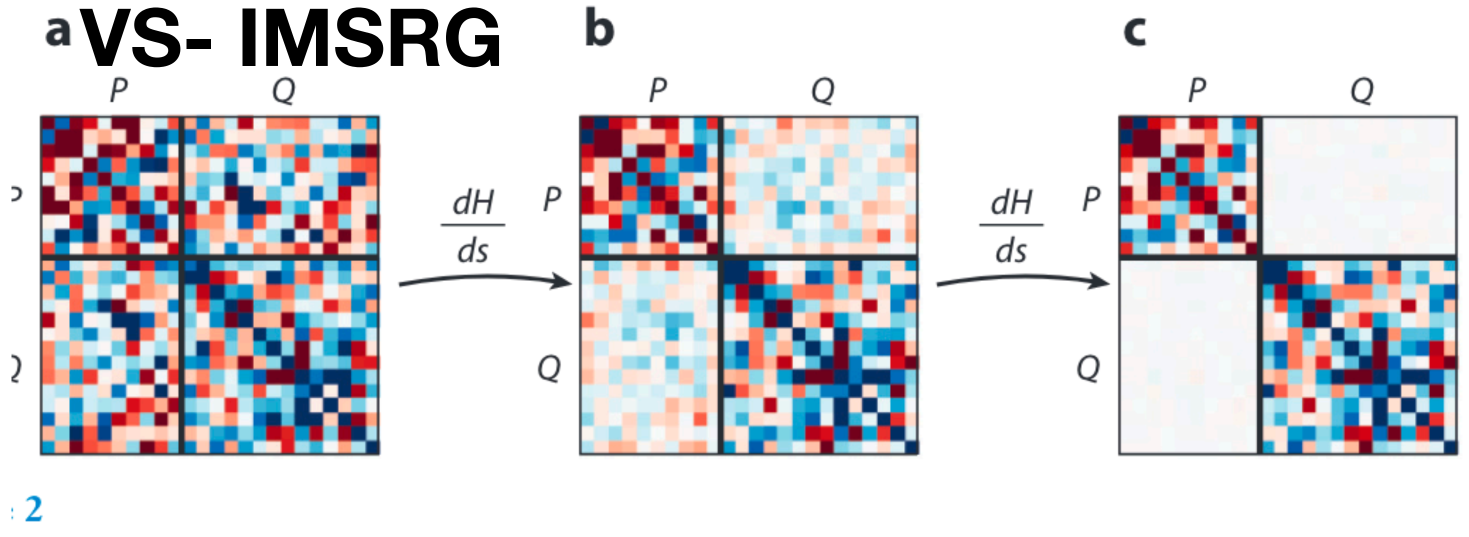


νHamil

T. Miyagi, EPJA 59, 150 (2023)

efficiently store three body potentials

VS- IMSRG



S. R. Stroberg et.al., Ann. Rev. Nucl. Part. Sci. 69, 307 (2019)

evolve effective interactions from χ-EFT

KSHELL

N. Shimizu et.al., Comp. Phys. Comm. 244, 372 (2019)

perform diagonalization

Training Samples

$E_{^{24}\mathrm{O}}$ $E_{^{27}\mathrm{O}}$ $E_{^{28}\mathrm{O}}$ at $\hbar\omega = 16\,\mathrm{MeV},\ \mathrm{e}_{\mathrm{max}} = 12,\ \mathrm{E}_{3\mathrm{max}} = 18$

300 G.S. Energies

~ 2000 Node * Hours on Pegasus Supercomputer @ CCS Tsukuba

~ 700 Node * Hours on Miyabi-G with MIG

MEP | PMM

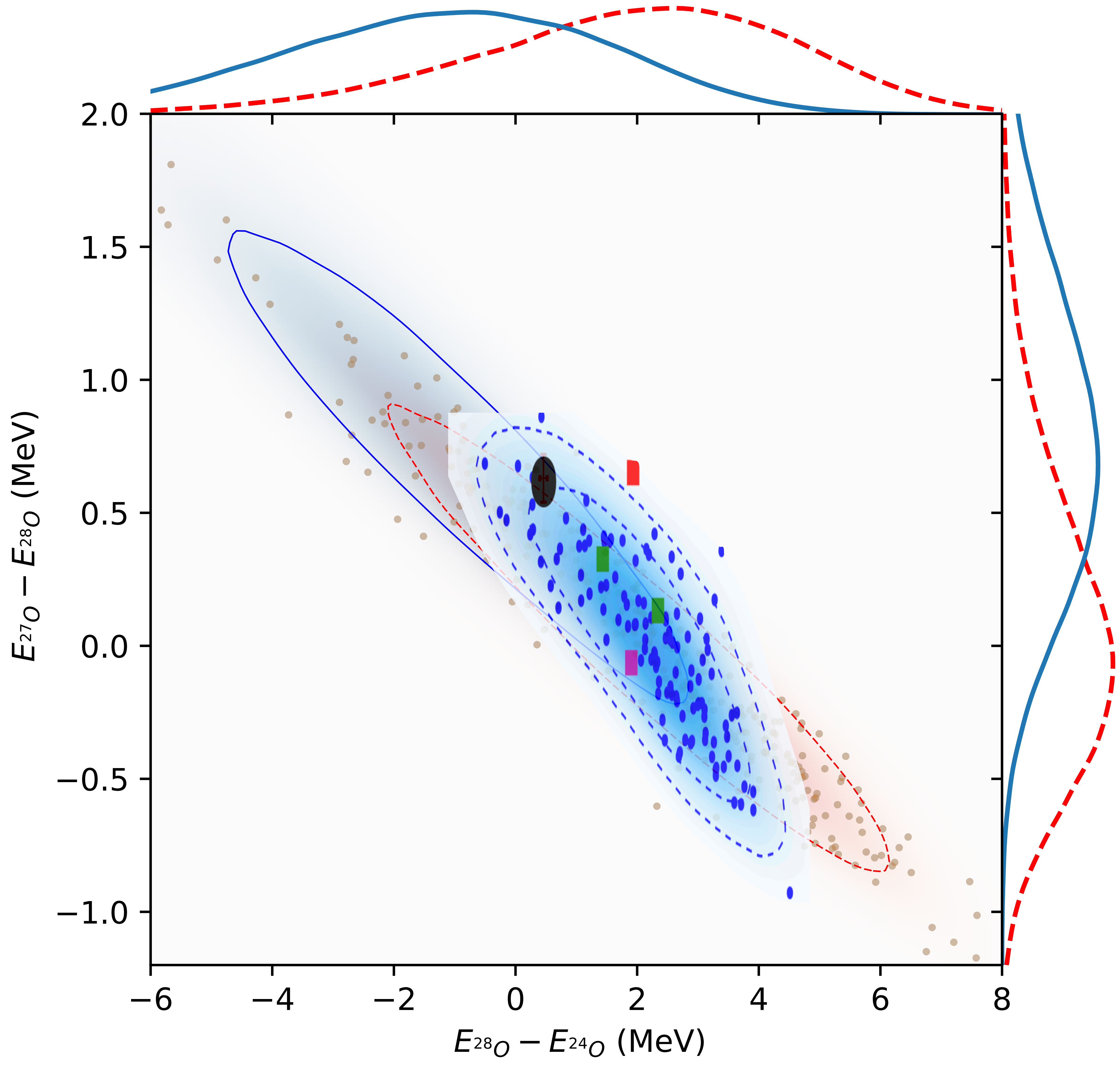
Application

A = 2 ~ 24 Observables

According to A = 2~4 NI measure

W.G. Jiang et.al. PRC 109 (2024) 064314

$P(O_1, O_2, \ldots) \sim$ **Multivariate Gaussian**



Y. Kondo et.al. *Nature* 620 (2023) 797

MEP | PMM

Application

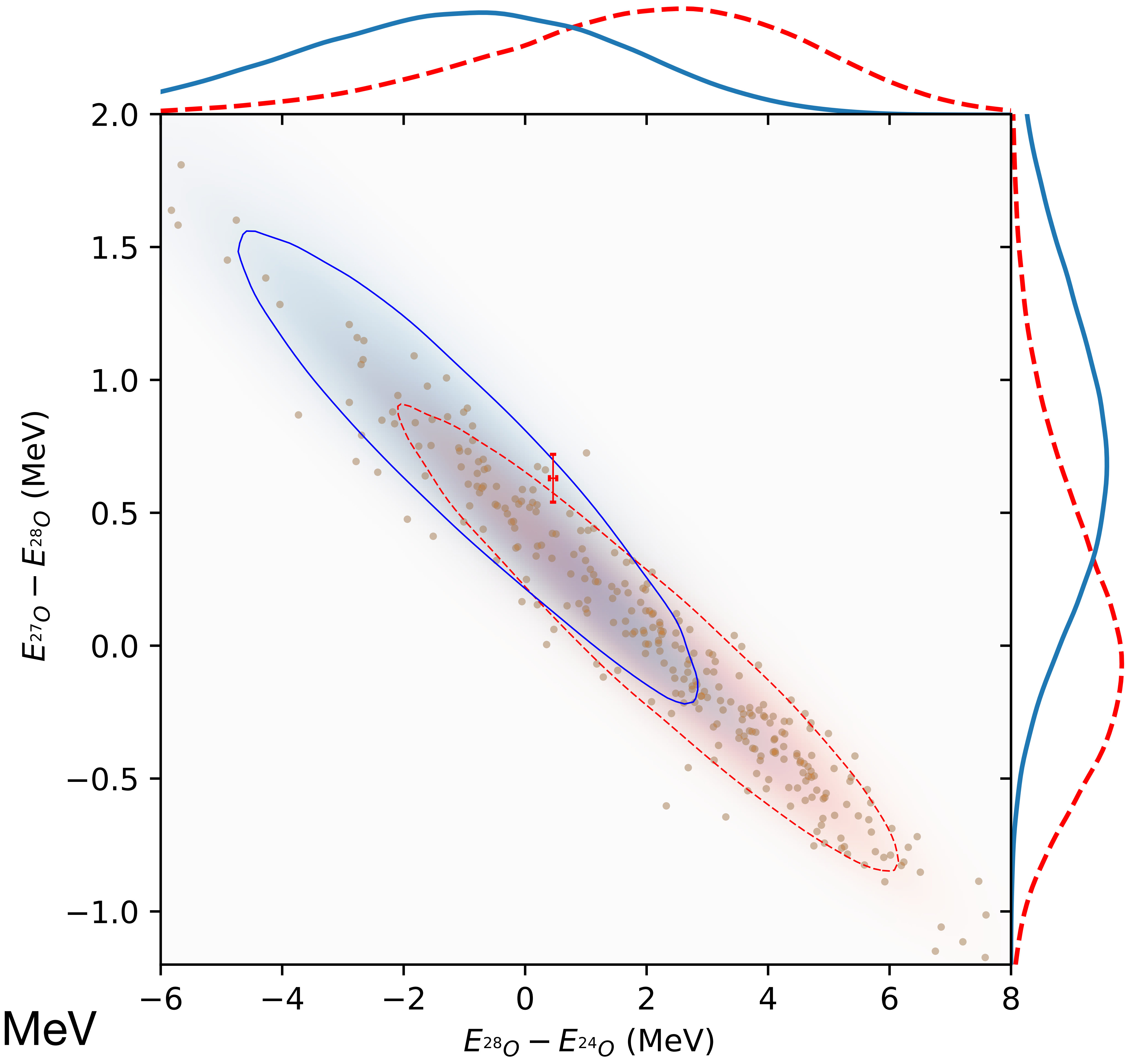
A = 2 ~ 24 Observables

According to A = 2~4 NI measure

Plus constraints of G.S. $^{16}\mathrm{O}, ^{24}\mathrm{O}$

$$E_{^{16}\mathrm{O}} = 127(2)\mathrm{MeV}$$

$$E_{^{24}\mathrm{O}} = 168(3)\mathrm{MeV}$$

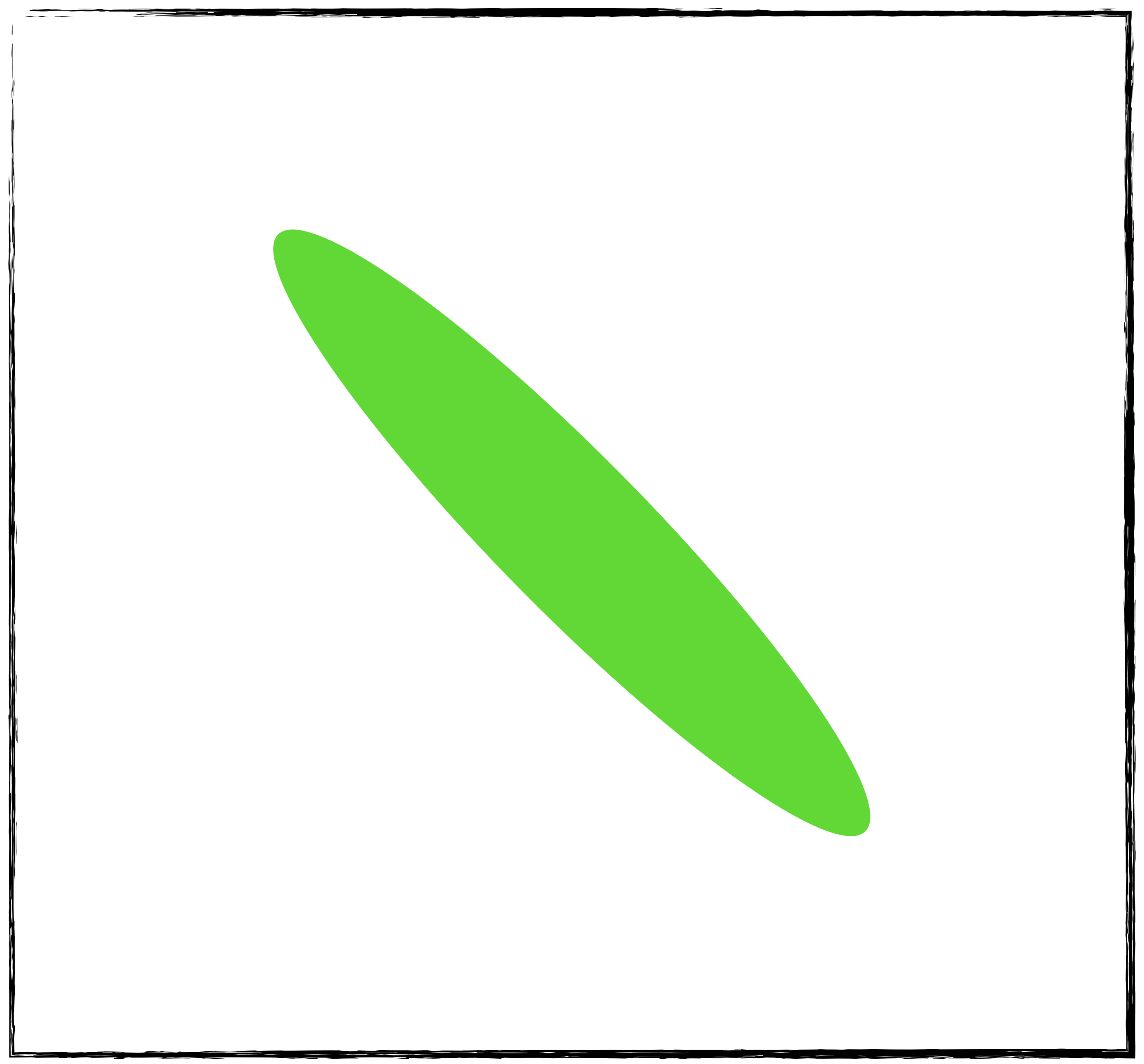


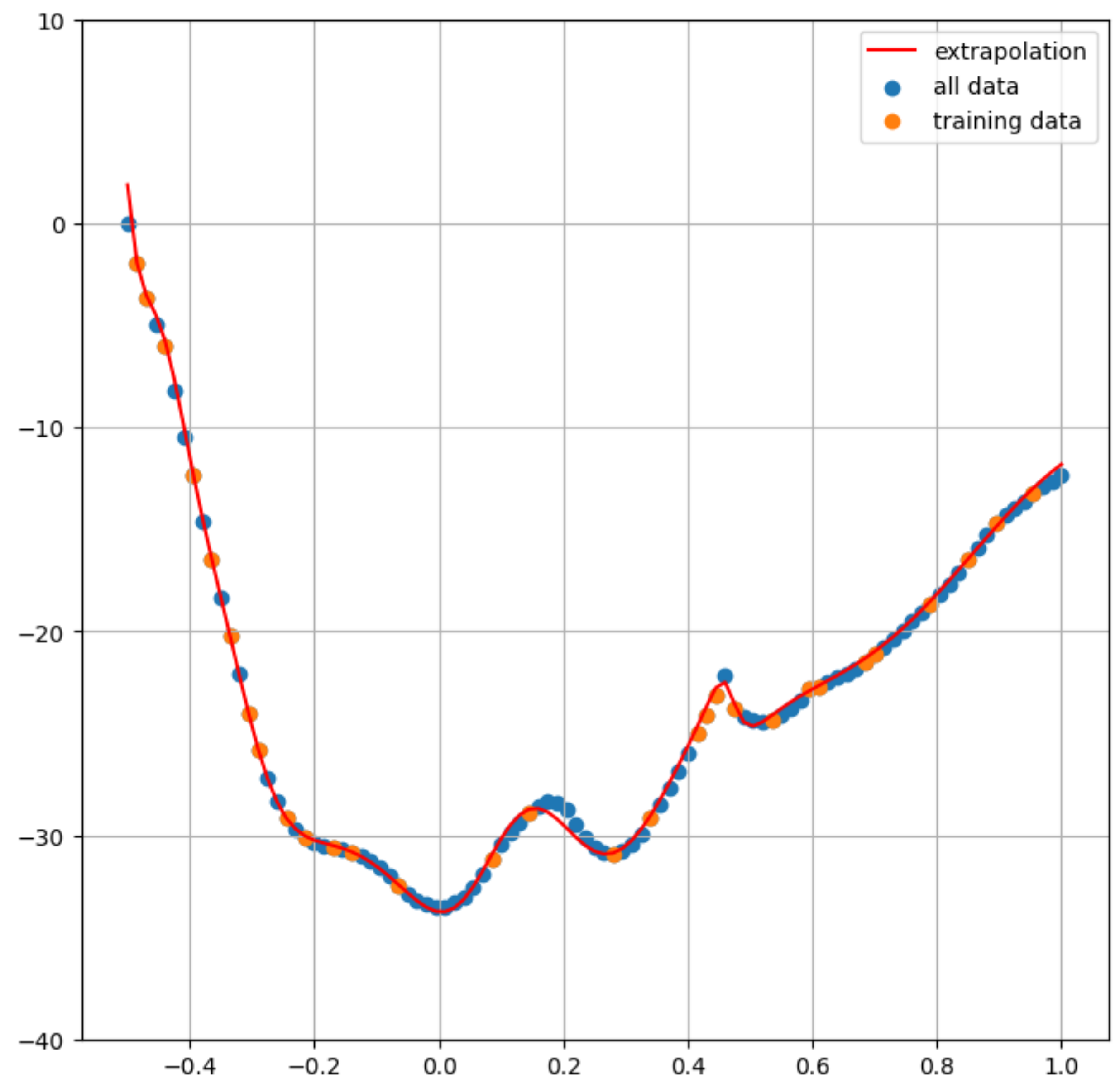
PMM error (100 bootstrapping x 10^5 samples): 0.2 MeV

Continuum: 0.5 ~ 1 MeV

G. Hagen, et al. Phys. Scripta 91 063006 (2016)

Outlook





Improving Emulator for Potential Energy Surface

Using Augmented Lagrangian Method
[Eur. Phys. J. A 46, 85–90 (2010)]

Summary

- We developed a connection emulator
- An efficient and deterministic substitution of statistical workflow
- Prob critical point in solution space
- A customizable hybrid surrogate model
- Currently: (phase shifts), eigenstates…

Next: General observables via PT/ALM

Thank You!