Ab initio nuclear scattering calculations using traps

Emulators for scattering using eigenvector continuation

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NSCL Virtual Theory Seminar, Sep. 2020

Thank my collaborators:

S. R. Stroberg, P. Navrátil, Chan Gwak, J. A. Melendez,

R. J. Furnstahl, J. D. Holt, A. J. Garcia, and P. J. Millican

Outline

- Background on ab initio calculations
- Our method adapts the principle of the Luscher method from Lattice QCD
- Benchmarks $(\mathrm{n}-\alpha)$ and applications for heavier system $(\mathrm{n}-{}^{24}O)$
- Summary and outlook I

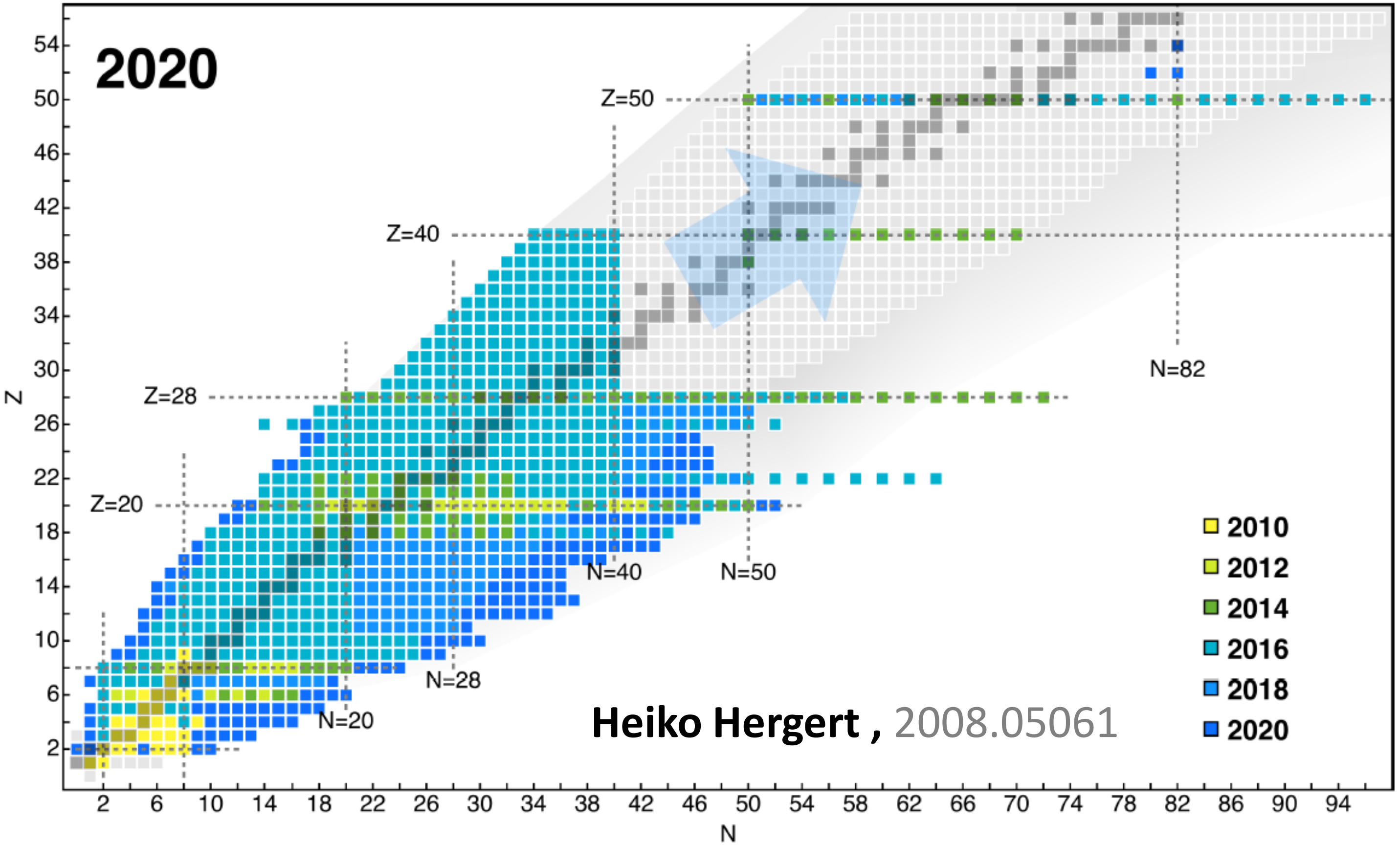
- Broad applications of emulators for bound and scattering states
- Eigenvector continuation emulators for scatterings
- Summary and outlook II

“Ab initio calculations of low-energy nuclear scattering using confining potential traps,”

XZ, S. R. Stroberg, P. Navrátil, Chan Gwak, J. A. Melendez, R. J. Furnstahl, and J. D. Holt, PRL **125**, 112503 (2020) [2004.13575]

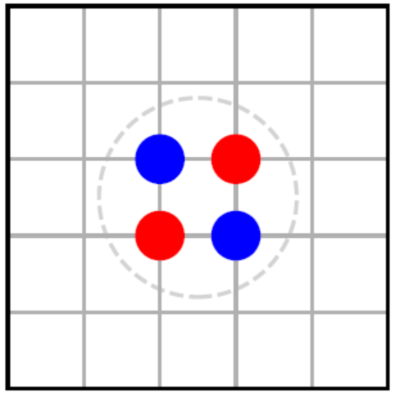
FRIB

- Nuclear reaction with astrophysical relevance
- Reactions as the tools at FRIB
- Consistent treatment of structure and scattering/reactions for drip-line nuclei
- Ab initio structure calculations have made amazing progress, while scattering/reactions are limited

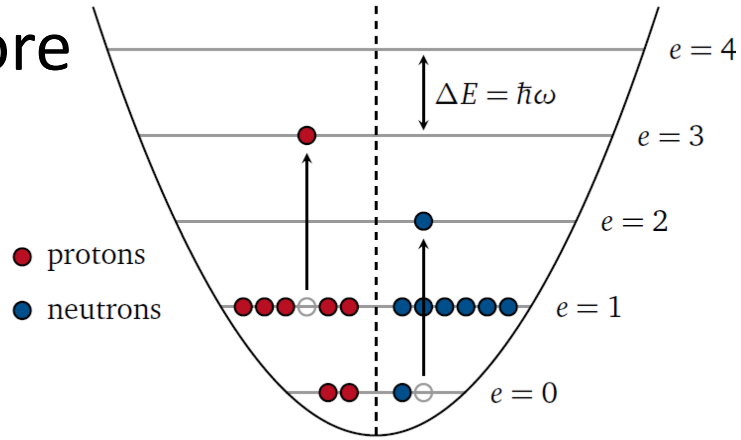


Can we take advantage of progress to compute scattering/reactions?

Ab initio calculations of bound nuclei

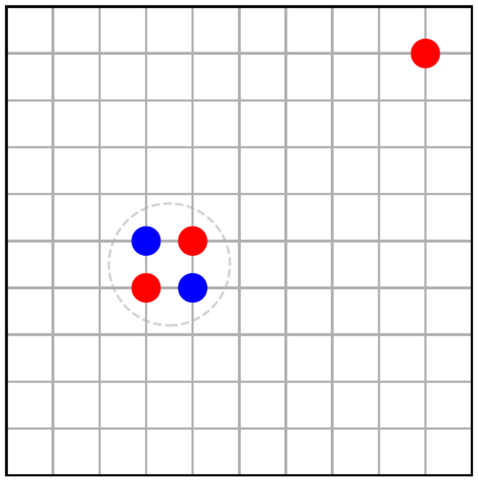


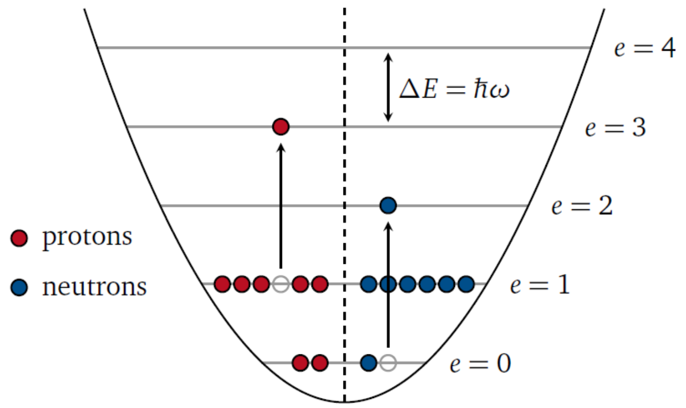
- Degrees of freedom (DOF): $\boldsymbol{r}$ and $\boldsymbol{s}$. Different treatments:
  - Monte Carlo (MC) sampling: Green's function MC, nuclear lattice effective field theory (NLEFT) (also similarly in lattice QCD)
  - Basis method, e.g. Hamiltonian diagonalization in no-core shell model (NCSM) and in-medium similarity renormalization group (IMSRG), and coupled-cluster



Ab initio calculations of scattering/reactions

- For scattering/reactions: much more DOF. Various methods:
  - Again MC-sampling of important configurations: NLEFT, GFMC, Lattice QCD
  - NCSM+continuum
  - Gamow shell-model
  - Ab initio optical potential





Key idea for **two-body** scattering

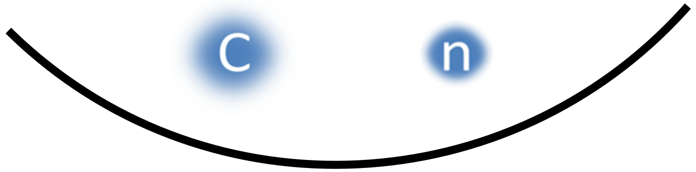
$$\sigma_l(E) = \frac{4\pi}{p^2} \times (2l+1)\sin^2\delta_l(E)$$

$$(\boldsymbol{E}, \boldsymbol{\omega_T}) \rightarrow \boldsymbol{\delta_l(E)}$$

- Eigen-energies of trapped projectile-target systems output from ab initio calculations → scattering (phase-shift) at those energies.

- Works with systems computable by structure methods (trap makes unbound system artificially bound)

Keep an example in your mind: neutron-alpha scattering



Luscher's method in Lattice QCD

Discrete eigen-energies for pi-pi in a finite volume gives the phase shift at those energies

$$(E, V_{Lattice}) \rightarrow \delta_l(E)$$

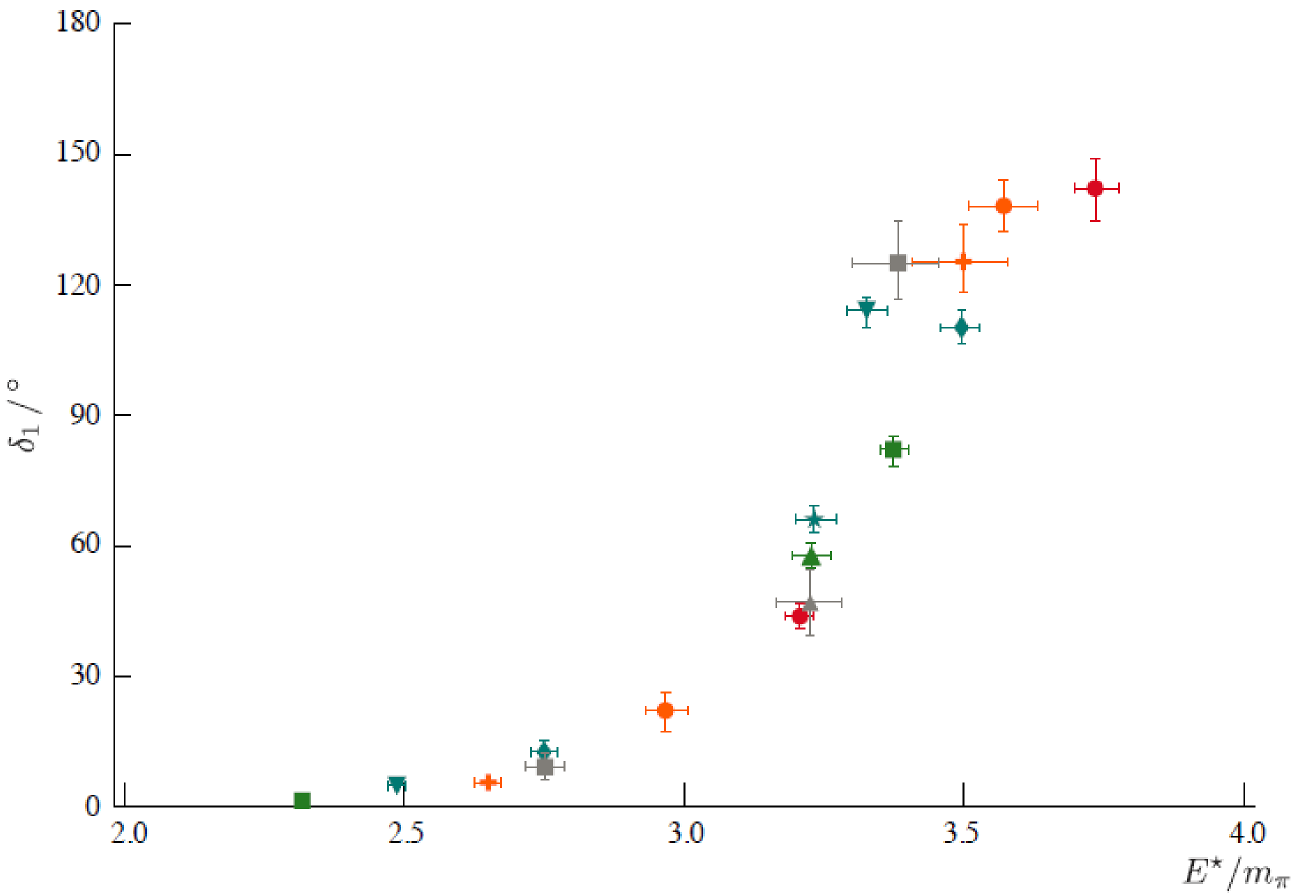
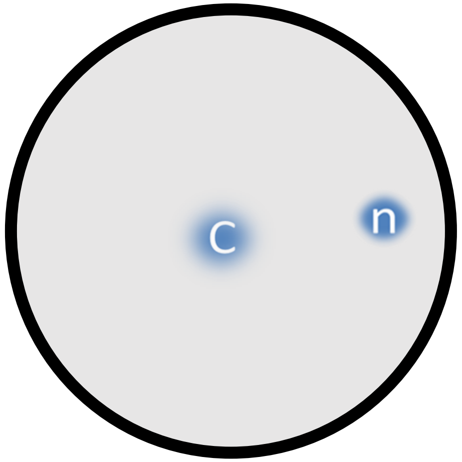


FIG. 14 Elastic $I = 1$ $\pi\pi$ scattering phase-shifts in P-wave determined from finite-volume spectra computed the same $m_\pi \sim 236$ MeV configurations as used in the calculation

Briceno et.al., RMP.90.025002 (2018)

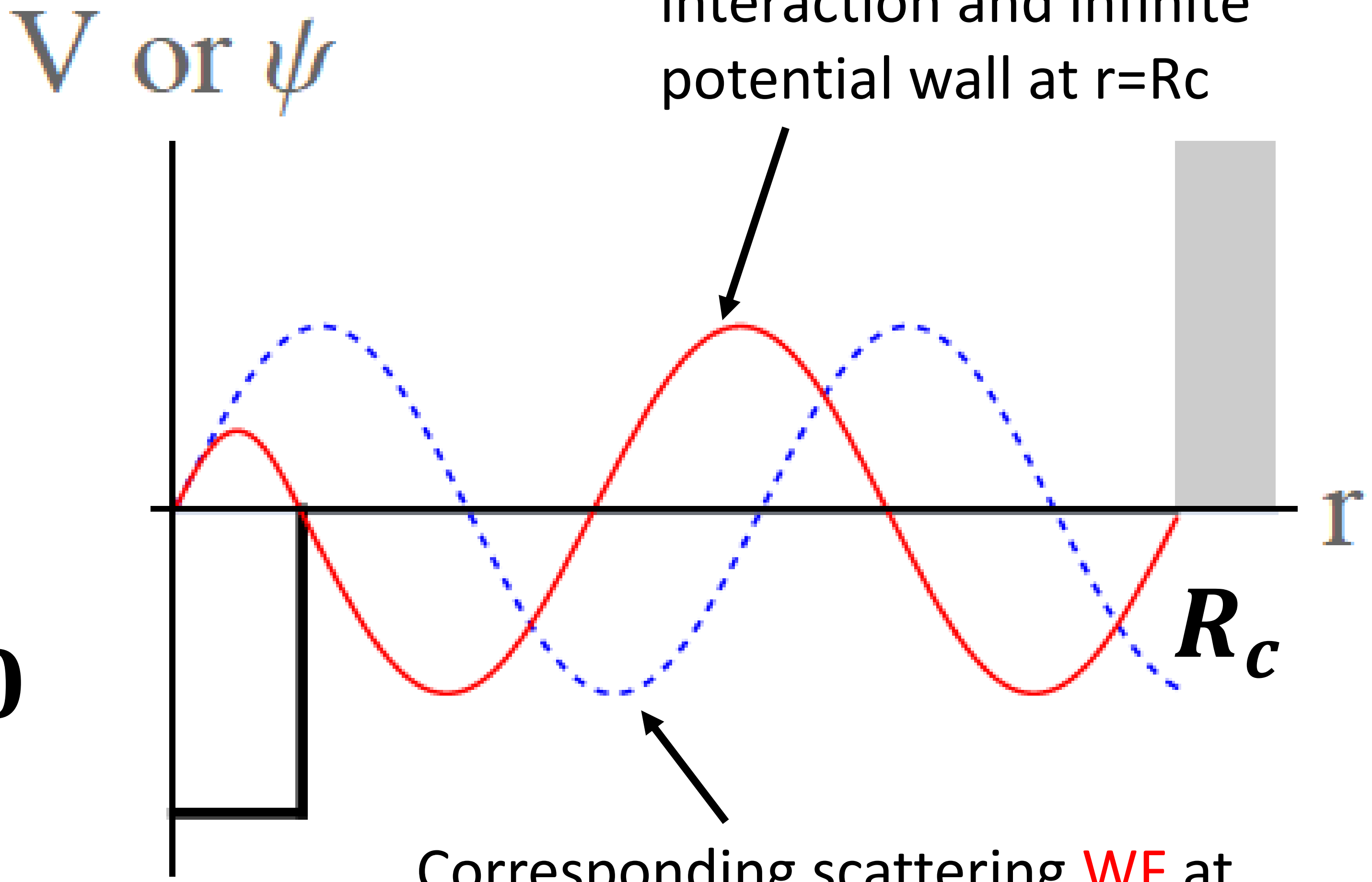
Cavity boundary condition (for relative motion)



$$\tan\delta_l \times n_l(kR_c) + j_l(kR_c) = 0$$

I.e., $(E, R_c) \rightarrow \delta_l(E)$

Scattering wave function (WF) at **E** with strong-interaction and infinite potential wall at r=Rc



Corresponding scattering WF at **E** in free space without any potential

However trapping nucleons using harmonic potential is well suited for nuclear calculations

- Reduces DOF → enable ab initio calculations
- Decouples the center of mass (CM) and internal DOFs
- Preserves rotational invariance

A different perspective: computer experiment

V_s

Continuum

Trap them in $\frac{1}{2} M_N \omega_T^2 r^2$ potential
within ab initio calculations

Bound State

Constrain EFT (or model on V_s) and use it to compute scattering and reaction

A universal formula at low energy→ BERW (Busch) formula

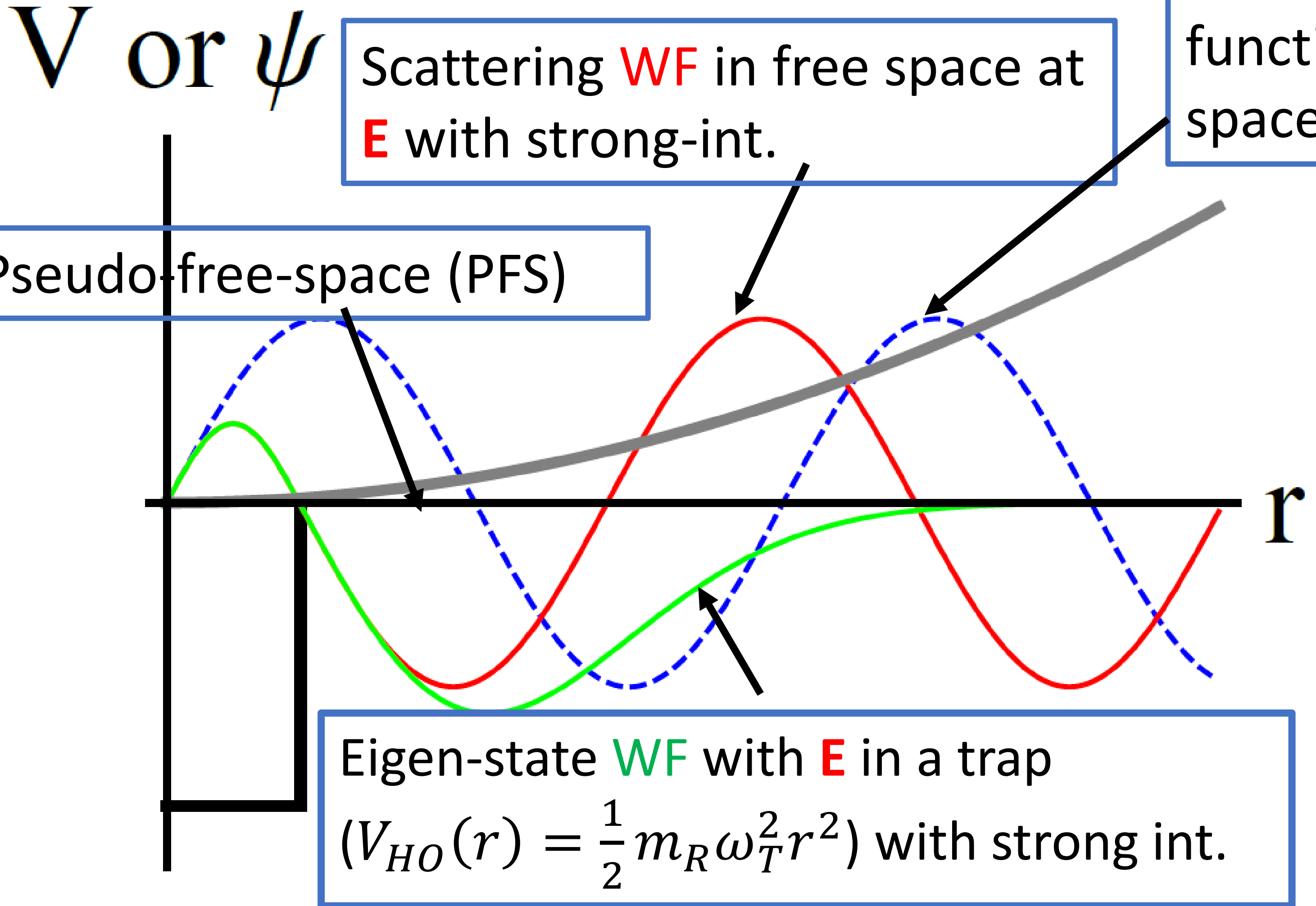
$$(E, \omega_T) \rightarrow \delta_l(E)$$

BERW formula: intuition

Busch, et.al., (1998); Blume & Greene (2002); Block & Holthaus (2002); Bolda, et.al., (2002); Stetcu, et.al., (2007, 2010); Luu, et.al., (2010).

$$p^{2l+1}cot\delta_l = (-1)^{l+1}(4\, M_R\omega_T)^{l+1/2}\frac{\Gamma(\frac{3}{4}+\frac{l}{2}-\frac{E}{2\omega_T})}{\Gamma(\frac{1}{4}-\frac{l}{2}-\frac{E}{2\omega_T})}$$

Suppose we know the eigen-energy (E) of the sys. in a trap for s-wave.



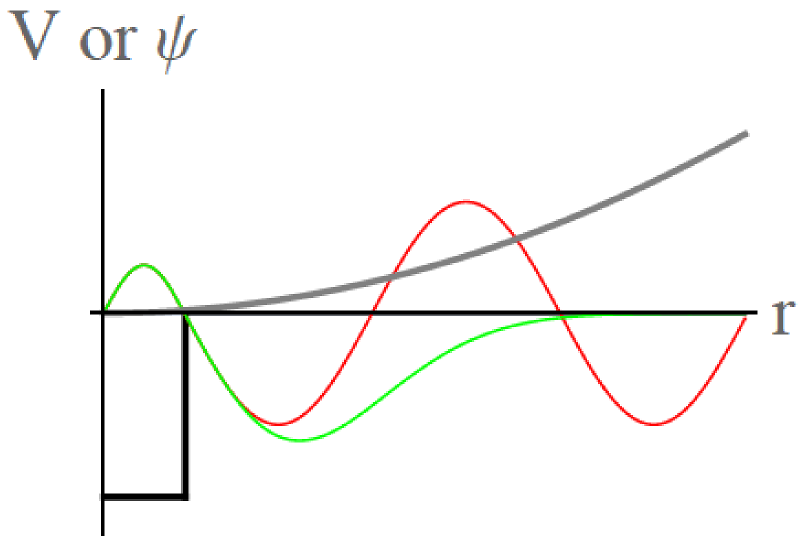
- The full WF dies off at large r. Integrate Schrodinger eq. inward → WF outside strong int. range. I.e., it is determined by **E** and ω_T.

$$\left[-\frac{\partial_R^2}{2m_R} + V_{HO}(r)\right]\psi(r) = E\psi(r)$$

- At PFS, the full WF is close to the scatt. WF, $\cos\delta\, j_0 + \sin\delta\, n_0$
- Matching them → BERW formula
- **BERW: left side → strong int.; right side [U(E)]→ (bound. cond.) long-dis. physics**

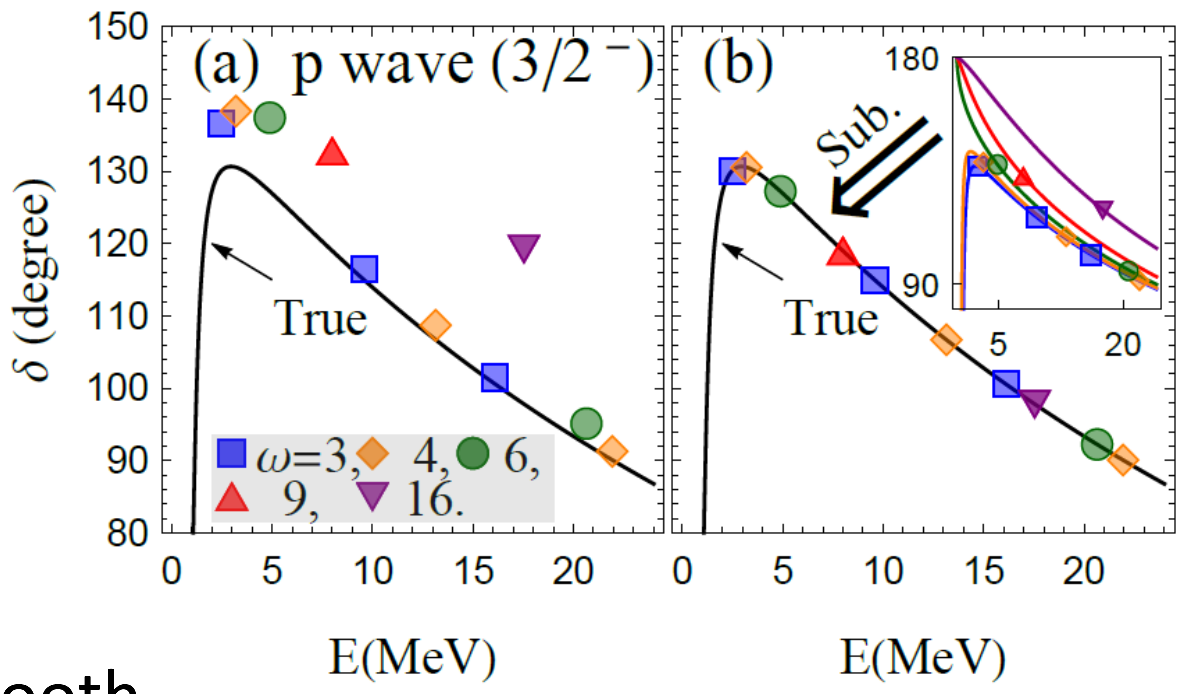
XZ, PRC.101.051602(R) (2020) [1905.05275]

BERW formula: the issue



However, PFS is not real free space.

$n-\alpha$ two-body potential model



- ω_T^2 dependence of extracted $\delta(E)$ is smooth
- Modify BERW's left side→ generalized effective range expansion (GERE)

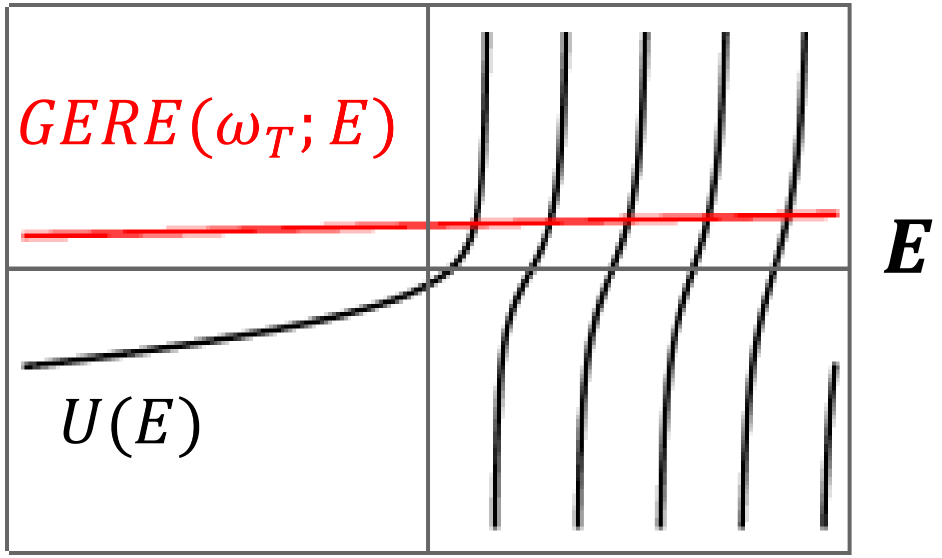
$$\sum_{i,j=0}^{+\infty} C_{i,j}(M_R\omega_T)^{2i}p^{2j} = U(E)$$

The perfect computer expt. (no errors!)

Quantization conditions:

$$\sum_{i,j=0}^{+\infty} C_{i,j}(M_R\omega_T)^{2i}p^{2j} = U(E)$$

$$p^{2l+1}cot\delta_l = \sum_{j=0}^{+\infty} C_{i=0,j}p^{2j}$$

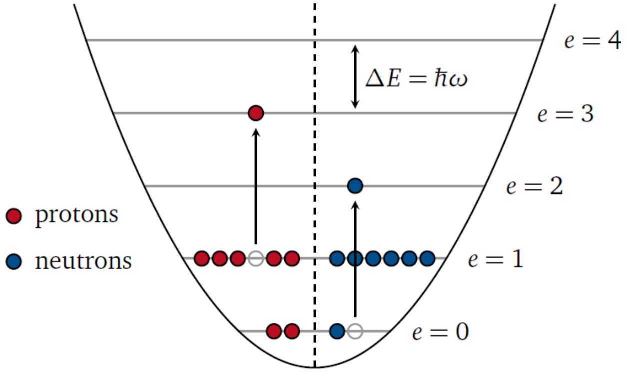


C n → Trap them within ab initio calculations

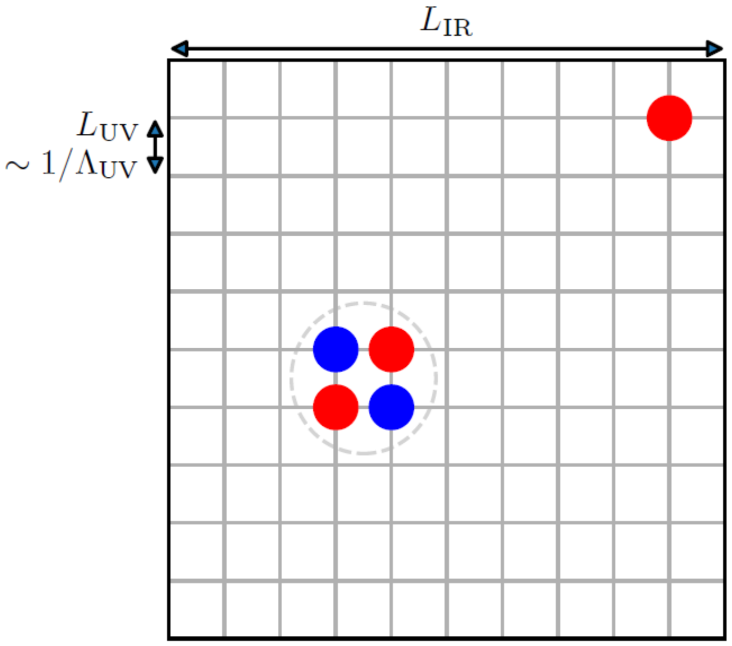
Bound State

→ U(E) at E → Fit them using GERE expansion → $C_{i=0,j}$ gives phase shift as func. of E

Imperfect expts: ab-initio calculations have truncations on Hilbert-space (regulator)



- Use two harmonic-oscillator-WF-based ab intio methods
  - NCSM : E < $N_{max}\ \omega$; IMSRG : e < $e_{max}\ \omega$
- Regulators modify both IR (long distance) and UV (short-distance) physics→ systematic errors
- To model the IR impact → change U function
- To model the UV impact→ the extracted GERE parameters $C_{i,j}$ depends on the resolution scale Λ_{uv}
- $C_{i,j}\ (\Lambda_{uv}) \xrightarrow{\Lambda_{uv}\to\infty}$ **reality**



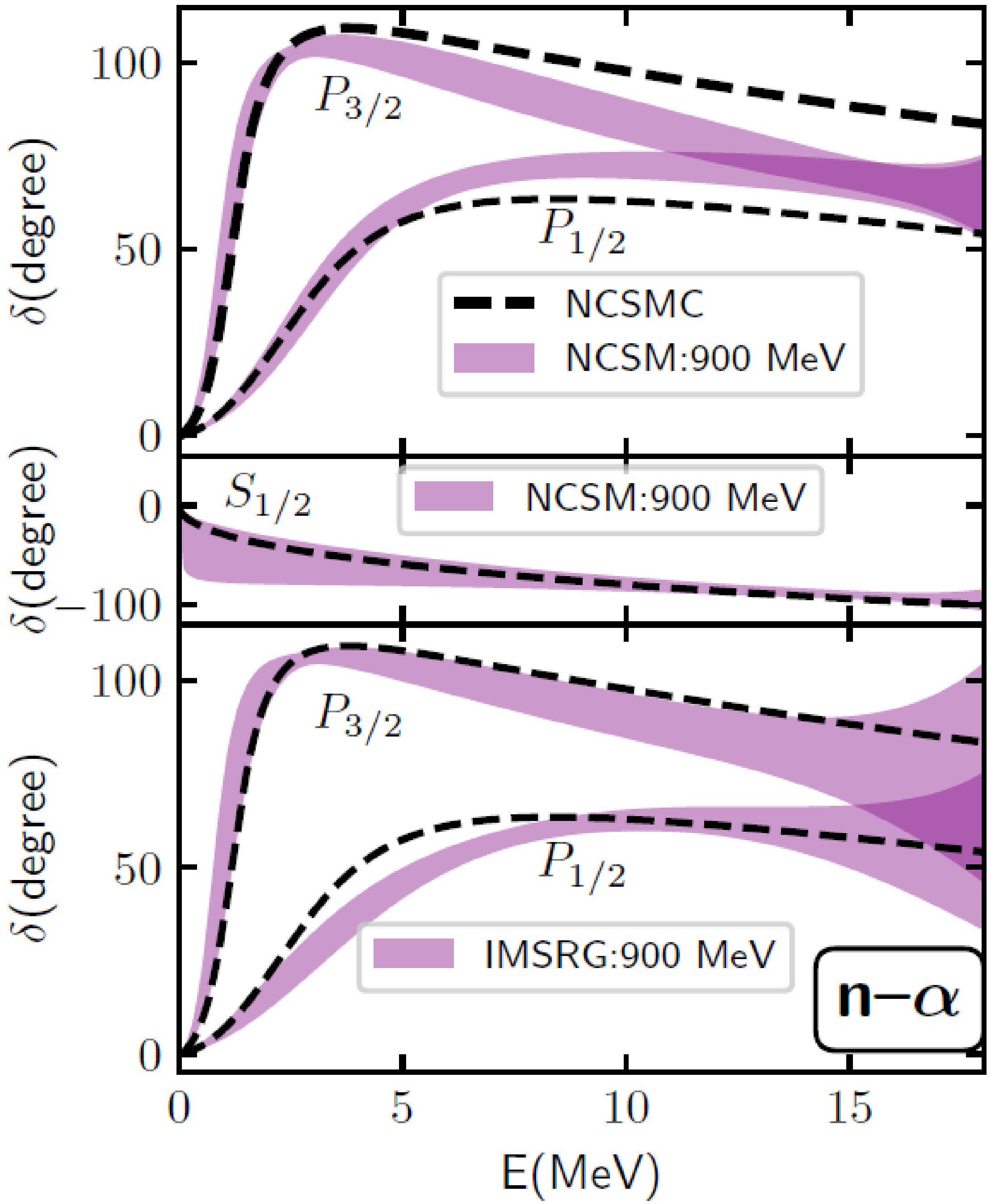
Ok, does it work?

Two sets of results based on NCSM and IMSRG output

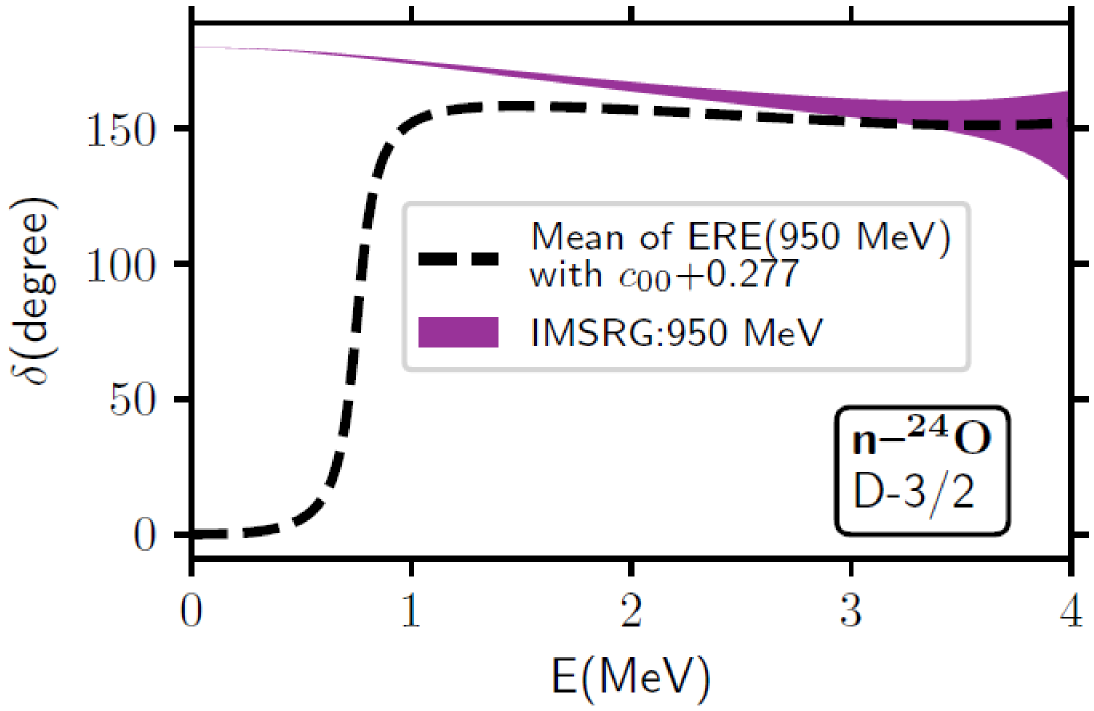
n-α scatterings in s and p waves

- The NCSM extraction agrees with NCSMC below 5 MeV
- The IMSRG agrees with NCSMC in p-3/2 but not in p-1/2
- Results at different Λ_{uv}

N: NCSM, IM: IMSRG,
Dashed line: NCSM+continuum



n-O24 scattering in d-3/2 channel



- Exists a low-energy bound state with 75% prob. and BE = −1.4 $\pm$ 0.54 MeV
- Use the mean value of Cs(950 MeV) and increase C00 by about 0.28→ dashed curve (res. at 0.75 MeV and Γ = 135 keV, close to expt. info.).
- Tuning nucleon int. could improve the prediction

Summary and outlook I

- The Luscher approach is modified for using traps
- Benchmarks: n-α scatterings
- Works for heavier systems heavier: n- O24 scattering
- Report results as functions of UV resolution scale

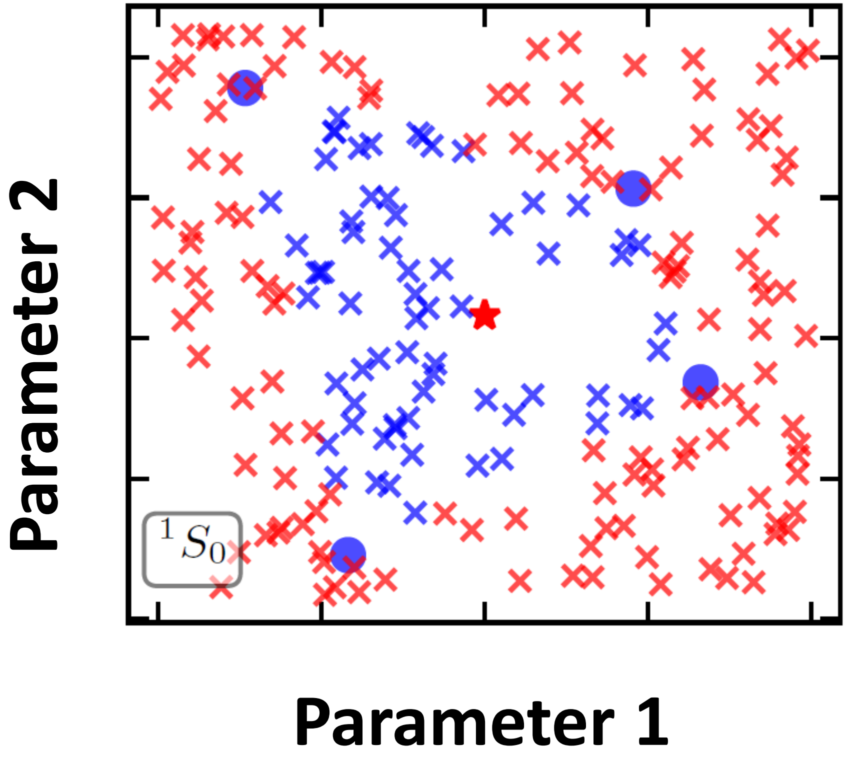
- Reduce the error bars
- Generalization for charged-particle scattering and reactions
- Apply GFMC to compute trapped systems
- And…

How about three-cluster system?

Emulators could open one avenue.

Emulator

- Compute model prediction many times in model fittings and error propagations (Bayesian inference and χ^2)
- About 10^6 samplings in my various studies.
- A bottleneck issue: computation time
- Need efficient and accurate emulators for models (training points in blue dots)



“Efficient emulators for scattering using eigenvector continuation”

R. J. Furnstahl, A. J. Garcia, P. J. Millican, and XZ ,
PLB **809,** 135719 (2020) [2007.03635]

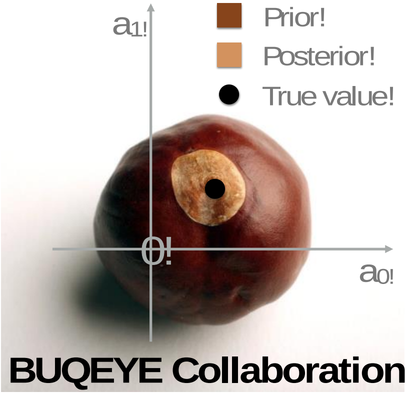
My S@INT seminar talk is available online.
(https://sites.google.com/uw.edu/int/seminars/sint)
Or search online for “INT seminar Xilin Zhang”.

Bayesian inference in low energy nuclear phy.

One main paradigm since 90s:

QCD, LQCD → Chiral EFT for NN and NNN (L(N,pi; **C**))

Study EFT truncation errors: infinite para. Space to finite one



https://buqeye.github.io

Few-nucleon systems

- Bound state
- Scattering/reactions

Many-nucleon systems

- Compact nuclei
- Dripline nuclei
- scattering/reactions

Bayesian Analysis of Nuclear Dynamics (BAND) Framework
https://bandframework.github.io/

Need emulators for bound state and scattering

One main program

FRIB

Emulators could enable

- an ab initio calculation of scattering/reactions
- Fit Chiral NN from LQCD

Eigenvector continuation (EC)

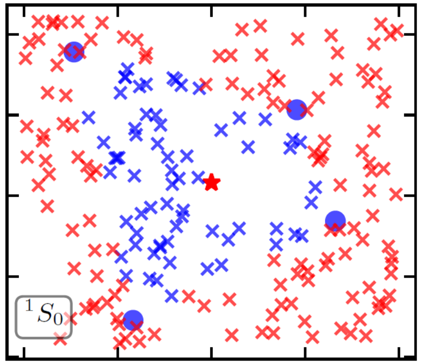
D. Frame, et.al., *Eigenvector continuation with subspace learning*, *PRL* 121 (2018) 3, 032501

$$\widehat{H}(\boldsymbol{\theta}) = \widehat{T} + \widehat{V}(\boldsymbol{\theta})$$

$$\widehat{H}(\boldsymbol{\theta}_i) \rightarrow |\psi_{\mathrm{gs}}(\boldsymbol{\theta}_i)\rangle$$

The traced wave functions (WFs) along $\boldsymbol{\theta}$ trajectory in parameter space lives in a low-dimension space

EC emulator for bound state calculations



$$|\psi_{\rm trial}\rangle = \sum_{i=1}^{N_b} c_i |\psi_{\rm gs}(\boldsymbol{\theta}_i)\rangle$$

$$\delta\left[\langle\psi_{\rm trial}|\widehat{H}(\boldsymbol{\theta})|\psi_{\rm trial}\rangle - \lambda(\langle\psi_{\rm trial}|\psi_{\rm trial}\rangle - 1)\right] = 0$$

$$\sum_k (H_{jk} - \lambda N_{jk}) c_k = 0$$

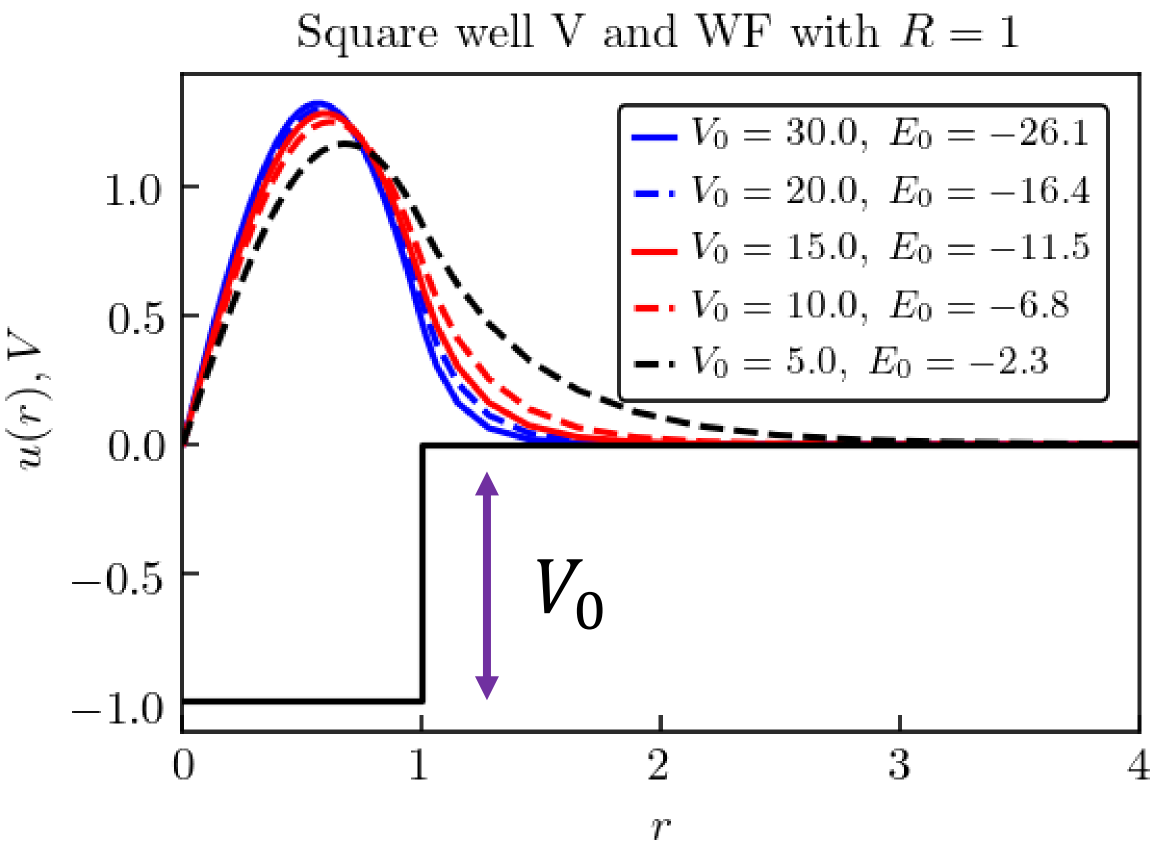
N_b-dim linear algebra

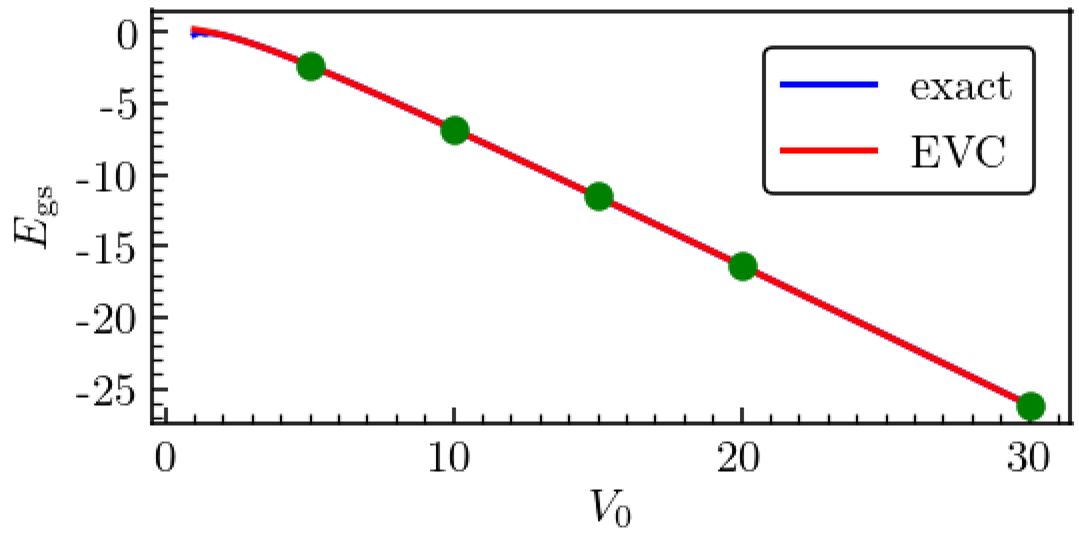
$$H_{ij}(\boldsymbol{\theta}) \equiv \langle\psi_{\rm gs}(\boldsymbol{\theta}_i)|\widehat{H}(\boldsymbol{\theta})|\psi_{\rm gs}(\boldsymbol{\theta}_j)\rangle \quad \text{and} \quad N_{ij} \equiv \langle\psi_{\rm gs}(\boldsymbol{\theta}_i)|\psi_{\rm gs}(\boldsymbol{\theta}_j)\rangle$$

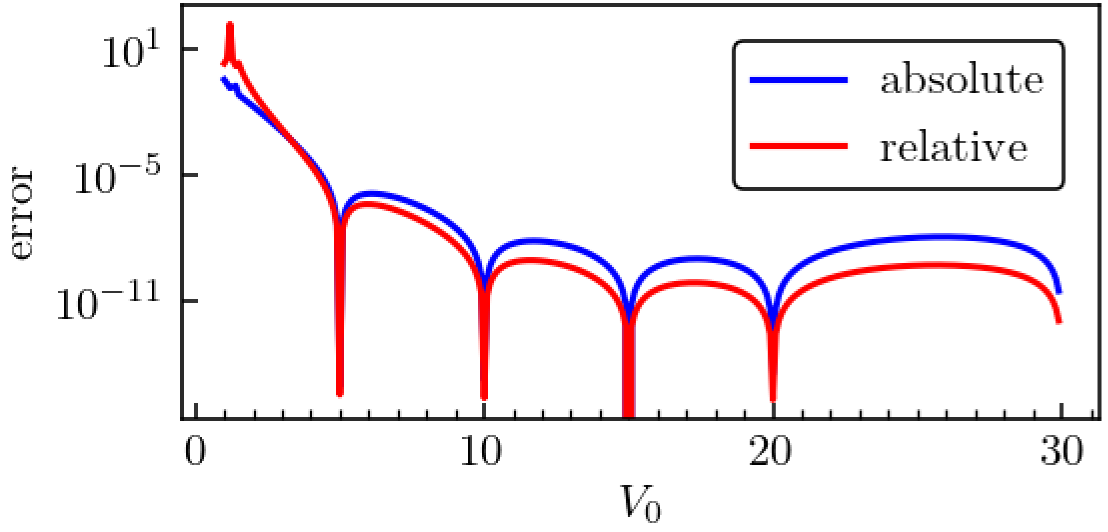
Ground state energy (λ)

Ground state WF (c_k)

EC emulator for bound state: square well







EC emulator for bound state: many-body calculations

S. König, A. Ekström, K. Hebeler, D. Lee, A. Schwenk
Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantification
arXiv:1909.08446

A. Ekström and G. Hagen
Global sensitivity analysis of bulk properties of an atomic nucleus
PRL **123** (2019) 25, 252501, 1910.02922

"about 1 Million sample in 16-dim space, 20 years calculation → 1 hour on a standard laptop."

Kohn variational method for scattering

$$\beta[u_{\mathrm{t}}] = \tau_{\mathrm{trial}} - \int_0^\infty dr\, u_{\mathrm{t}}(r) D u_{\mathrm{t}}(r)$$

$$D \equiv -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + U(r) - p^2$$

$$u_{\mathrm{t}}(r) \underset{r\to\infty}{\longrightarrow} \frac{1}{p}\sin(pr - \frac{1}{2}\ell\pi) + \tau_{\mathrm{trial}}\cos(pr - \frac{1}{2}\ell\pi)$$

$$\beta[u_{\mathrm{exact}}] = \frac{1}{p}[\tan\delta_\ell(E)]_{\mathrm{exact}}$$

$$\delta\beta = \delta\tau - \int_0^\infty dr\, u_{\mathrm{exact}}(r) D\delta u(r) + \mathcal{O}(\delta u^2)$$

$$\delta\beta = 0 + \mathcal{O}(\delta u^2)$$

Emulators for two-body scattering: Kohn + EC

$$u_t(r) = \sum_i c_i u_i(r; E)$$

u_i : scattering WFs of $\widehat{H}(\boldsymbol{\theta}_i)$

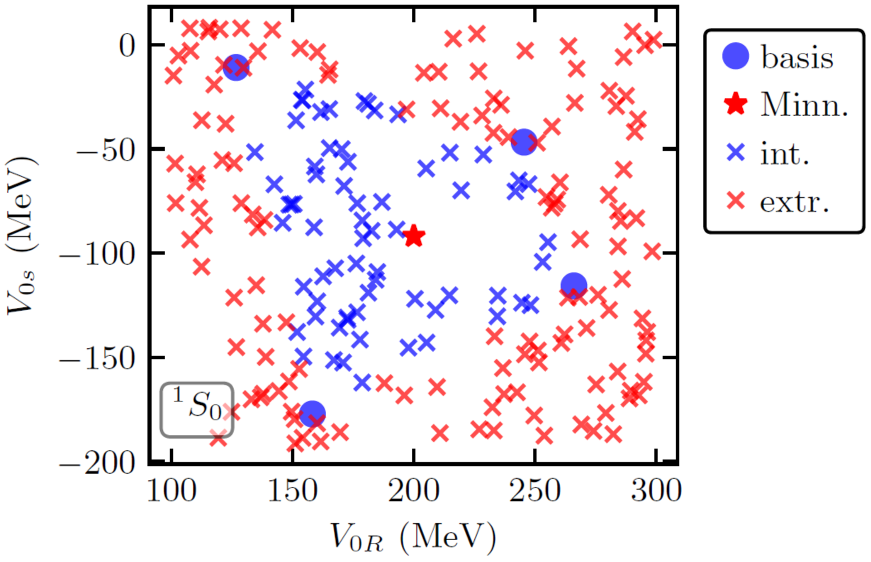
$$u_t(r) \underset{r\to\infty}{\longrightarrow} \left(\sum_{i=1}^{N} c_i\right) \frac{1}{p} \sin(pr - \frac{1}{2}\ell\pi) + \left(\sum_{i=1}^{N} c_i \tau_i\right) \cos(pr - \frac{1}{2}\ell\pi)$$

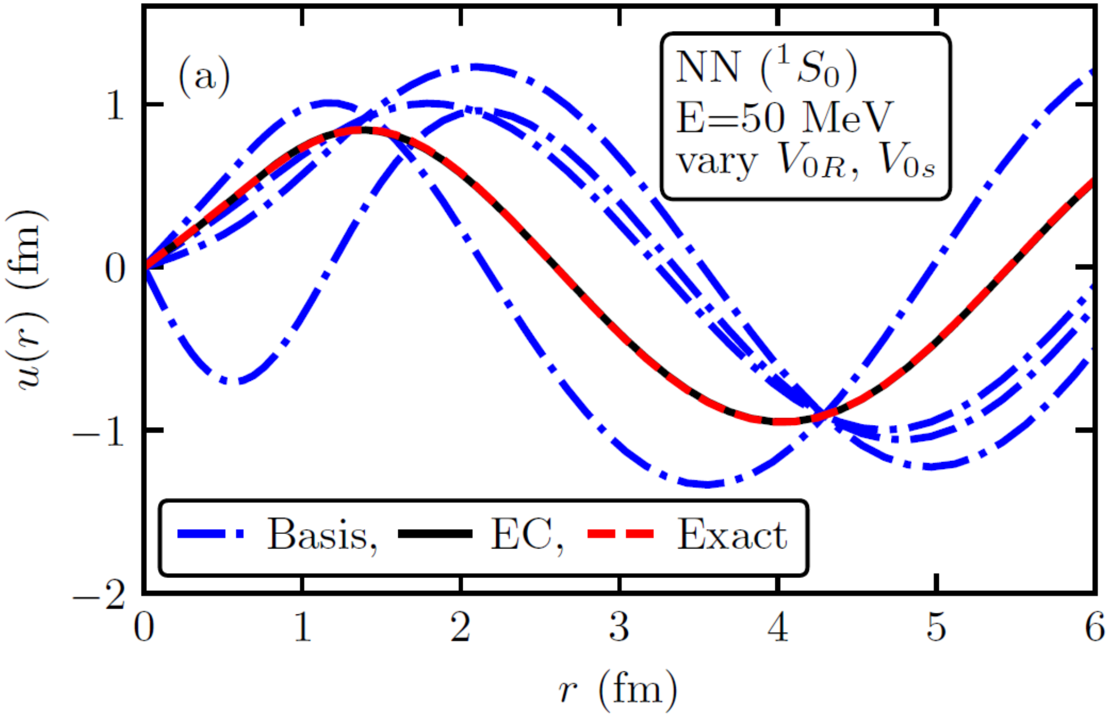
$$\sum_j \left(\Delta U^\intercal + \Delta U\right)_{ij} c_j = \tau_i - \lambda$$

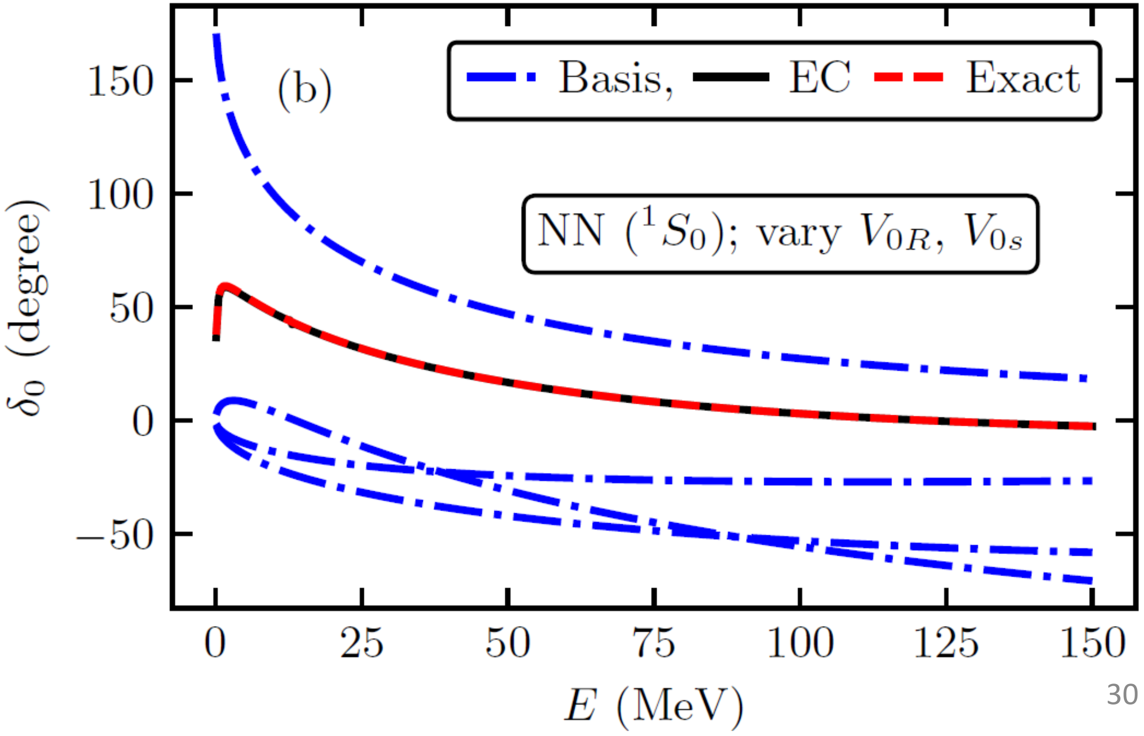
$$\Delta U_{jk} \equiv \int_0^\infty dr\, u_j(r; E)(2\mu)\left[V(r; \boldsymbol{\theta}) - V_k(r)\right] u_k(r; E)$$

- N_b-dim linear algebra
- The long-range part cancelled
- Reduce comp.

Tests of the emulators: NN scattering

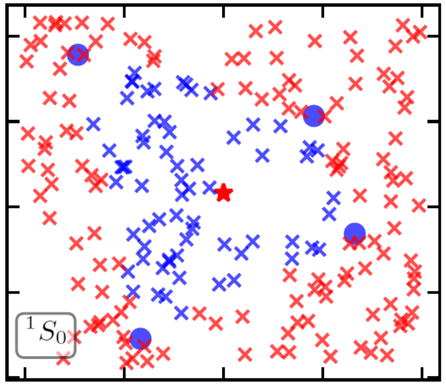






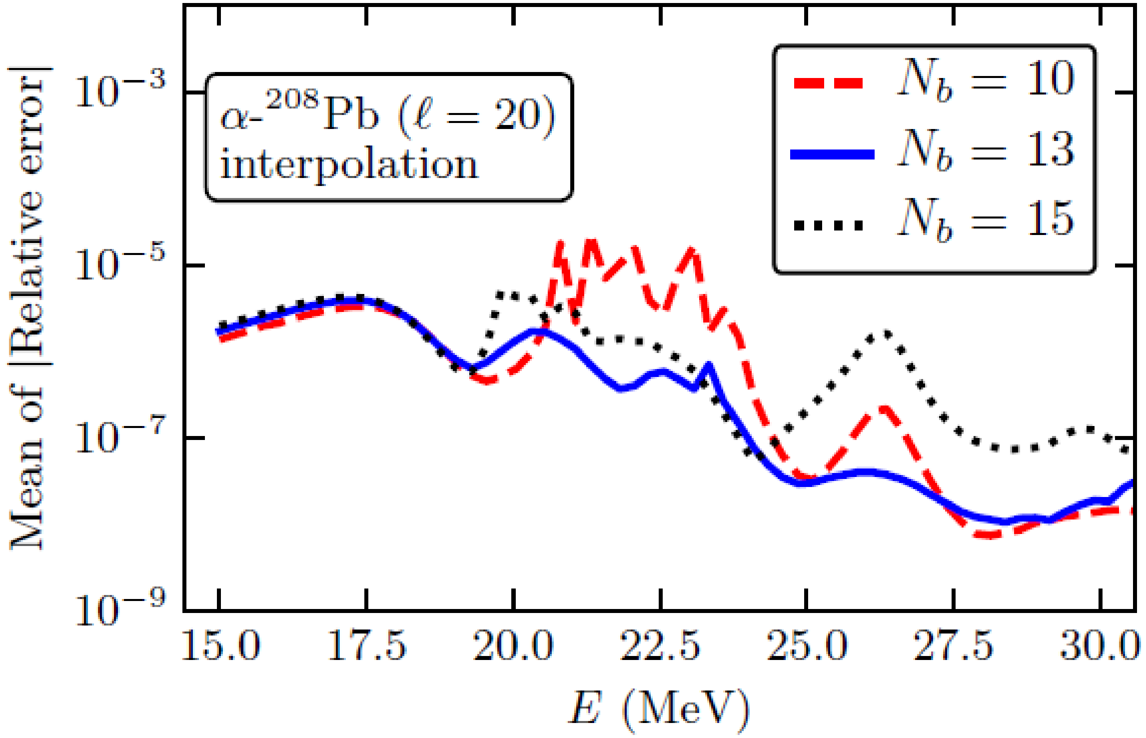
$$V_{^1S_0}(r) \equiv V_{0R}e^{-\kappa_R r^2} + V_{0s}e^{-\kappa_s r^2}$$

Tests of the emulators: alpha-Pb scattering



$$V(r) = V_0\ f(r, R_R, a_R) + iW_0\ f(r, R_I, a_I)$$

Wood-Saxon form



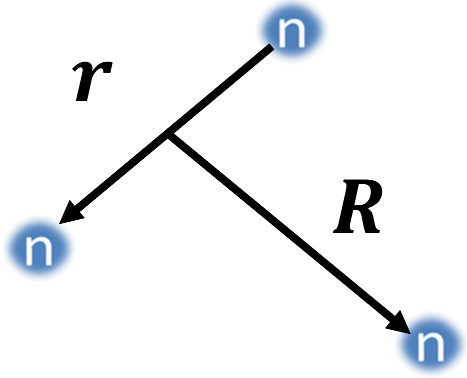
$$V_0 = -100 \text{ MeV} \quad W_0 = -10 \text{ MeV}$$

$$\boldsymbol{\theta}_i = \{V_0, W_0\}$$

Vary parameters by +- 50% around the “best” values.

Generalization to coupled channel is straightforward and ongoing.

Generalization to three-body scattering: below breakup threshold



$$H = T_r + T_R + V_{2-body} + V_{3-body}$$

For indistinguishable particles:

$$\Psi(\boldsymbol{r}, \boldsymbol{R}) \xrightarrow{R\to\infty} \phi_b(\boldsymbol{r}) \left[\frac{1}{P}\sin\left(PR - \frac{l\pi}{2}\right) + \tau\cos\left(PR - \frac{l\pi}{2}\right)\right]$$

$$\beta[\psi_t] = \tau_t - 2\mu\langle\psi_t|\hat{H}(\boldsymbol{\theta}) - E|\psi_t\rangle$$

Generalization to three-body scattering: above breakup threshold

KOHN VARIATIONAL PRINCIPLE FOR THREE-PARTICLE SCATTERING*

J. Nuttall
Texas A & M University, College
(Received 30 June 196

The Kohn variational principle is extended to apply t
particle bound state is broken up by a third particle.

Few-Body Systems 30, 39–63 (2001)

Few-Body Systems

PHYSICAL REVIEW D VOLUME 5,

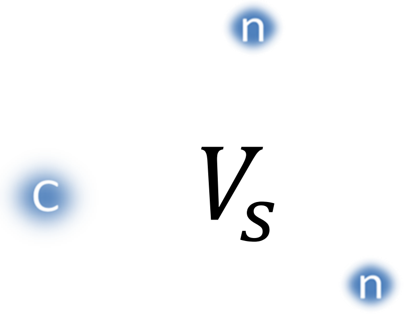
Kohn-Type Variational Principle fo

M. Lieber,† Leonard Ros
Department of Physics, New York
(Received 2

The Kohn Variational Principle for Elastic Proton-Deuteron Scattering Above Deuteron Breakup Threshold*

M. Viviani[1], A. Kievsky[1], and S. Rosati[1,2]

Fit three-cluster V_s to experimental data and ab initio results using EC emulators



Fit Chiral 3N force from data and LQCD results using EC emulators

PHYSICAL REVIEW VOLUME 87, NUMBER 3 AUGUST 1, 1952

Variational Methods for Periodic Lattices*

W. Kohn†
Carnegie Institute of Technology, Pittsburgh, Pennsylvania, and Institute for Theoretical Physics, Copenhagen, Denmark
(Received April 21, 1952)

The problem of finding the propagating solutions of the Schrödinger equation in periodic lattices is formulated as a variational principle. This may be used as a starting point to establish the general properties of bands. Furthermore it is shown that by introducing various approximations into the variational principle, the chief existing approximation methods can all be derived from it. Improvements of these methods are suggested. Numerical illustrations are presented and the possibilities of the variational method for more accurate calculations of the energy bands of solids are discussed.

Summary and outlook II

- The EC emulators for scattering are efficient and accurate in various two-body scattering cases

- Ongoing generalizations to 3-body systems (coupled-channels, too)

- Applications in fitting and error propagations:
  - Chiral 3N interactions against experimental data (e.g., Nd) and LQCD results
  - nuclear optical potentials against data
  - cluster-cluster interactions to ab initio calculations using traps