New results on eigenvector continuation and quantum mechanical bootstrap

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Outline

1. Analyticity and unitarity
   - Analytic properties of eigensolutions
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   - From analytic continuation to eigenvector continuation
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   - *R*-matrix EC and its applications in nuclear reactions
3. Quantum mechanical bootstrap
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   - Quantum anharmonic oscillators
   - Bootstrapping the deuteron
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Analyticity and unitarity

Analyticity and **unitarity** are fundamentally important in quantum physics.

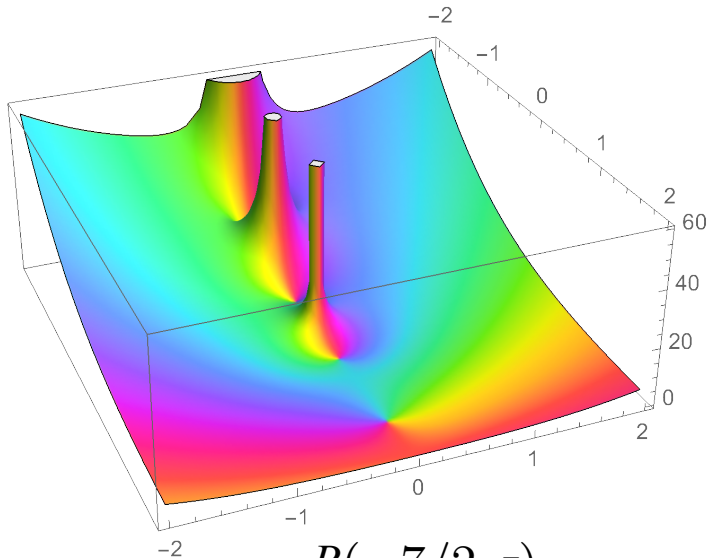
Loosely speaking, **analyticity** says that physical quantities (e.g., wave functions and scattering amplitudes) are generally smooth functions even when some variables go from the real axis to the complex plane. Occasionally, there are singularities and branch cuts. But their properties should be understandable.

- Beta function:

$$B(x,y) = \int_0^1 \mathrm{d}t\, t^{x-1}(1-t)^{y-1}$$

  $\rightarrow$ Veneziano amplitude ✔

- Dirichlet function: nowhere continuous ✖



$B(-7/2,z)$

Loosely speaking, **unitarity** says that quantum mechanical systems should evolve in such a way that the probability is conserved and the evolution is reversible.

***S*-matrix:**

$$
\begin{aligned}
S\,|\text{in}\rangle = |\text{out}\rangle &\xrightarrow{\text{measure}} |\text{out}_1\rangle \\
&\xrightarrow{\text{measure}} |\text{out}_2\rangle \\
&\xrightarrow{\text{measure}} |\text{out}_3\rangle \\
&\cdots
\end{aligned}
$$

with $SS^\dagger = S^\dagger S = 1$.

- Black hole information paradox:

  $|\Psi\rangle$ (pure state) $\rightarrow$ BH $\rightarrow$ Hawking radiation (mixed state)

  Unitarity seems to be violated $\rightarrow$ puzzle for decades

Analytic properties of eigensolutions

Consider the Schrödinger equation with a short-range potential $U(r)$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - c\,U(r) + p^2\right]\phi_{p,l,c}(r) = 0.$$

- **Regular eigensolution:**

$$\phi_{p,l,c}(r) \to \widehat{j}_l(pr), \qquad r \to 0,$$

$$\Rightarrow \phi_{p,l,c}(r) \to \frac{i}{2}\left[\mathscr{S}_{l,c}(p)H_l^{(-)}(pr) - \mathscr{S}_{l,c}(p)^* H_l^{(+)}(pr)\right], \qquad r \to \infty,$$

where $\mathscr{S}_{l,c}(p)$ is the Jost function, $\widehat{j}_l(z) \equiv z j_l(z)$ is the Riccati-Bessel function, and $H_l^{(\mp)}(pr)$ are the incoming and outgoing Hankel functions.

- **Normalized eigensolution:**

$$\psi_{p,l,c}(r) \equiv \phi_{p,l,c}(r)/\mathscr{S}_{l,c}(p),$$

$$\Rightarrow \psi_{p,l,c}(r) \to \frac{i}{2}\left[H_l^{(-)}(pr) - S_{l,c}(p)H_l^{(+)}(pr)\right], \qquad r \to \infty,$$

where $S_{l,c}(p) \equiv \mathscr{S}_{l,c}(p)^*/\mathscr{S}_{l,c}(p)$ is the S-matrix element.

Regular eigensolution:

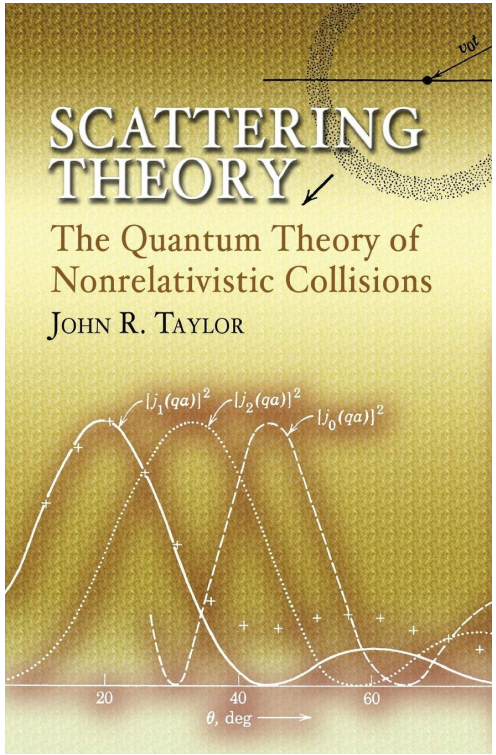
1. $\phi_{p,l,c}(r)$ is an entire function of the coupling constant $c \in \mathbb{C}$.
2. $\phi_{p,l,c}(r)$ is an entire function of the momentum $p \in \mathbb{C}$.
3. $\phi_{p,l,c}(r)$ is analytic in the angular momentum l for $\mathrm{Re}(l) > -1/2$.

Normalized eigensolution:

$$\psi_{p,l,c}(r) \equiv \phi_{p,l,c}(r)/\mathscr{S}_{l,c}(p).$$

convolute the analytic properties of the regular eigensolution $\phi_{p,l,c}(r)$ with the Jost function $\mathscr{S}_{l,c}(p)$.

- $\mathscr{S}_{l,c}(p)$ is an entire function of the coupling constant $c \in \mathbb{C}$.



Positivity constraint

Positivity constraint: non-negativity of norm

$$\langle\Psi|\Psi\rangle \geq 0 \Rightarrow \text{Probability should never be negative.}$$

Question: For quantum harmonic oscillators, the annihilation and creation operators satisfy $[a, a^\dagger] = 1$. Is there a state $|\Psi\rangle \neq 0$ satisfying $a^\dagger |\Psi\rangle = 0$?

Answer: No!

$$0 = \langle\Psi|aa^\dagger|\Psi\rangle = \langle\Psi|\Psi\rangle + \langle\Psi|a^\dagger a|\Psi\rangle$$

$$\Rightarrow \langle\Psi|a^\dagger a|\Psi\rangle = -\langle\Psi|\Psi\rangle$$

$\Rightarrow$ violate positivity constraint $\square$

Also, for electromagnetic fields, a naive Lorentz covariant quantization gives

$$[a^0_{\boldsymbol{p}}, a^{0\dagger}_{\boldsymbol{q}}] = -(2\pi)^3\delta^{(3)}(\boldsymbol{p}-\boldsymbol{q})$$

$$\Rightarrow \langle \boldsymbol{p}, 0|\boldsymbol{q}, 0\rangle = \langle 0|a^0_{\boldsymbol{p}} a^{0\dagger}_{\boldsymbol{q}}|0\rangle = -(2\pi)^3\delta^{(3)}(\boldsymbol{p}-\boldsymbol{q}) < 0$$

$\Rightarrow$"violation" of unitarity $\Rightarrow$ gauge fixing $\Rightarrow$ Gupta-Bleuler formalism

Eigenvector continuation: motivations

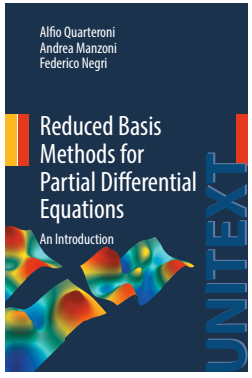
Eigenvector continuation (EC) is proposed by D. Frame *et al.*, Phys. Rev. Lett. **121**, 032501 (2018).

Similar ideas:

H. Rabitz and R. Conn, Phys. Rev. A **7**, 577 (1973).

E. R. Davidson, Comput. Phys. Commun. **53**, 49 (1989).

A. Quarteroni, A. Manzoni, and F. Negri, *Reduced Basis Methods for Partial Differential Equations* (2016).

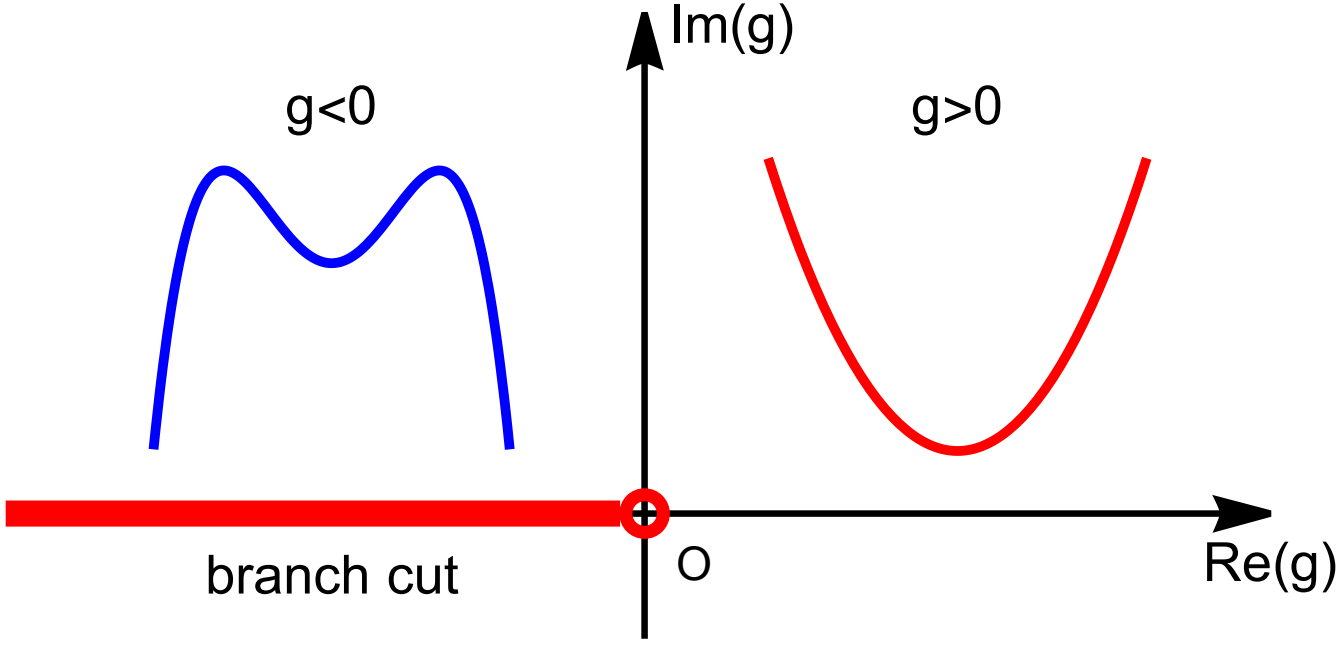


- What can EC do?
  1. resum the perturbation series when it diverges;
  2. speed up variational calculations that have to be repeated for a large number of times.
- Killer apps:
  1. resummation of perturbative expansions
  2. sensitivity analysis
  3. uncertainty quantification (especially based on Bayesian analysis)

Resummation of perturbative expansions

Perturbation expansions in quantum mechanics often diverge.

- Quantum anharmonic oscillator $H = p^2/2 + x^2/2 + gx^4$



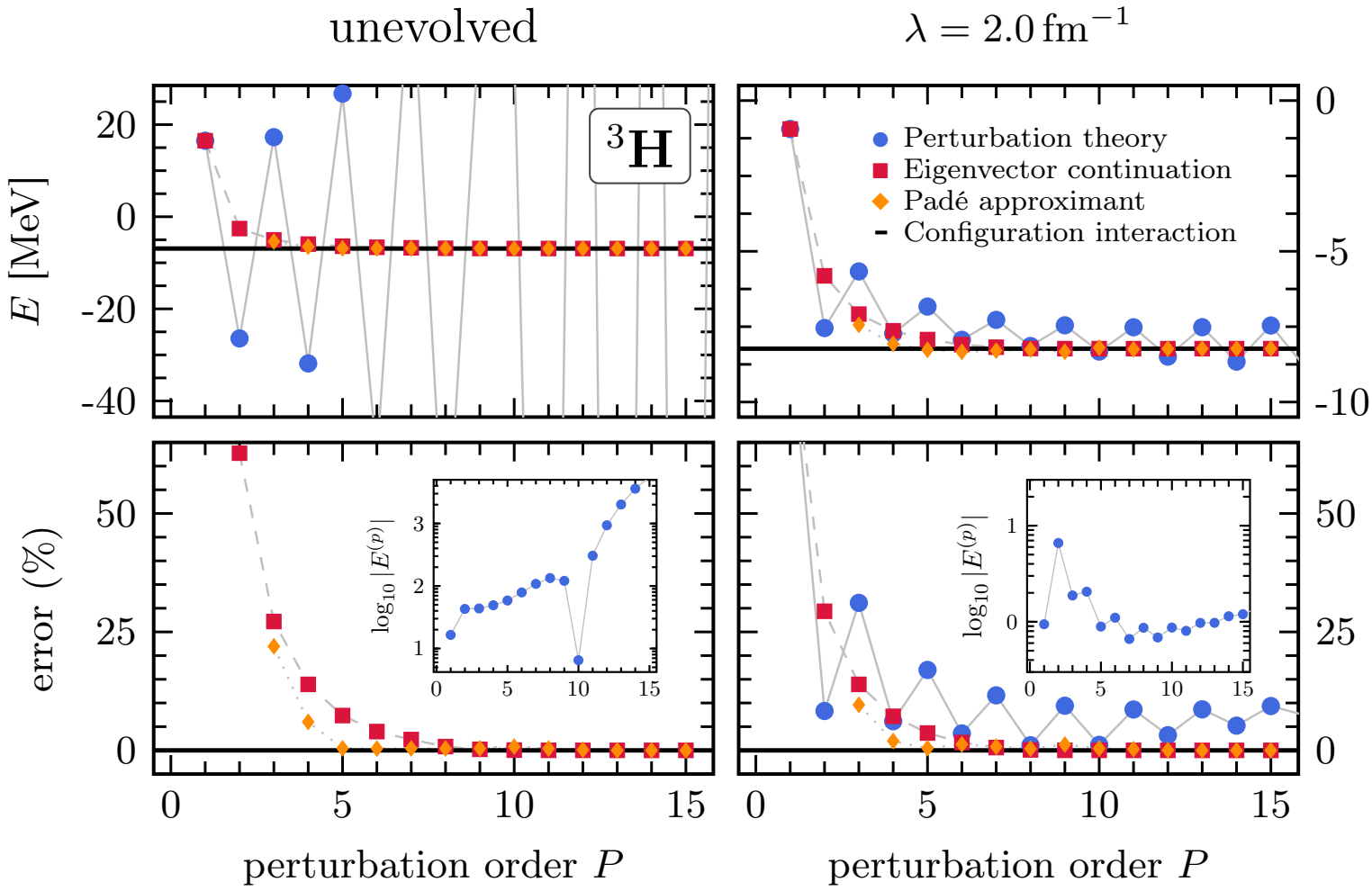
Perturbative expansion around $g = 0$ does not converge for any g.

C. M. Bender and T. T. Wu, Phys. Rev. D **7**, 1620 (1973).

EC can do the resummation.

M. C. Franzke *et al.*, arXiv:2108.02824.

- Many-body perturbation theory (^{3}H from EM500 with/without SRG evolution)



P. Demol *et al.*, Phys. Rev. C **101**, 041302(R) (2020).

Sensitivity analysis

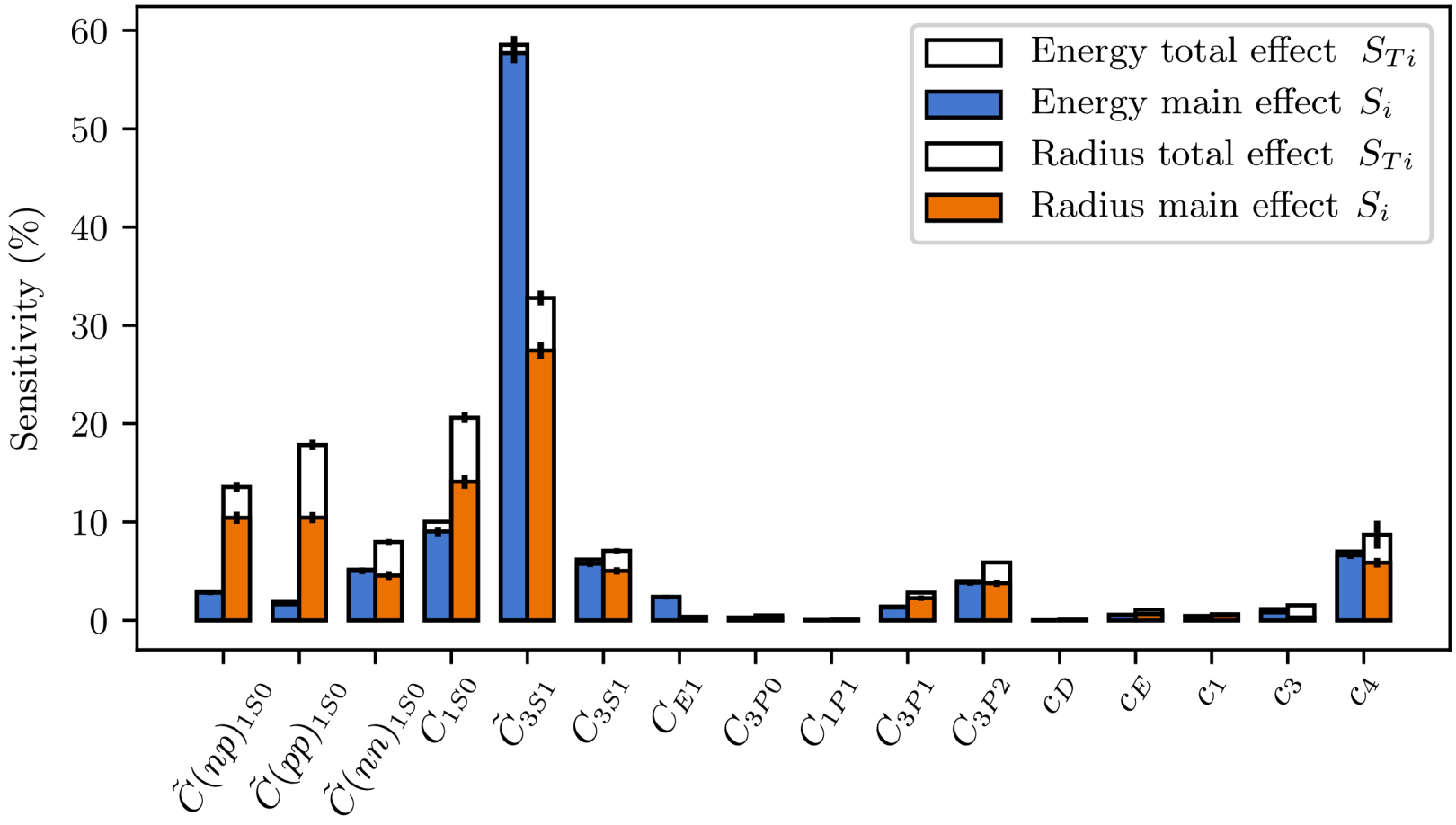
Wikipedia: "**Sensitivity analysis** *is the study of how the uncertainty in the output of a mathematical model or system (numerical or otherwise) can be divided and allocated to* **different sources of uncertainty in its inputs**. *A related practice is* **uncertainty analysis**, *which has a greater focus on* **uncertainty quantification** *and* **propagation of uncertainty.**"

- chiral potentials:
  #LEC: 2+@LO, 9+@NLO/N^{2}LO, 26+@N^{3}LO, $\cdots$
- nuclear reaction models: $\sim$ 10 parameters in the optical potential

Difficulties:

A huge number of samples are needed,
but running time $\propto$ the number of samples.

With standard methods, 10^6 CCSD calculations for ^{16}O take **20 years**.
With **EC**, they can be done in **1h** on a standard laptop!



A. Ekström and G. Hagen, Phys. Rev. Lett. **123**, 252501 (2019).

Uncertainty quantification

quantifying the reliability of outcomes from a model

$\Leftarrow$ experimental, model, method, numerical, $\cdots$

Bayes' theorem

$$P(H|D) = \frac{P(D|H)P(H)}{P(D)} \Rightarrow \text{Bayesian statistics}$$

- $P(H|D)$ posterior, $P(H)$ prior, $P(D|H)$ likelihood

Likelihood

$$P(D|H) \propto \exp(-\chi^2/2) \Rightarrow \text{labouring}$$

S. König *et al.*, Phys. Lett. B **810**, 135814 (2020)

S. Yoshida and N. Shimizu, arXiv:2105.08256

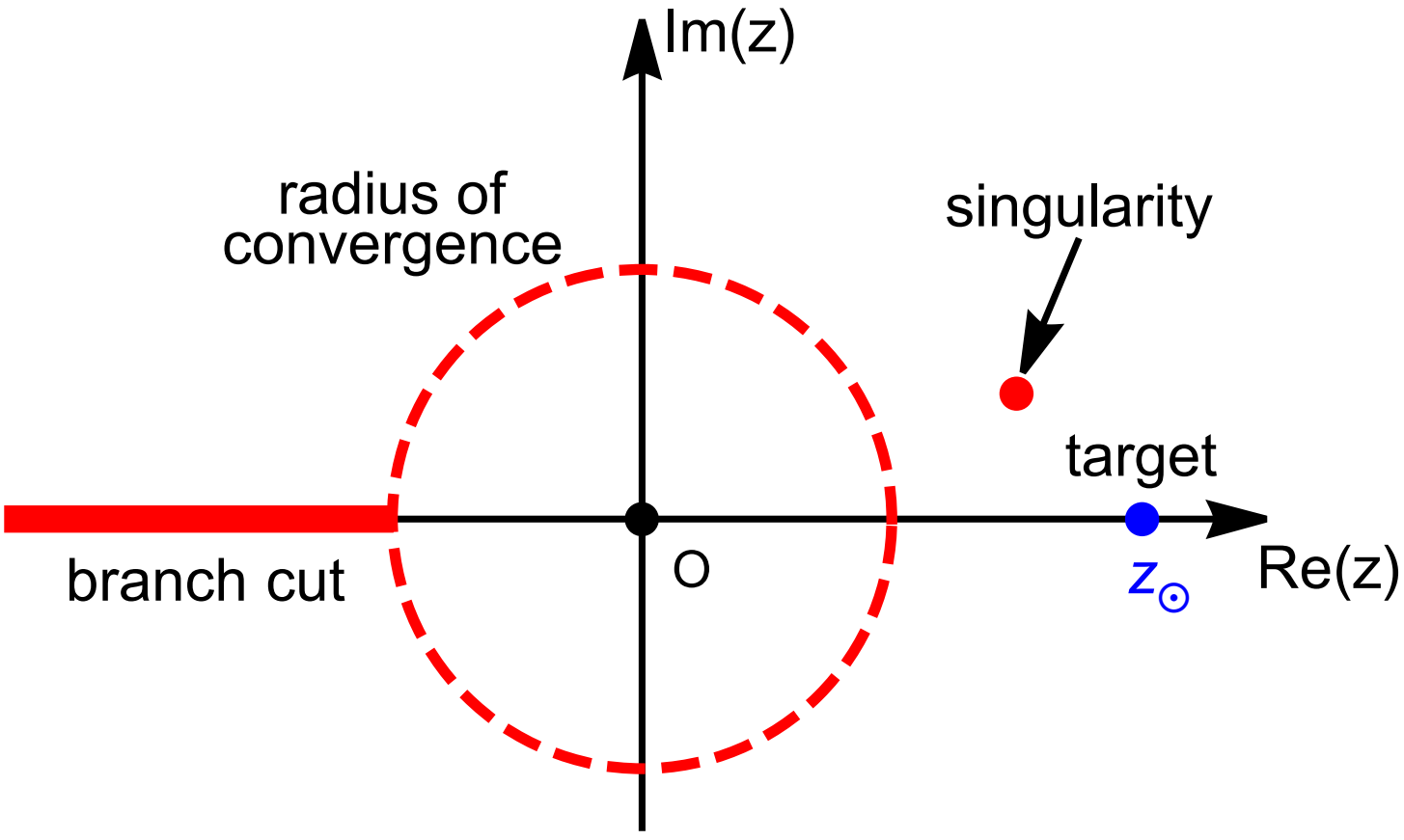
S. Wesolowski *et al.*, Phys. Rev. C **104**, 064001 (2021)

T. Djärv *et al.*, arXiv:2108.13313

B. Hu *et al.*, arXiv:2112.01125

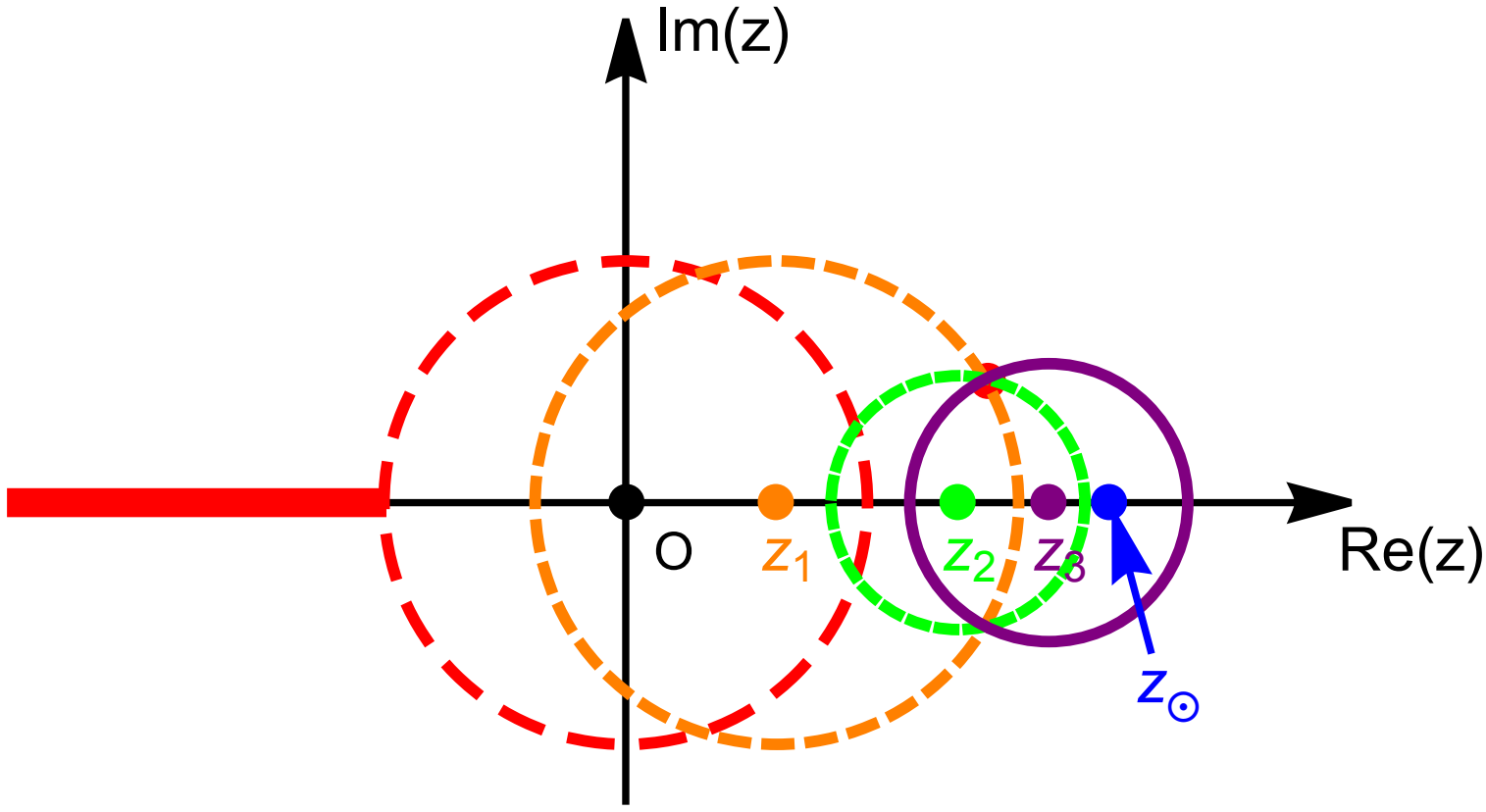
From analytic continuation to eigenvector continuation

Consider the eigensolution $\Psi(z)$ well-defined at $z \geq 0$, where z can be the momentum p, the angular momentum l, or the coupling constant c.



The target point $z_\odot$ is outside the radius of convergence at $z = 0$.

Analytic continuation



With the reference points z_1, z_2, and z_3, the target point $z_\odot$ is related to perturbative expansions around $z = 0$.

Perturbation theory

$$\Psi(z_1) = \sum_{i_1=0}^{\infty} \Psi^{(i_1)}(0)\, z_1^{i_1}/i_1!,$$

$$\Psi(z_2) = \sum_{i_2=0}^{\infty} \Psi^{(i_2)}(z_1)(z_2 - z_1)^{i_2}/i_2!,$$

$$\Psi(z_3) = \sum_{i_3=0}^{\infty} \Psi^{(i_3)}(z_2)(z_3 - z_2)^{i_3}/i_3!,$$

$$\Psi(z_\odot) = \sum_{i_4=0}^{\infty} \Psi^{(i_4)}(z_3)(z_\odot - z_3)^{i_4}/i_4!.$$

$$\Rightarrow \Psi(z_\odot) = \sum_{i_1=0}^{\infty}\sum_{i_2=0}^{\infty}\sum_{i_3=0}^{\infty}\sum_{i_4=0}^{\infty} \Psi^{(i_1+i_2+i_3+i_4)}(0)(z_\odot - z_3)^{i_4}(z_3 - z_2)^{i_3} \times (z_2 - z_1)^{i_2} z_1^{i_1}/(i_4! i_3! i_2! i_1!).$$

$$\boldsymbol{\Psi(z_\odot) = \#_0 \Psi^{(0)}(0) + \#_1 \Psi^{(1)}(0) + \#_2 \Psi^{(2)}(0) + \cdots.}$$

Finite difference representation

$$\Psi^{(1)}(0) \sim [\Psi(z) - \Psi(0)]/z,$$
$$\Psi^{(2)}(0) \sim [\Psi(2z) - 2\Psi(z) + \Psi(0)]/z^2, \cdots$$

$$\boldsymbol{\Psi(z_\odot) = \#_0 \Psi(\omega_0) + \#_1 \Psi(\omega_1) + \#_2 \Psi(\omega_2) + \cdots.}$$

Question:

How to determine the values of $\#_0, \#_1, \#_2, \cdots$?

Answer: In EC, via the variational principle for structural problems.

With $\{\Psi^{(i)}(0)\}$ or $\{\Psi(\omega_i)\}$ as the variational basis functions $\{v_i\}$, solve

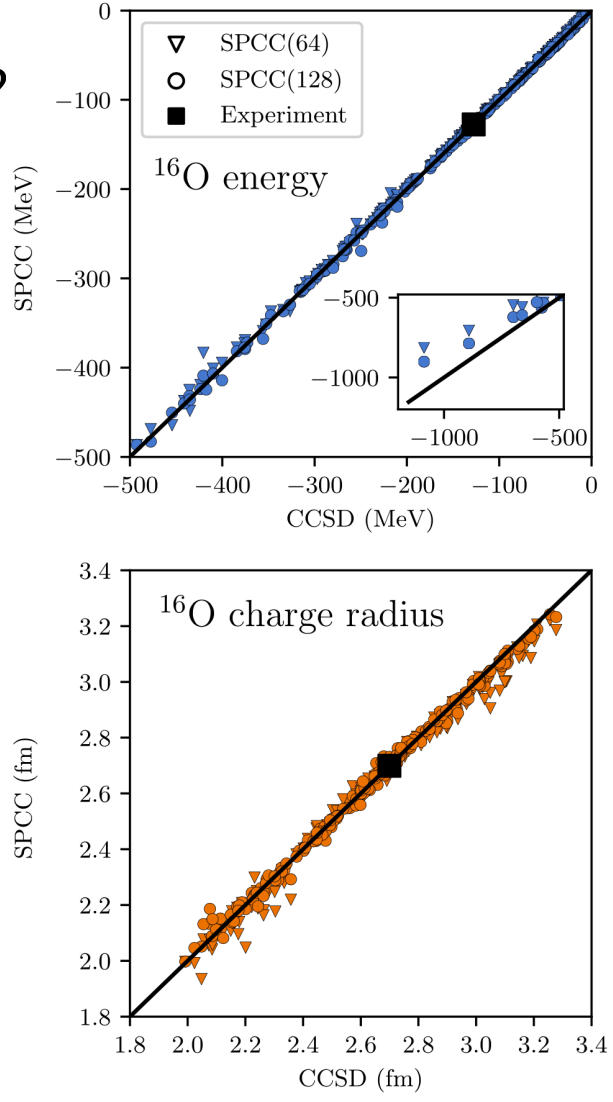
$$\mathcal{H}(z_\odot)\vec{v} = E\mathcal{N}\vec{v}, \quad \text{广义本征值问题}$$

with $[\mathcal{H}(z_\odot)]_{ij} = \langle v_i|H(z_\odot)|v_j\rangle$ and $[\mathcal{N}]_{ij} = \langle v_i|v_j\rangle$.

Example: sensitivity analysis

Still remember Ekström and Hagen (2019)?

- The technical details of CCSD are a bit complicated. Let's focus on the EC part.
- **Training points:** $N_{\mathrm{EC}} = 64$ and 128 points in a domain surrounds the nominal LEC values of $\mathrm{NNLO_{sat}}$ within 20% relative variation, $\cdots$.
- **Emulator:** trading the accuracy of an exact calculation for a significant speed-up.



Ekström and Hagen (2019)

Mathematical properties of EC:

- Convergence properties of EC

  A. Sarkar and D. Lee, Phys. Rev. Lett. **126**, 032501 (2021).

- **Eigenenergy errors of EC**

  D. Bai and Z. Ren (2021)

  See also A. Sarkar and D. Lee, 2107.13449.

Definition: for the pth eigenstate

$$\Delta E^{(p)}_{\mathrm{EC}}(\boldsymbol{c}_{\odot}) \equiv E^{(p)}_{\mathrm{EC}}(\boldsymbol{c}_{\odot}) - E^{(p)}_{\mathrm{exact}}(\boldsymbol{c}_{\odot}).$$

Direct method: exact calculations are needed for test sets besides training sets $\rightarrow$ additional computational time

Indirect method: emulator for eigenenergy errors of EC $\leftarrow$ mathematical properties of eigenenergy errors of EC

Rigorous upper bounds for variational eigenenergy errors:

- Weinstein's upper bound (1932)

$$\Delta E_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot) \leq \sigma_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot),$$

with $E_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot) \leq \frac{1}{2}[E^{(p)}(\boldsymbol{c}_\odot) + E^{(p+1)}(\boldsymbol{c}_\odot)]$ and

Hamiltonian variance

$$\sigma_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot)^2 = \langle \phi_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot) | \, H(\boldsymbol{c}_\odot)^2 \, | \phi_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot) \rangle - E_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot)^2.$$

- Temple's upper bound (1928)

$$\Delta E_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot) \leq \frac{\sigma_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot)^2}{\beta - E_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot)},$$

with $E_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_\odot) < \beta \leq E^{(p+1)}(\boldsymbol{c}_\odot)$.

M. A. Abdel-Raouf, Phys. Rept. **84**, 163 (1982) (citations: 42)

Rediscovered for several times in history and generally less-known!? E.g., C. Gros, *Criterion for a good variational wave function*, Phys. Rev. B **42**, 6835(R) (1990).

S. Goedecker and K. Maschke, *Comment on "· · ·"*, PRB (1991):

"Exact relations of this kind which give bounds on the error in energy as a function of the variance have been known for a long time. Such a criterion was proposed by Weinstein in 1934. Even though those criteria are very useful, they cannot be found in most textbooks on quantum mechanics, one exception being the textbook by Pauling and Wilson (1935)."

Applications in nuclear physics in the 1960s:

E. W. Schmid, Y. C. Tang, and R. C. Herndon, Nucl. Phys. **42**, 95 (1963).
Y. C. Tang, R. C. Herndon, and E. W. Schmid, Phys. Rev. 134, B743 (1964).
Y. C. Tang, E. W. Schmid, R. C. Herndon, Nucl. Phys. **65**, 203 (1965).
Y. C. Tang and R. C. Herndon, Nucl. Phys. A **93**, 692 (1967).

In general, **Temple's bound** is more stringent.

Approximate factorization of eigenenergy error in EC

$$\Delta E_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_{\odot}) \approx A(\boldsymbol{c}_{\odot}) \times \sigma_{\mathrm{EC}}^{(p)}(\boldsymbol{c}_{\odot})^2.$$

The prefactor $A(\boldsymbol{c}_{\odot})$ is mainly determined by the target values of the control parameters $\boldsymbol{c}_{\odot}$ and less sensitive to either training points or target low-lying eigenstates.

Three testing problems:

(1) one-parameter Hamiltonian

$$H(c_{\odot}) = H_0 + c_{\odot} H_1.$$

Here, H_0 and H_1 are two 100×100 Hermitian matrices, with random matrix elements $[H_0]_{ij}$ and $[H_1]_{ij}$ from $[-1, 1]$.

(2) two-parameter Hamiltonian

$$H(c_\odot, d_\odot) = H_0 + c_\odot H_1 + d_\odot H_2.$$

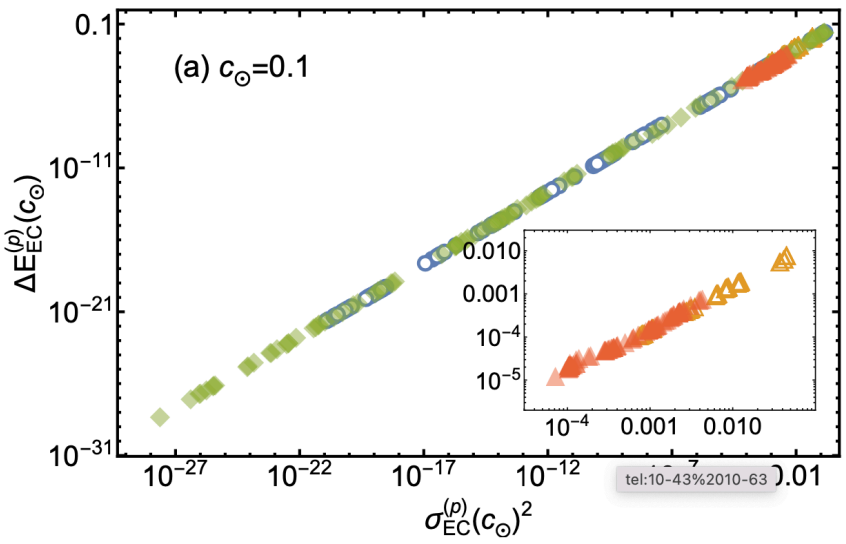
Here, H_0, H_1, H_2 are three 100×100 random Hermitian matrices with random matrix elements $[H_0]_{ij}$, $[H_1]_{ij}$, and $[H_2]_{ij}$ from $[-1, 1]$.

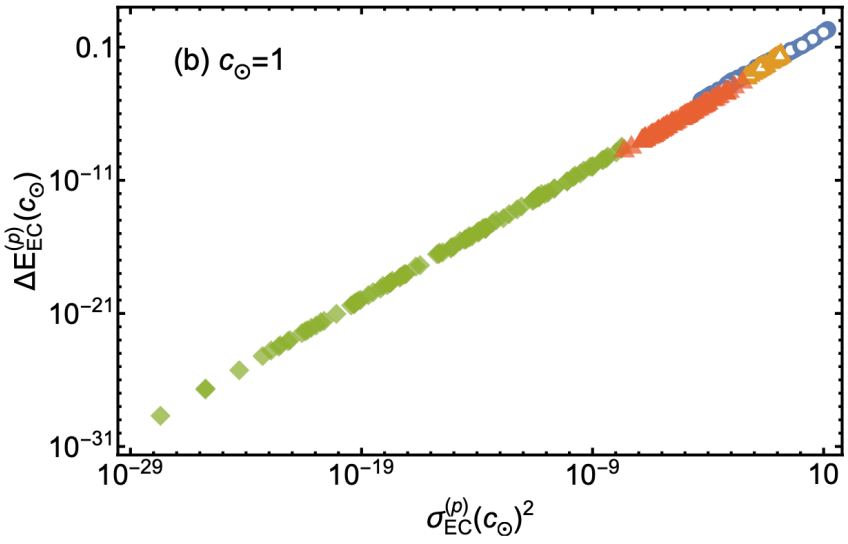
(3) deuteron

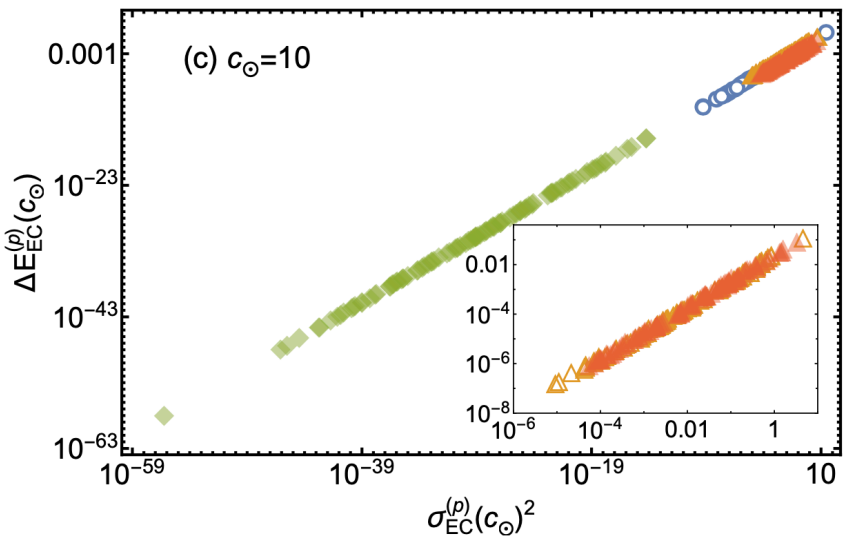
$$H(c_\odot, d_\odot, e_\odot) = H_0 + c_\odot H_1 + d_\odot H_2 + e_\odot H_3,$$

with $(c_\odot, d_\odot, e_\odot) = (\widetilde{C}_{^3S_1}, C_{^3S_1}, C_{^3S_1\text{-}^3D_1})$ for the deuteron Hamiltonian at $\mathrm{N^2LO}$.

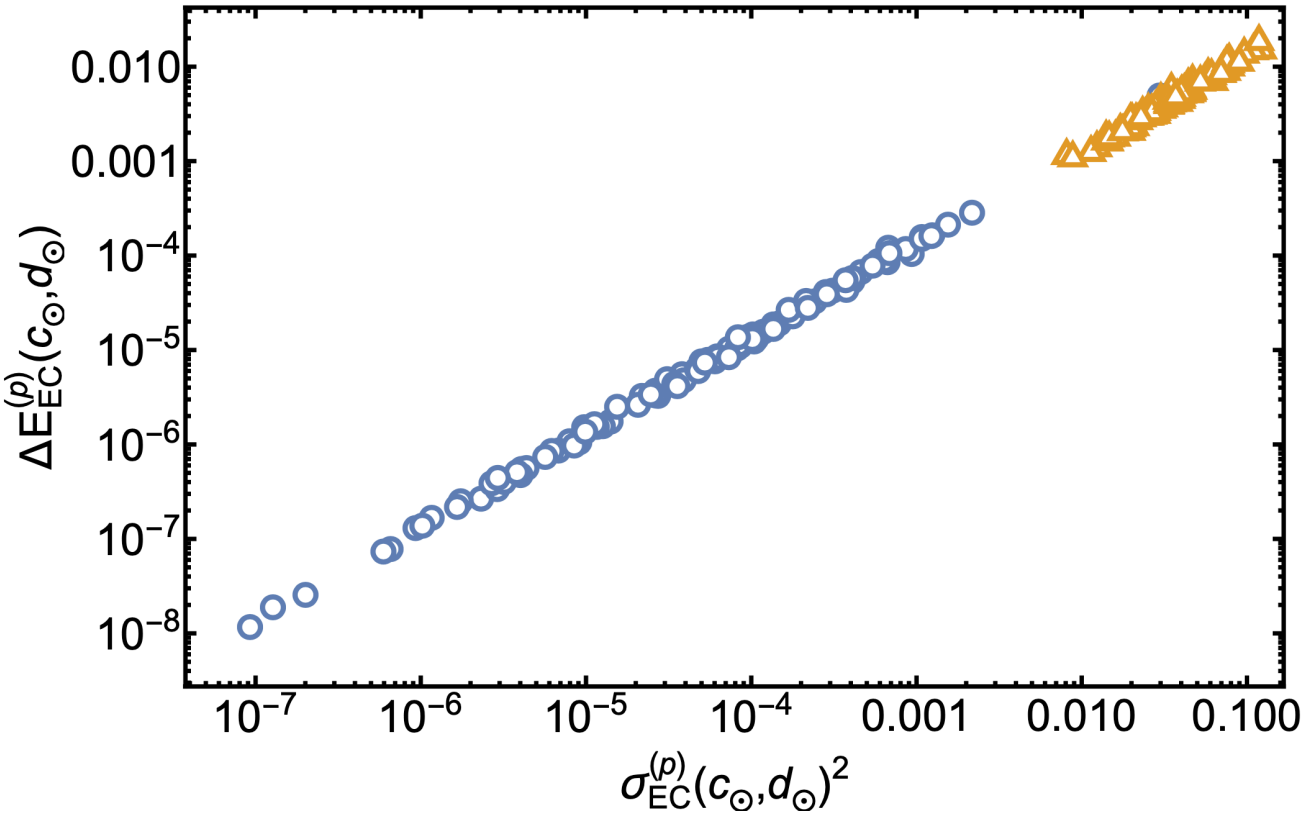
One-parameter Hamiltonian



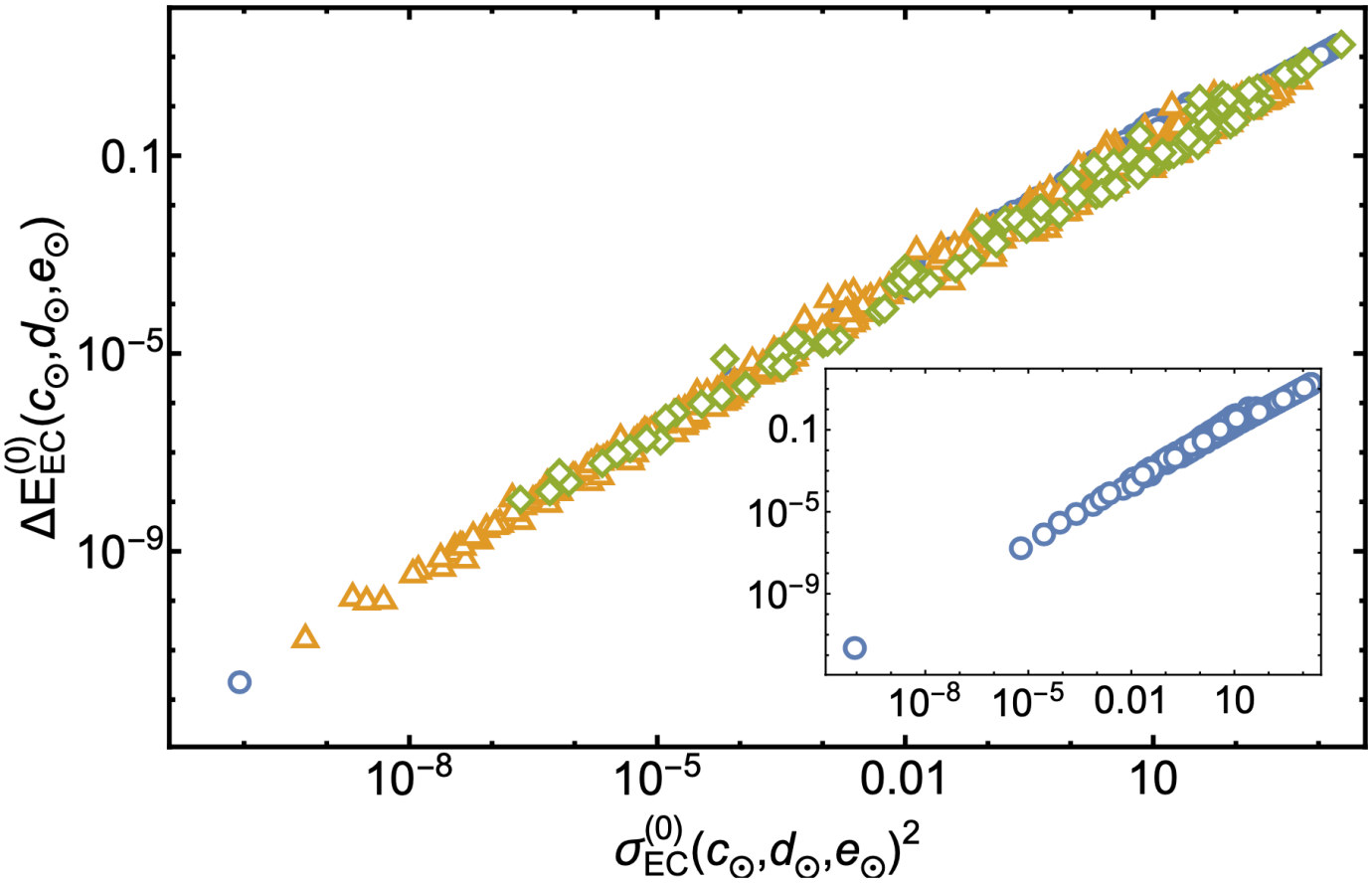




Two-parameter Hamiltonian



Deuteron


0.1
10^{-5}
10^{-9}
$\Delta E_{EC}^{(0)}(c_\odot, d_\odot, e_\odot)$
10^{-8}
10^{-5}
0.01
10
$\sigma_{EC}^{(0)}(c_\odot, d_\odot, e_\odot)^2$
0.1
10^{-5}
10^{-9}
10^{-8}
10^{-5}
0.01
10

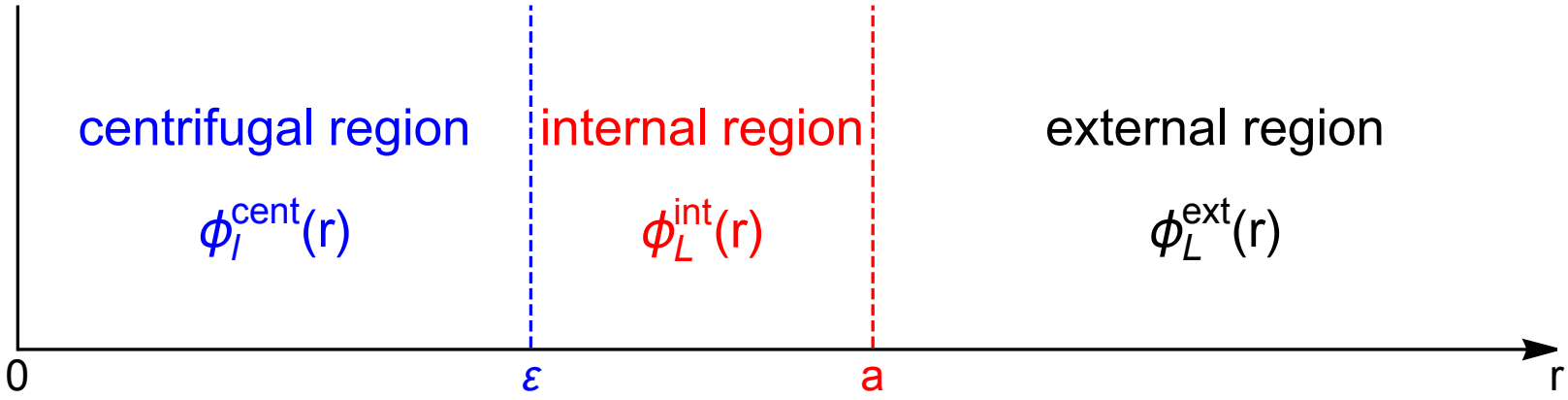
R-matrix EC and its applications in nuclear reactions

Generalize EC from nuclear structures to **nuclear reactions**

- Kohn variational principle
  1. R. J. Furnstahl *et al.*, Phys. Lett. B **809**, 135719 (2020).
  2. J. A. Melendez *et al.*, Phys. Lett. B **821**, 136608 (2021).
  3. C. Drischler *et al.*, Phys. Lett. B **823**, 136777 (2021).
  4. X. Zhang and R. J. Furnstahl, arXiv:2110.04269.
- *R*-matrix theory
  1. D. Bai and Z. Ren, Phys. Rev. C **103**, 014612 (2021).
  2. D. Bai, to appear (2022).
- Reaction observables from bound-state calculations (to be explored)

Advantages of *R*-matrix EC: based on the rich ecosystem of the *R*-matrix theory, including bound states, resonant states, elastic/inelastic scatterings, transfer reactions, breakup reactions, and fusion reactions.

The *R*-matrix theory



For regular boundary condition

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - c\,U(r) + p^2 - \mathcal{L}(a) + \mathcal{L}(\varepsilon)\right]\phi^{\mathrm{int}}_{p,l,c}(r)$$

$$= -\mathcal{L}(a)\phi^{\mathrm{ext}}_{p,l,c}(r) + \mathcal{L}(\varepsilon)\phi^{\mathrm{cent}}_{p,l,c}(r),$$

$$\phi^{\mathrm{int}}_{p,l}(a) = \phi^{\mathrm{ext}}_{p,l}(a) = \frac{i}{2}\left[\mathscr{S}_l(p)H_l^{(-)}(pa) - \mathscr{S}_l(p)^* H_l^{(+)}(pa)\right],$$

$$\phi^{\mathrm{int}}_{p,l}(\varepsilon) = \phi^{\mathrm{cent}}_{p,l}(\varepsilon) = (2l+1)!!\,\widehat{j}_l(p\varepsilon),$$

where $\mathcal{L}(R) = \delta(r-R)\mathrm{d}/\mathrm{d}r$ is the Bloch operator.

Taking the variational trial wave function

$$\phi^{\text{int}}_{p,l,c}(r) = \sum_{i=1}^{N_{\text{EC}}} \zeta_i \phi^{\text{int}}_{z_i}(r),$$

where z_i could be the momentum p_i, the angular momentum l_i, or the coupling constant c_i

$$\sum_{j=1}^{N_{\text{EC}}} \left(\phi^{\text{int}}_{z_i} \left| \frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - U(r) + p^2 - \mathcal{L}(a) + \mathcal{L}(\varepsilon) \right| \phi^{\text{int}}_{z_j} \right) \zeta_j$$

$$= - \left(\phi^{\text{int}}_{z_i} \left| \mathcal{L}(a) \right| \phi^{\text{ext}}_{p,l,c} \right) + \left(\phi^{\text{int}}_{z_i} \left| \mathcal{L}(\varepsilon) \right| \phi^{\text{cent}}_{p,l,c} \right),$$

$$\sum_{i=1}^{N_{\text{EC}}} \phi^{\text{int}}_{z_i}(a)\zeta_i = \frac{i}{2} \left[\mathscr{S}_l(p) H_l^{(-)}(pa) - \mathscr{S}_l(p)^* H_l^{(+)}(pa) \right],$$

$$\sum_{i=1}^{N_{\text{EC}}} \phi^{\text{int}}_{z_i}(\varepsilon)\zeta_i = (2l+1)!! \widehat{j}_l(p\varepsilon),$$

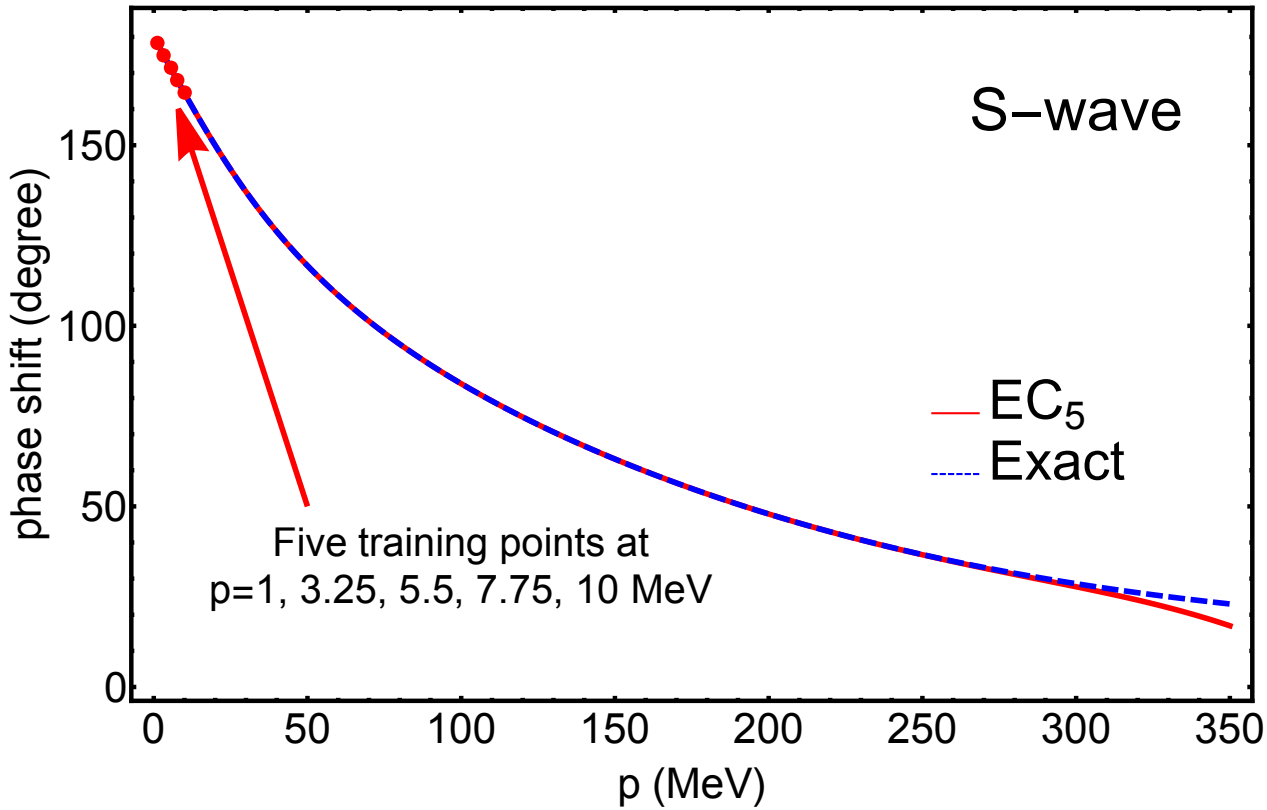
Remember the analytic properties of the regular eigensolution?

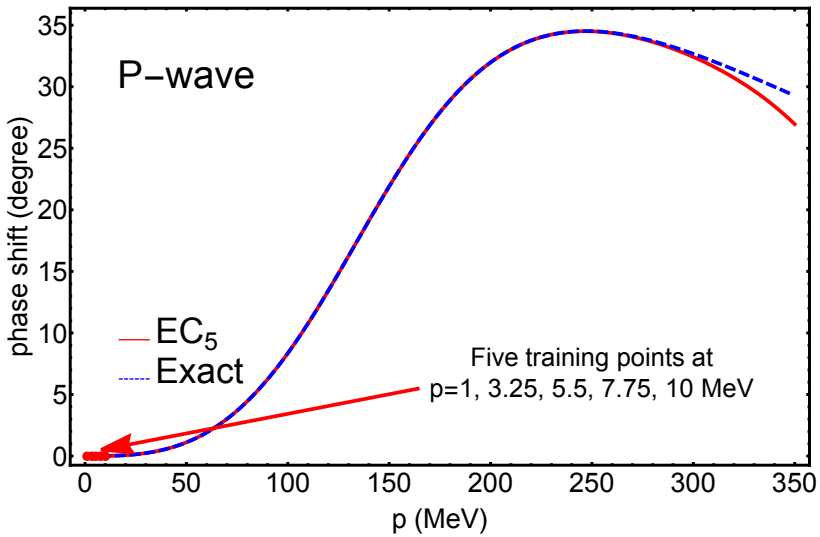
EC in momentum

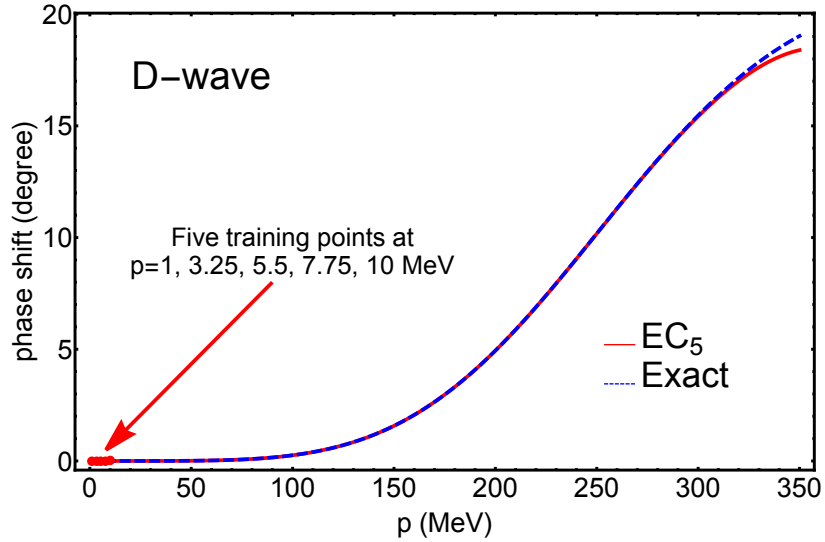
Minnesota-like potential

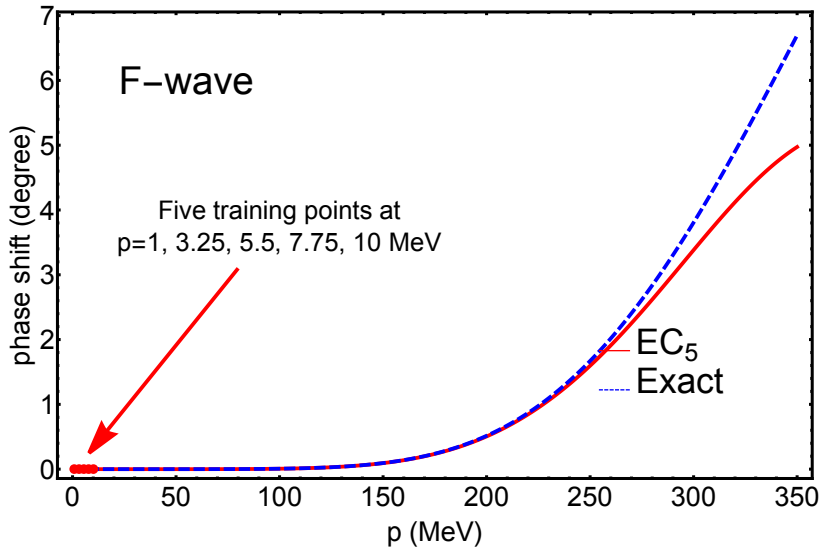
$$V_{\rm NN}(r) = V_{\rm r}\exp(-\kappa_{\rm r} r^2) + V_{\rm a}\exp(-\kappa_{\rm a} r^2),$$

with $V_{\rm r} = 200$ MeV, $V_{\rm a} = -178$ MeV, $\kappa_{\rm r} = 1.487$ fm^{-2}, and $\kappa_{\rm a} = 0.639$ fm^{-2}.



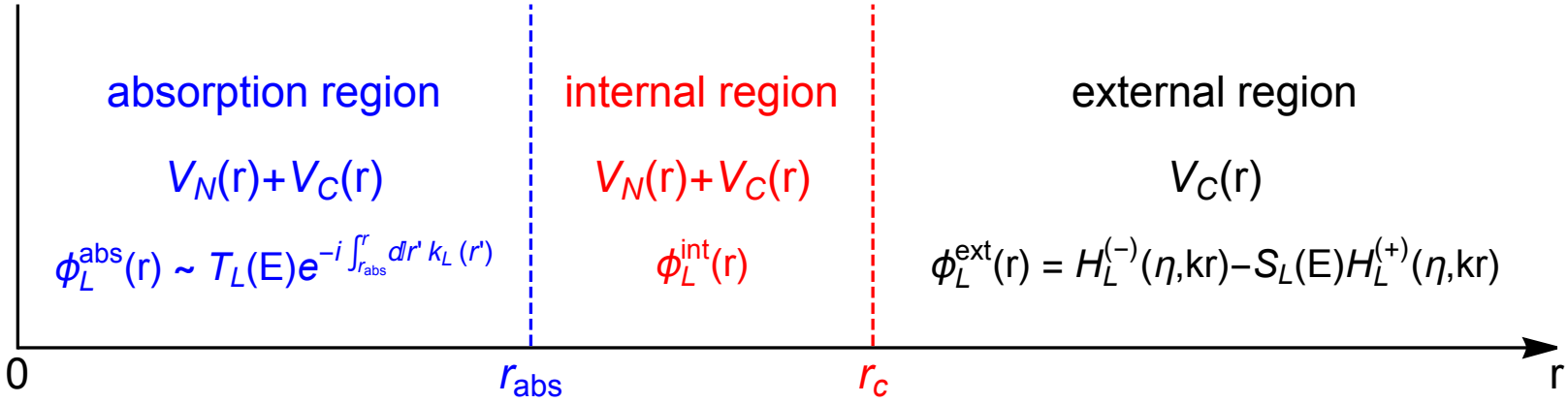

P−wave
phase shift (degree)
p (MeV)
EC5
Exact
Five training points at
p=1, 3.25, 5.5, 7.75, 10 MeV


D−wave
phase shift (degree)
p (MeV)
Five training points at
p=1, 3.25, 5.5, 7.75, 10 MeV
EC5
Exact

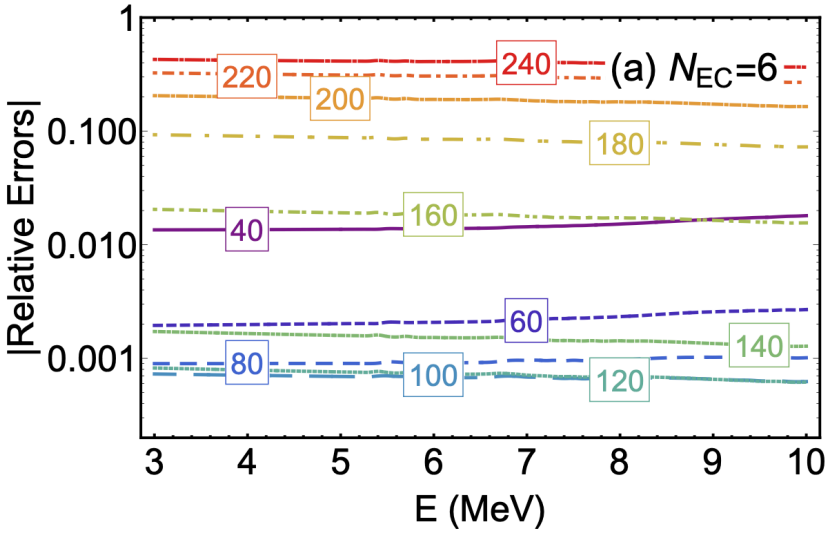

F−wave
phase shift (degree)
p (MeV)
Five training points at
p=1, 3.25, 5.5, 7.75, 10 MeV
EC5
Exact

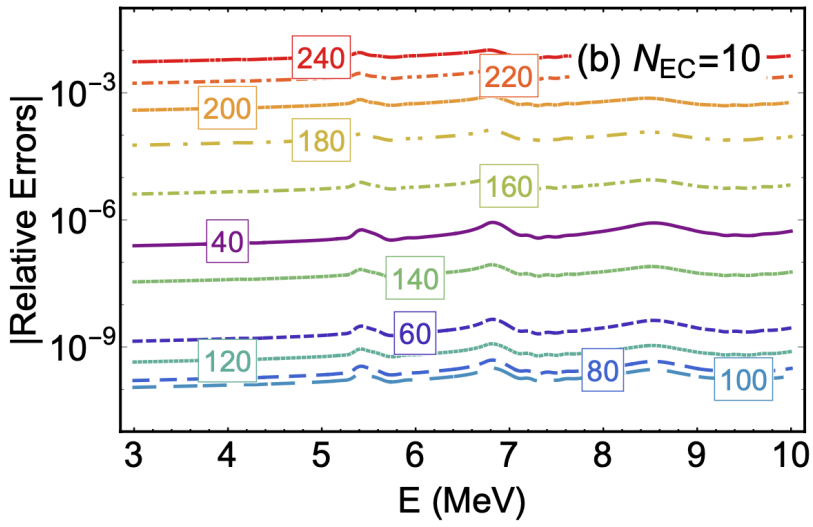
R-matrix EC for fusion reactions

Modifying the *R*-matrix theory for the **incoming wave boundary condition**,



the $^{14}N + {}^{12}C$ fusion, Woods-Saxon potential



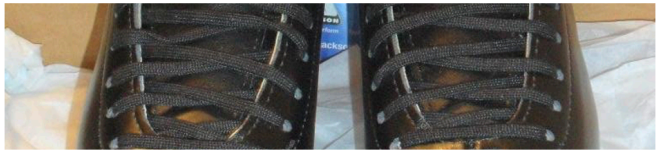


History

- Geoffrey Chew (1924-2019)
  "Nature is as it is because this is the only possible nature consistent with itself."
- Initially as an approach to the strong interaction in the 1960s, known as the S-matrix approach at that time.
- "Compete" with quantum field theory and "lose" in the era of QCD.

solving the problem!

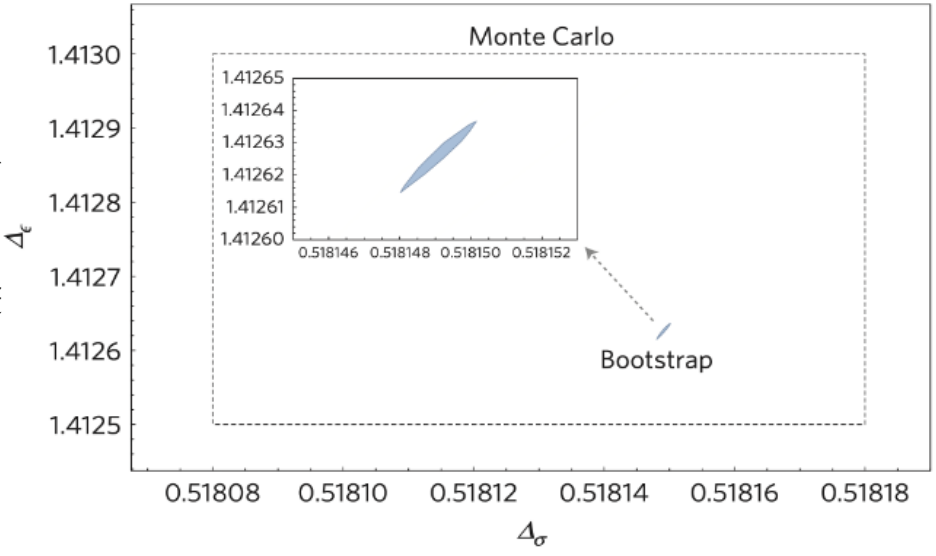
self-consistency



physical principles

Revival

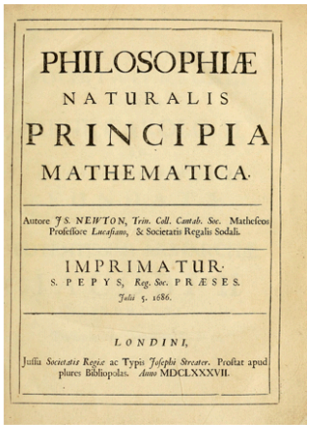
- **Conformal bootstrap**
  conformal bootstrap + primary operators + crossing symmetry + unitarity + a small number of auxiliary assumptions (tagging the theory)
- **Traditionally,** quantum fields, Lagrangian, Feynman rules, Feynman diagrams, dimensional regularization, ϵ expansion, Wilson-Fisher fixed point, $\cdots$
  Where is analyticity? Where is unitarity? Where is crossing symmetry?



critical point of 3D Ising model (1603.04436)

Wishes

Historical Hints: From Newtonian to Lagrangian and Hamiltonian


PHILOSOPHIÆ
NATURALIS
PRINCIPIA
MATHEMATICA

Autore Is. NEWTON, Trin. Coll. Cantab. Soc. Matheseos Professore Lucasiano, & Societatis Regalis Sodali.

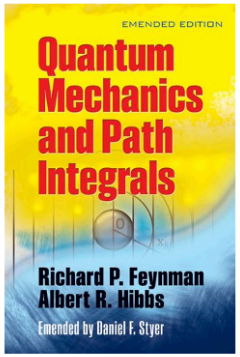
IMPRIMATUR
S. PEPYS, Reg. Soc. PRÆSES.
Julii 5. 1686.

LONDINI,
Jussu Societatis Regiæ ac Typis Josephi Streater. Prostat apud plures Bibliopolas. Anno MDCLXXXVII.

"geometric" language

$$S[x(t)] = \int_{t_1}^{t_2} L(x(t), \dot{x}(t), t)dt$$

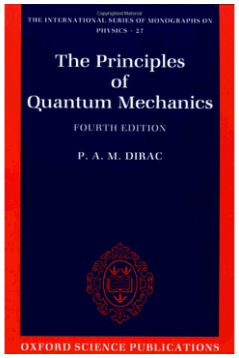
virtual displacement



$$\frac{dq}{dt} = \frac{\partial H}{\partial p}$$

$$\frac{dp}{dt} = \frac{\partial H}{\partial q}$$

Poisson bracket



What are the "Lagragian" and "Hamiltonian" in the quantum era?
Springboard to new revolutions?

Quantum anharmonic oscillators

Generalize bootstrap from relativistic QFT to nonrelativistic QM

- X. Han, S. A. Hartnoll, and J. Kruthoff, Phys. Rev. Lett. **125**, 041601 (2020), inspired by H. W. Lin, J. High Energ. Phys. **2020**, 90 (2020).

Define the model

- Hamiltonian

$$H = p^2 + x^2 + gx^4$$

- Commutation relation

$$[x, p] = i$$

Self-consistency: defining eigenstate

- Condition I

$$\langle E|[H, \mathcal{O}]|E\rangle \equiv \langle [H, \mathcal{O}]\rangle_E = 0$$

- Condition II

$$\langle \mathcal{O}H\rangle_E = E\,\langle O\rangle_E$$

Self-consistency: concretization

- For Condition I, take

$$\mathcal{O} = x^s \quad \text{and} \quad \mathcal{O} = x^t p$$

- For Condition II, take

$$\mathcal{O} = x^{t-1}$$

Self-consistency: simplification

- Condition I

$$4t \langle x^{t-1} p^2 \rangle_E = 8g \langle x^{t+3} \rangle_E + 4 \langle x^{t+1} \rangle_E - t(t-1)(t-2) \langle x^{t-3} \rangle_E$$

- Condition II

$$\langle x^{t-1} p^2 \rangle_E = E \langle x^{t-1} \rangle_E - \langle x^{t+1} \rangle_E - g \langle x^{t+3} \rangle_E$$

Self-consistency: finalization

- Recursive relation

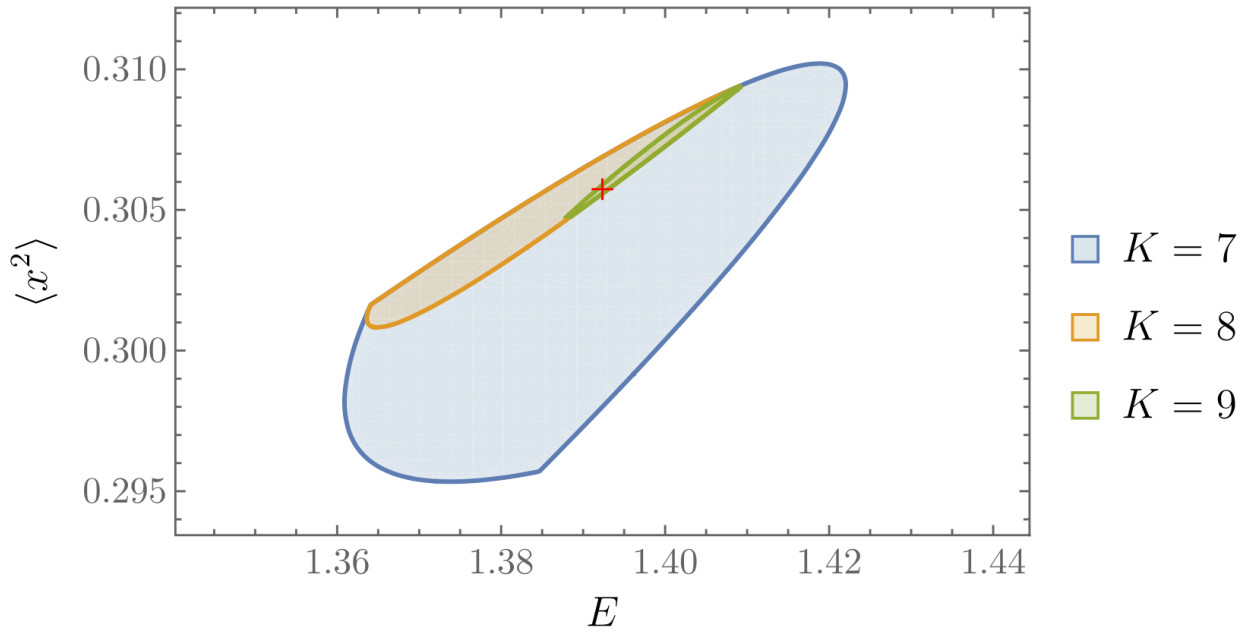
$$4tE\langle x^{t-1}\rangle_E + t(t-1)(t-2)\langle x^{t-3}\rangle_E - 4(t+1)\langle x^{t+1}\rangle_E$$
$$-4g(t+2)\langle x^{t+3}\rangle_E = 0$$

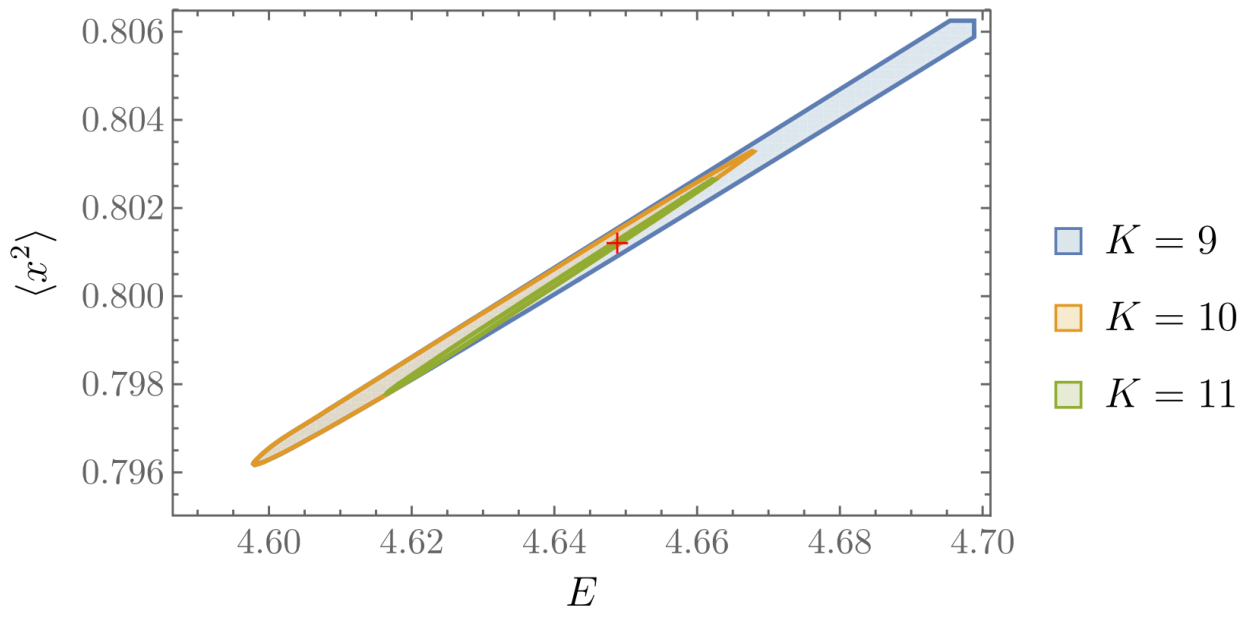
Physical principle

- Positivity constraint

$$\langle \mathcal{O}^\dagger \mathcal{O}\rangle_E \geq 0, \quad \mathcal{O} = \sum_{i=0}^{K} c_i x^i$$

$\Rightarrow$ the bootstrap matrix $\mathcal{M}$ of size $(K+1)\times(K+1)$ with $\mathcal{M}_{ij} = \langle x^{i+j}\rangle_E$ should be positive semidefinite.


0.310
0.305
0.300
0.295
$\langle x^2 \rangle$
1.36
1.38
1.40
1.42
1.44
E
$K = 7$
$K = 8$
$K = 9$


0.806
0.804
0.802
0.800
0.798
0.796
$\langle x^2 \rangle$
4.60
4.62
4.64
4.66
4.68
4.70
E
$K = 9$
$K = 10$
$K = 11$

Bootstrapping the deuteron

More applications of quantum mechanical bootstrap: harmonic oscillator, hydrogen atom, double-well potential, Bloch Band, etc. **Recursive relations** play a crucial role, restricting the forms of potentials to polynomial and trigonometric.

Consider the deuteron Hamiltonian from pionless EFT in harmonic oscillator space

$$H_{N_{\max}} = \sum_{i,j=0}^{N_{\max}} H_{ij} \left|i\right\rangle \left\langle j\right| \equiv \sum_{i,j=0}^{N_{\max}} \left(T_{ij} + V_{ij}\right) \left|i\right\rangle \left\langle j\right| ,$$

$$T_{ij} = \langle i|T|j\rangle = \frac{\omega}{2}\left[(2j+3/2)\delta_{ij} - \sqrt{j(j+1/2)}\delta_{i+1,j} - \sqrt{(j+1)(j+3/2)}\delta_{i-1,j}\right],$$

$$V_{ij} = \langle i|V|j\rangle = V_0 \delta_{j0}\delta_{ij}.$$

E. F. Dumitrescu *et al.*, Phys. Rev. Lett. **120**, 210501 (2018).

S. Binder *et al.*, Phys. Rev. C **93**, 044332 (2016).

A. Bansal *et al.*, Phys. Rev. C **98**, 054301 (2018).

The bootstrap matrix

Positivity constraint

$$\langle \Psi | \mathcal{O}^\dagger \mathcal{O} | \Psi \rangle \geq 0$$

Let $\mathcal{O} = \sum_{i=0}^{K} \alpha_i \mathcal{O}_i$

$$\mathcal{M} \succeq 0, \qquad \mathcal{M}_{ij} = \langle \mathcal{O}_i^\dagger \mathcal{O}_j \rangle_E.$$

For deuteron, consider

$$\mathcal{O} = \sum_{i \leq j} \alpha_{ij} |i\rangle \langle j| \equiv \sum_{i \leq j} \alpha_{ij} \mathcal{O}_{ij} = \alpha_{00}\mathcal{O}_{00} + \cdots + \alpha_{0N}\mathcal{O}_{0,N_{\max}} + \alpha_{11}\mathcal{O}_{11} + \cdots$$
$$+ \alpha_{1,N_{\max}}\mathcal{O}_{1,N_{\max}} + \cdots + \alpha_{N_{\max}-1,N_{\max}-1}\mathcal{O}_{N_{\max}-1,N_{\max}-1}$$
$$+ \alpha_{N_{\max}-1,N_{\max}}\mathcal{O}_{N_{\max}-1,N_{\max}} + \alpha_{N_{\max},N_{\max}}\mathcal{O}_{N_{\max},N_{\max}}.$$

The bootstrap matrix is of $N_{\mathcal{M}} \times N_{\mathcal{M}}$, with $N_{\mathcal{M}} \equiv (N_{\max}+1)(N_{\max}+2)/2$.

See also J. G. Li *et al.*, Phys. Rev. C **103**, 064324 (2021).

The bootstrap matrix: examples

- $N_{\max} = 2$

$$\mathcal{M}_2 = \begin{pmatrix} \langle \mathcal{O}_{00} \rangle_{E_2} & \langle \mathcal{O}_{01} \rangle_{E_2} & \langle \mathcal{O}_{02} \rangle_{E_2} & 0 & 0 & 0 \\ \langle \mathcal{O}_{01} \rangle_{E_2} & \langle \mathcal{O}_{11} \rangle_{E_2} & \langle \mathcal{O}_{12} \rangle_{E_2} & 0 & 0 & 0 \\ \langle \mathcal{O}_{02} \rangle_{E_2} & \langle \mathcal{O}_{12} \rangle_{E_2} & \langle \mathcal{O}_{22} \rangle_{E_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \langle \mathcal{O}_{11} \rangle_{E_2} & \langle \mathcal{O}_{12} \rangle_{E_2} & 0 \\ 0 & 0 & 0 & \langle \mathcal{O}_{12} \rangle_{E_2} & \langle \mathcal{O}_{22} \rangle_{E_2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \langle \mathcal{O}_{22} \rangle_{E_2} \end{pmatrix}$$

- $N_{\max} = 3$

$$\mathcal{M}_3 = \begin{pmatrix} \langle \mathcal{O}_{00} \rangle_{E_3} & \langle \mathcal{O}_{01} \rangle_{E_3} & \langle \mathcal{O}_{02} \rangle_{E_3} & \langle \mathcal{O}_{03} \rangle_{E_3} & 0 & 0 & 0 & 0 & 0 & 0 \\ \langle \mathcal{O}_{01} \rangle_{E_3} & \langle \mathcal{O}_{11} \rangle_{E_3} & \langle \mathcal{O}_{12} \rangle_{E_3} & \langle \mathcal{O}_{13} \rangle_{E_3} & 0 & 0 & 0 & 0 & 0 & 0 \\ \langle \mathcal{O}_{02} \rangle_{E_3} & \langle \mathcal{O}_{12} \rangle_{E_3} & \langle \mathcal{O}_{22} \rangle_{E_3} & \langle \mathcal{O}_{23} \rangle_{E_3} & 0 & 0 & 0 & 0 & 0 & 0 \\ \langle \mathcal{O}_{03} \rangle_{E_3} & \langle \mathcal{O}_{13} \rangle_{E_3} & \langle \mathcal{O}_{23} \rangle_{E_3} & \langle \mathcal{O}_{33} \rangle_{E_3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \langle \mathcal{O}_{11} \rangle_{E_3} & \langle \mathcal{O}_{12} \rangle_{E_3} & \langle \mathcal{O}_{13} \rangle_{E_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \langle \mathcal{O}_{12} \rangle_{E_3} & \langle \mathcal{O}_{22} \rangle_{E_3} & \langle \mathcal{O}_{23} \rangle_{E_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \langle \mathcal{O}_{13} \rangle_{E_3} & \langle \mathcal{O}_{23} \rangle_{E_3} & \langle \mathcal{O}_{33} \rangle_{E_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \langle \mathcal{O}_{22} \rangle_{E_3} & \langle \mathcal{O}_{23} \rangle_{E_3} & 0 \\ 0 & 0 & & 0 & 0 & 0 & 0 & \langle \mathcal{O}_{23} \rangle_{E_3} & \langle \mathcal{O}_{33} \rangle_{E_3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \langle \mathcal{O}_{33} \rangle_{E_3} \end{pmatrix}$$

Self-consistency conditions

- Completeness relation

$$\sum_{i=0}^{N_{\max}} \langle \mathcal{O}_{ii} \rangle_{E_{N_{\max}}} = 1$$

- Definition of eigenstate

$$\langle H_{N_{\max}} \mathcal{O}_{ij} \rangle_{E_{N_{\max}}} = E_{N_{\max}} \langle \mathcal{O}_{ij} \rangle_{E_{N_{\max}}}$$

$$\Rightarrow [ij]_{N_{\max}} \equiv \left(\sum_{k=0}^{N_{\max}} H_{(ki)} \langle \mathcal{O}_{(kj)} \rangle_{E_{N_{\max}}} - E_{N_{\max}} \langle \mathcal{O}_{ij} \rangle_{E_{N_{\max}}} = 0 \right)$$

for $i \leq j$.

One constraint has to be removed to avoid overcompleteness. **Which one?**

Numerical results: $N_{\max} = 2$

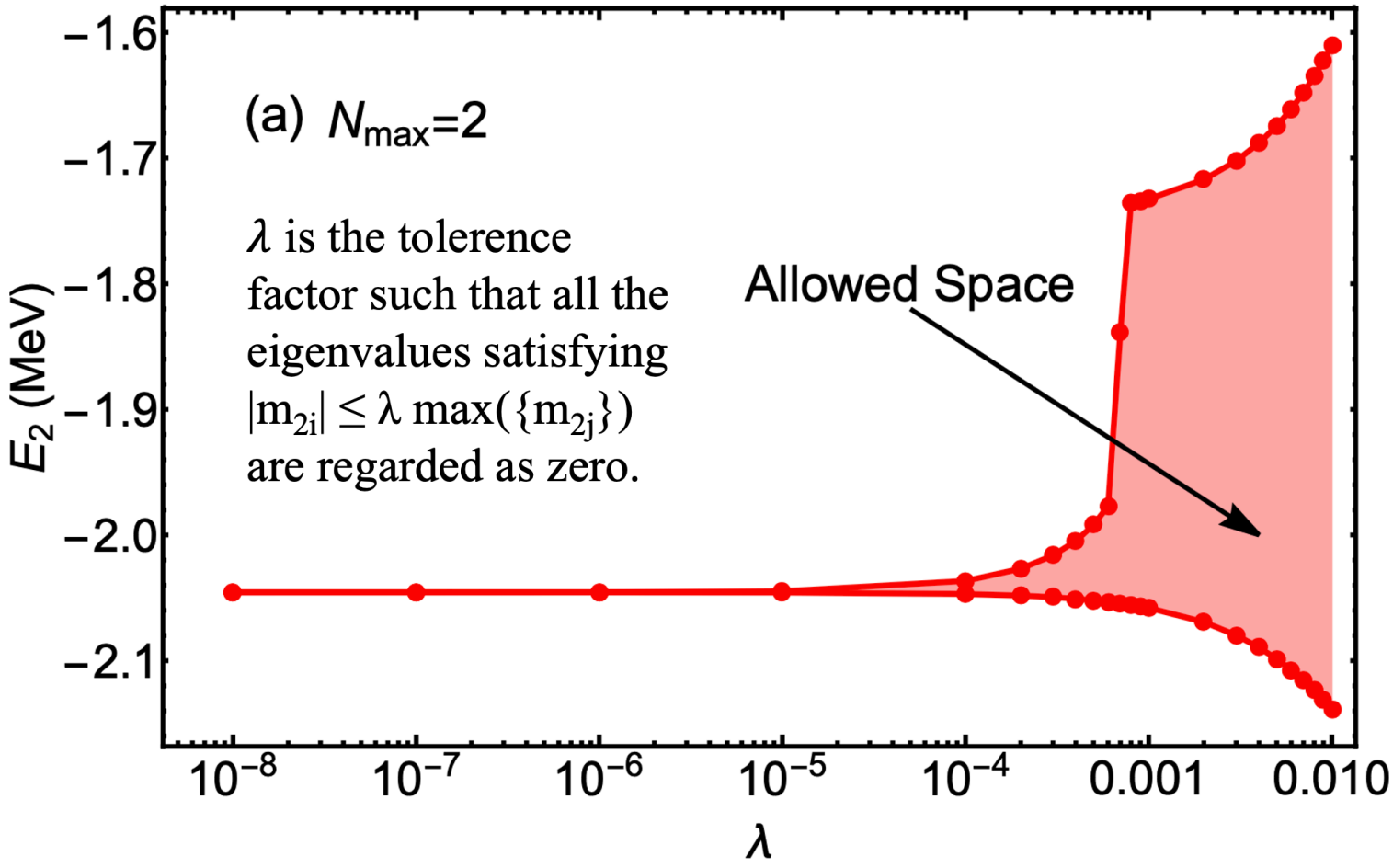
- Hamiltonian

$$H_2 = \begin{pmatrix} -0.436581 & -4.28661 & 0 \\ -4.28661 & 12.25 & -7.82624 \\ 0 & -7.82624 & 19.25 \end{pmatrix}$$

with the exact lowest eigenvalue found to be $E_2^{\text{exact}} = -2.045671$ MeV.

- Self-consistency conditions

$$\langle \mathcal{O}_{00} \rangle_{E_2} + \langle \mathcal{O}_{11} \rangle_{E_2} + \langle \mathcal{O}_{22} \rangle_{E_2} = 1,$$
$$[00]_2 \equiv \left(H_{00} \langle \mathcal{O}_{00} \rangle_{E_2} + H_{01} \langle \mathcal{O}_{01} \rangle_{E_2} + H_{02} \langle \mathcal{O}_{02} \rangle_{E_2} - E_2 \langle \mathcal{O}_{00} \rangle_{E_2} = 0 \right),$$
$$[01]_2 \equiv \left(H_{00} \langle \mathcal{O}_{01} \rangle_{E_2} + H_{01} \langle \mathcal{O}_{11} \rangle_{E_2} + H_{02} \langle \mathcal{O}_{12} \rangle_{E_2} - E_2 \langle \mathcal{O}_{01} \rangle_{E_2} = 0 \right),$$
$$[11]_2 \equiv \left(H_{01} \langle \mathcal{O}_{01} \rangle_{E_2} + H_{11} \langle \mathcal{O}_{11} \rangle_{E_2} + H_{12} \langle \mathcal{O}_{12} \rangle_{E_2} - E_2 \langle \mathcal{O}_{11} \rangle_{E_2} = 0 \right),$$
$$[12]_2 \equiv \left(H_{01} \langle \mathcal{O}_{02} \rangle_{E_2} + H_{11} \langle \mathcal{O}_{12} \rangle_{E_2} + H_{12} \langle \mathcal{O}_{22} \rangle_{E_2} - E_2 \langle \mathcal{O}_{12} \rangle_{E_2} = 0 \right),$$
$$[22]_2 \equiv \left(H_{02} \langle \mathcal{O}_{02} \rangle_{E_2} + H_{12} \langle \mathcal{O}_{12} \rangle_{E_2} + H_{22} \langle \mathcal{O}_{22} \rangle_{E_2} - E_2 \langle \mathcal{O}_{22} \rangle_{E_2} = 0 \right).$$



For $\lambda = 10^{-8}$, $\mathcal{M}_2$ is positive semidefinite at -2.045671 MeV $\leq E_2$ ≤ -2.0456701 MeV. $E_2^{\text{exact}} = -2.045671$ MeV

Numerical results: $N_{\max} = 3$

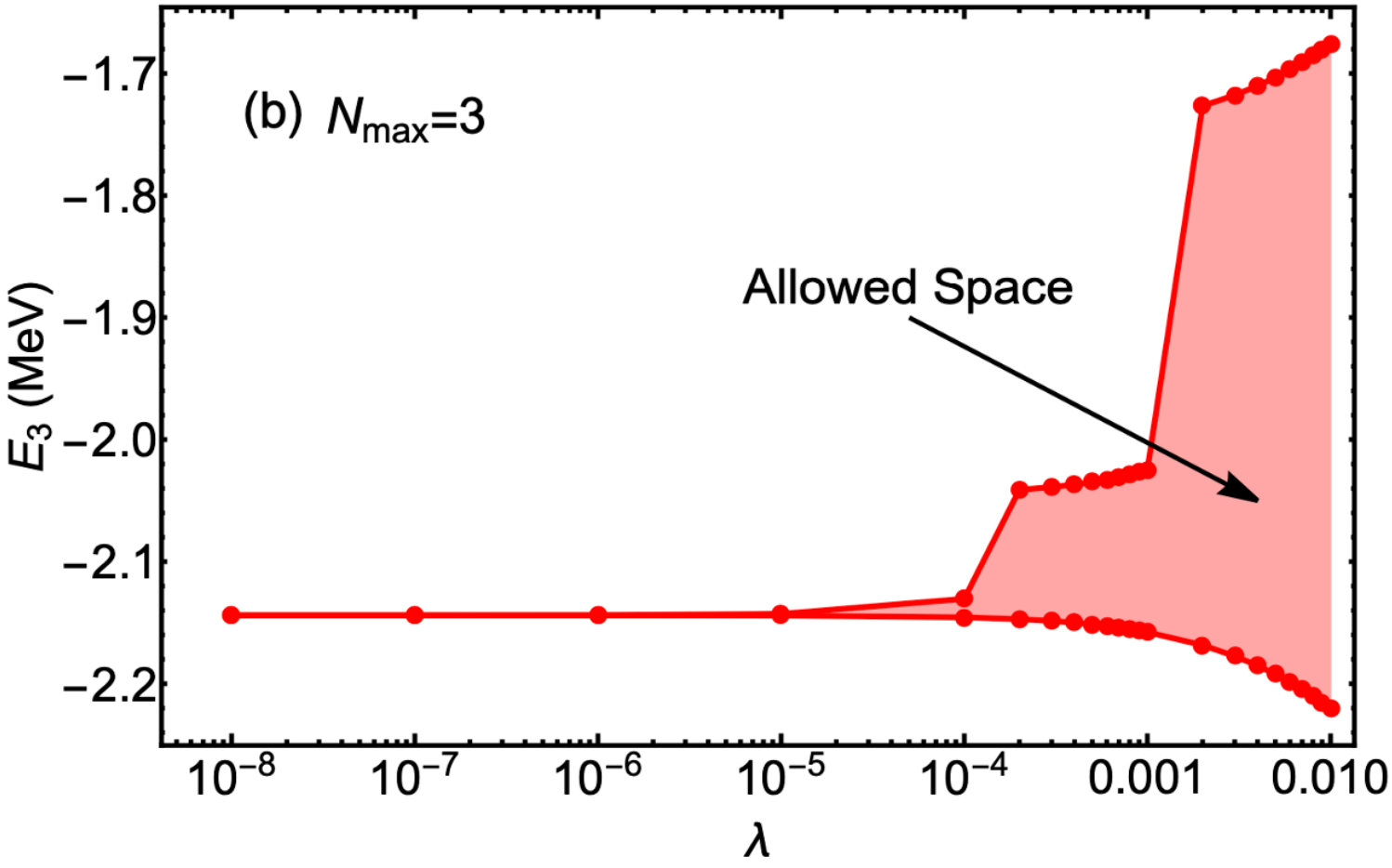
- Hamiltonian

$$H_3 = \begin{pmatrix} -0.436581 & -4.28661 & 0 & 0 \\ -4.28661 & 12.25 & -7.82624 & 0 \\ 0 & -7.82624 & 19.25 & -11.3413 \\ 0 & 0 & -11.3413 & 26.25 \end{pmatrix},$$

with the exact lowest eigenvalue found to be $E_3^{\text{exact}} = -2.143981$ MeV.

- Self-consistency conditions

$$\begin{aligned}
&\langle \mathcal{O}_{00} \rangle_{E_3} + \langle \mathcal{O}_{11} \rangle_{E_3} + \langle \mathcal{O}_{22} \rangle_{E_3} + \langle \mathcal{O}_{33} \rangle_{E_3} = 1, \\
&[00]_3 \equiv \left(H_{00} \langle \mathcal{O}_{00} \rangle_{E_3} + H_{01} \langle \mathcal{O}_{01} \rangle_{E_3} + H_{02} \langle \mathcal{O}_{02} \rangle_{E_3} + H_{03} \langle \mathcal{O}_{03} \rangle_{E_3} - E_3 \langle \mathcal{O}_{00} \rangle_{E_3} = 0 \right), \\
&[01]_3 \equiv \left(H_{00} \langle \mathcal{O}_{01} \rangle_{E_3} + H_{01} \langle \mathcal{O}_{11} \rangle_{E_3} + H_{02} \langle \mathcal{O}_{12} \rangle_{E_3} + H_{03} \langle \mathcal{O}_{13} \rangle_{E_3} - E_3 \langle \mathcal{O}_{01} \rangle_{E_3} = 0 \right), \\
&[02]_3 \equiv \left(H_{00} \langle \mathcal{O}_{02} \rangle_{E_3} + H_{01} \langle \mathcal{O}_{12} \rangle_{E_3} + H_{02} \langle \mathcal{O}_{22} \rangle_{E_3} + H_{03} \langle \mathcal{O}_{23} \rangle_{E_3} - E_3 \langle \mathcal{O}_{02} \rangle_{E_3} = 0 \right), \\
&[03]_3 \equiv \left(H_{00} \langle \mathcal{O}_{03} \rangle_{E_3} + H_{01} \langle \mathcal{O}_{13} \rangle_{E_3} + H_{02} \langle \mathcal{O}_{23} \rangle_{E_3} + H_{03} \langle \mathcal{O}_{33} \rangle_{E_3} - E_3 \langle \mathcal{O}_{03} \rangle_{E_3} = 0 \right), \\
&[11]_3 \equiv \left(H_{01} \langle \mathcal{O}_{01} \rangle_{E_3} + H_{11} \langle \mathcal{O}_{11} \rangle_{E_3} + H_{12} \langle \mathcal{O}_{12} \rangle_{E_3} + H_{13} \langle \mathcal{O}_{13} \rangle_{E_3} - E_3 \langle \mathcal{O}_{11} \rangle_{E_3} = 0 \right), \\
&[12]_3 \equiv \left(H_{01} \langle \mathcal{O}_{02} \rangle_{E_3} + H_{11} \langle \mathcal{O}_{12} \rangle_{E_3} + H_{12} \langle \mathcal{O}_{22} \rangle_{E_3} + H_{13} \langle \mathcal{O}_{23} \rangle_{E_3} - E_3 \langle \mathcal{O}_{12} \rangle_{E_3} = 0 \right), \\
&[22]_3 \equiv \left(H_{02} \langle \mathcal{O}_{02} \rangle_{E_3} + H_{12} \langle \mathcal{O}_{12} \rangle_{E_3} + H_{22} \langle \mathcal{O}_{22} \rangle_{E_3} + H_{23} \langle \mathcal{O}_{23} \rangle_{E_3} - E_3 \langle \mathcal{O}_{22} \rangle_{E_3} = 0 \right), \\
&[23]_3 \equiv \left(H_{02} \langle \mathcal{O}_{03} \rangle_{E_3} + H_{12} \langle \mathcal{O}_{13} \rangle_{E_3} + H_{22} \langle \mathcal{O}_{23} \rangle_{E_3} + H_{23} \langle \mathcal{O}_{33} \rangle_{E_3} - E_3 \langle \mathcal{O}_{23} \rangle_{E_3} = 0 \right), \\
&[33]_3 \equiv \left(H_{03} \langle \mathcal{O}_{03} \rangle_{E_3} + H_{13} \langle \mathcal{O}_{13} \rangle_{E_3} + H_{23} \langle \mathcal{O}_{23} \rangle_{E_3} + H_{33} \langle \mathcal{O}_{33} \rangle_{E_3} - E_3 \langle \mathcal{O}_{33} \rangle_{E_3} = 0 \right).
\end{aligned}$$



For $\lambda = 10^{-8}$, $\mathcal{M}_3$ is positive semidefinite at
-2.143981 MeV $\leq E_3 \leq -2.143980$ MeV. $E_3^{\text{exact}} = -2.143981$ MeV

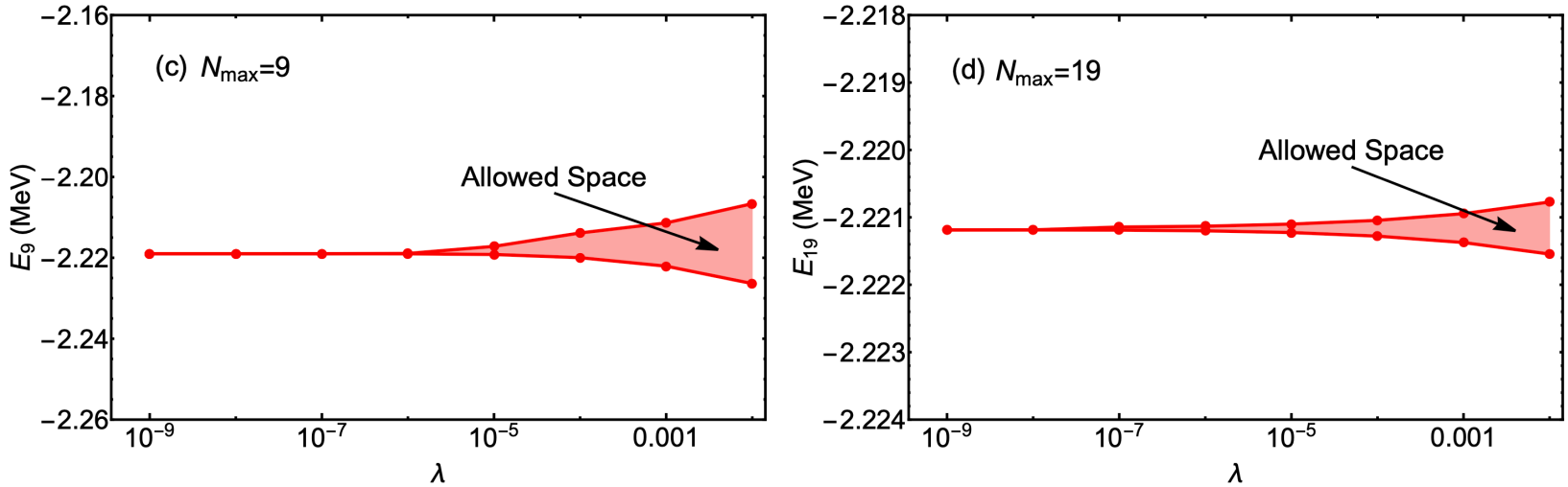
Numerical results: $N_{\max} = 9$ and $N_{\max} = 19$

- Hamiltonian

  The exact lowest eigenvalues are found to be $E_9^{\text{exact}} = -2.219002$ MeV and $E_{19}^{\text{exact}} = -2.221187$ MeV.

- Self-consistency conditions

  To bootstrap the lowest eigenvalues, the bootstrap constraints $\overline{[09]}_9$ and $\overline{[0,19]}_{19}$ are used for $N_{\max} = 9$ and $N_{\max} = 19$.



At $\lambda = 10^{-9}$, the bootstrap matrices $\mathcal{M}_9$ and $\mathcal{M}_{19}$ are positive semidefinite for -2.21900225 MeV $\leq E_9 \leq -2.21900217$ MeV and -2.22118726 MeV $\leq E_{19} \leq -2.22118714$ MeV.

Summary and outlook

Eigenvector continuation

- rooted in analyticity, combined with the variational method $\Rightarrow$ resumming perturbative expansions + efficient emulators
- R-matrix EC = EC + the R-matrix theory, proof of concept in simple reactions
- Future directions of R-matrix EC
  - from EC to sensitivity analysis and uncertainty quantification of nuclear reactions
  - Mathematical properties: convergence, errors, $\cdots$

Quantum mechanical bootstrap

- Bootstrap $\rightarrow$ quantum mechanical bootstrap ($\Leftarrow$ positivity constraint $\Leftarrow$ unitarity) $\rightarrow$ quantum anharmonic oscillator $\rightarrow$ deuteron
- Future directions
  - maybe few-body systems
  - maybe resonant states, keep thinking.


Thank you!
河海大学