Generalized Luscher method: an avenue for ab initio calculation of low-energy nuclear scattering and reactions

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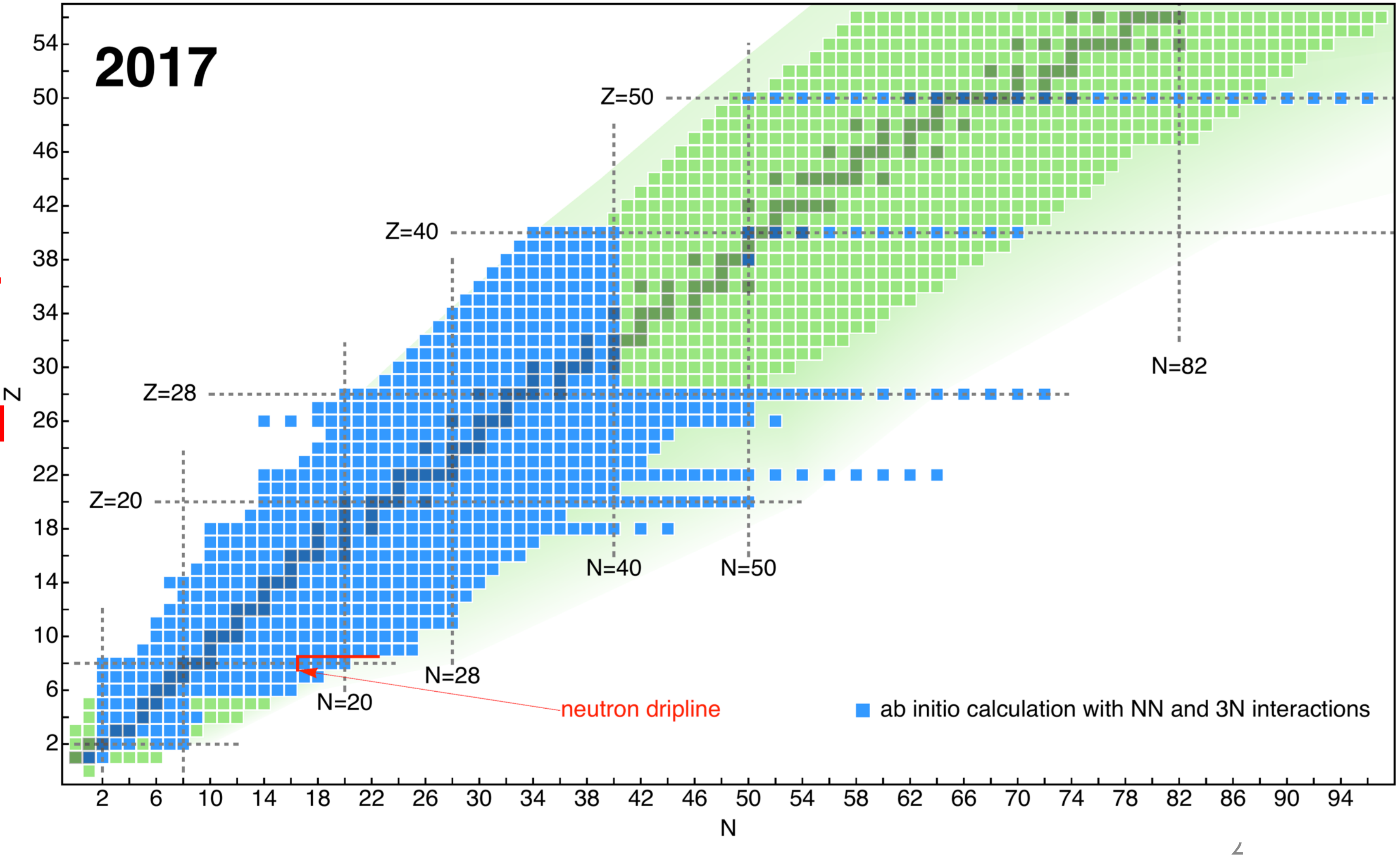
In collaboration with J. Melendez, and R. Furnstahl

The question

- Ab initio structure calculations have made amazing progress, while scattering/reactions are limited
- **Can we take advantage of this bound-state-calculation's progress and compute scattering/reactions?**
- Drip-line nuclei needs consistent treatment of structure and scattering/reactions



Key idea

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

- Eigen-energies of trapped projectile-target system computed by ab initio energy calculation → scattering info (phase-shift) at those energies
- Interpolating between eigen-energies gives the scattering phase-shift as function of scattering energy
- **The method should work with nuclear systems (e.g., neutron-nucleus) that can be computed by the ab initio structure methods.**

Outline

- Our method generalizes the Luscher method used in Lattice QCD
  - Perfect computer experiment
  - Imperfect computer experiment
- Benchmark our scattering calculations against the existing ab initio calculation $(\mathrm{n}-\alpha)$
- Show it also works for heavier system $(\mathrm{n}-{}^{24}O$, as recently measured)
- Modeling of errors in the imperfect computer experiment
- Comparison to other methods
- Summary and Outlook: inelastic reactions, and role of R-matrix/potential model

Luscher's method in Lattice QCD

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

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

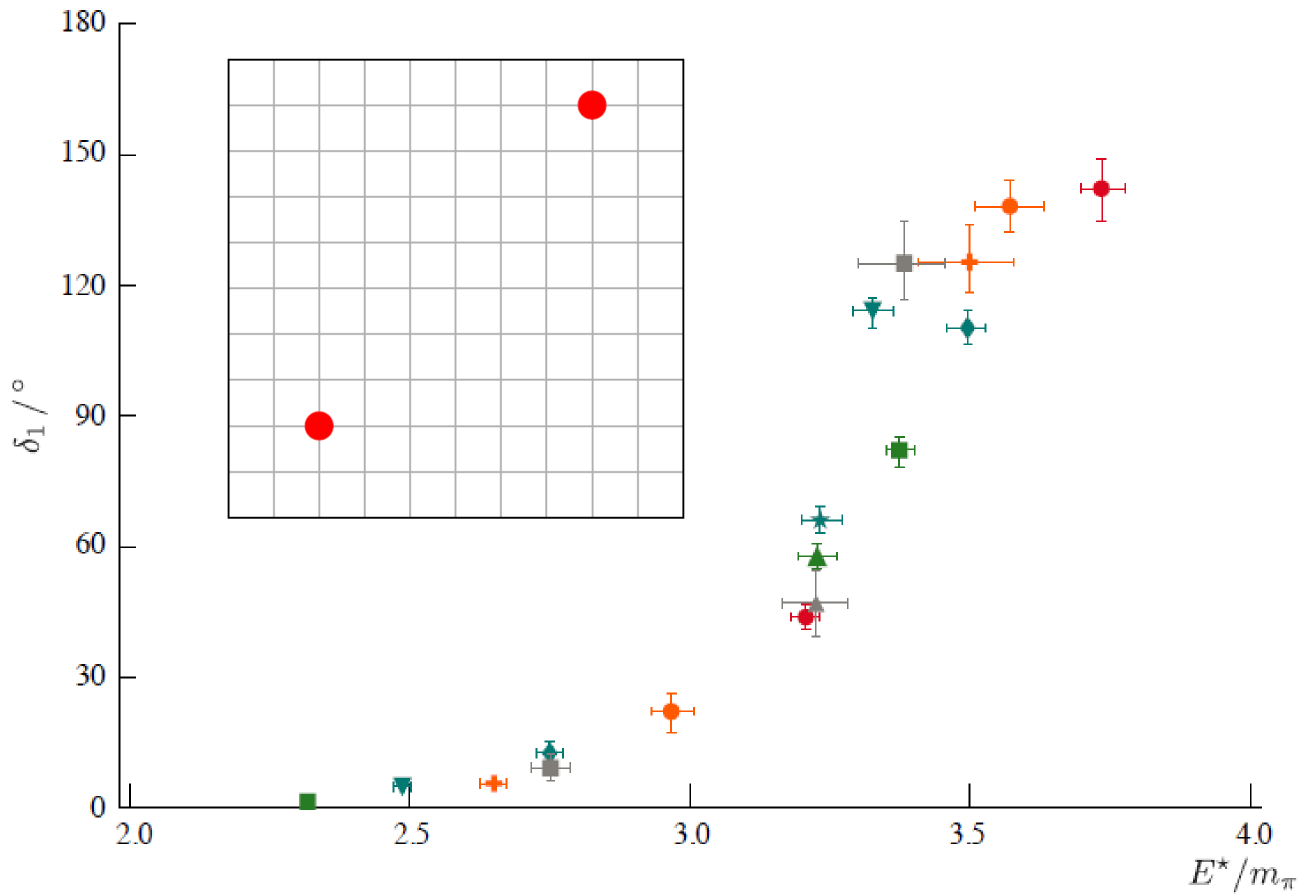


FIG. 14 Elastic $I = 1$ $\pi\pi$ scattering phase-shifts in P-wave determined from finite-volume spectra computed the same $m_\pi \sim 236$ MeV configurations as used in the calculation

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

However trapping nucleons in harmonic potential well is better suited for harmonic-oscillator-basis calculations

- Reduces degrees of freedom (DOF) → make ab initio calculations feasible
- The center of mass (CM) and internal DOF are **decoupled**
- Lattice regulator breaks rotational invariance

There is a "universal" formula for two-cluster system at low energy→ BERW (Busch) formula

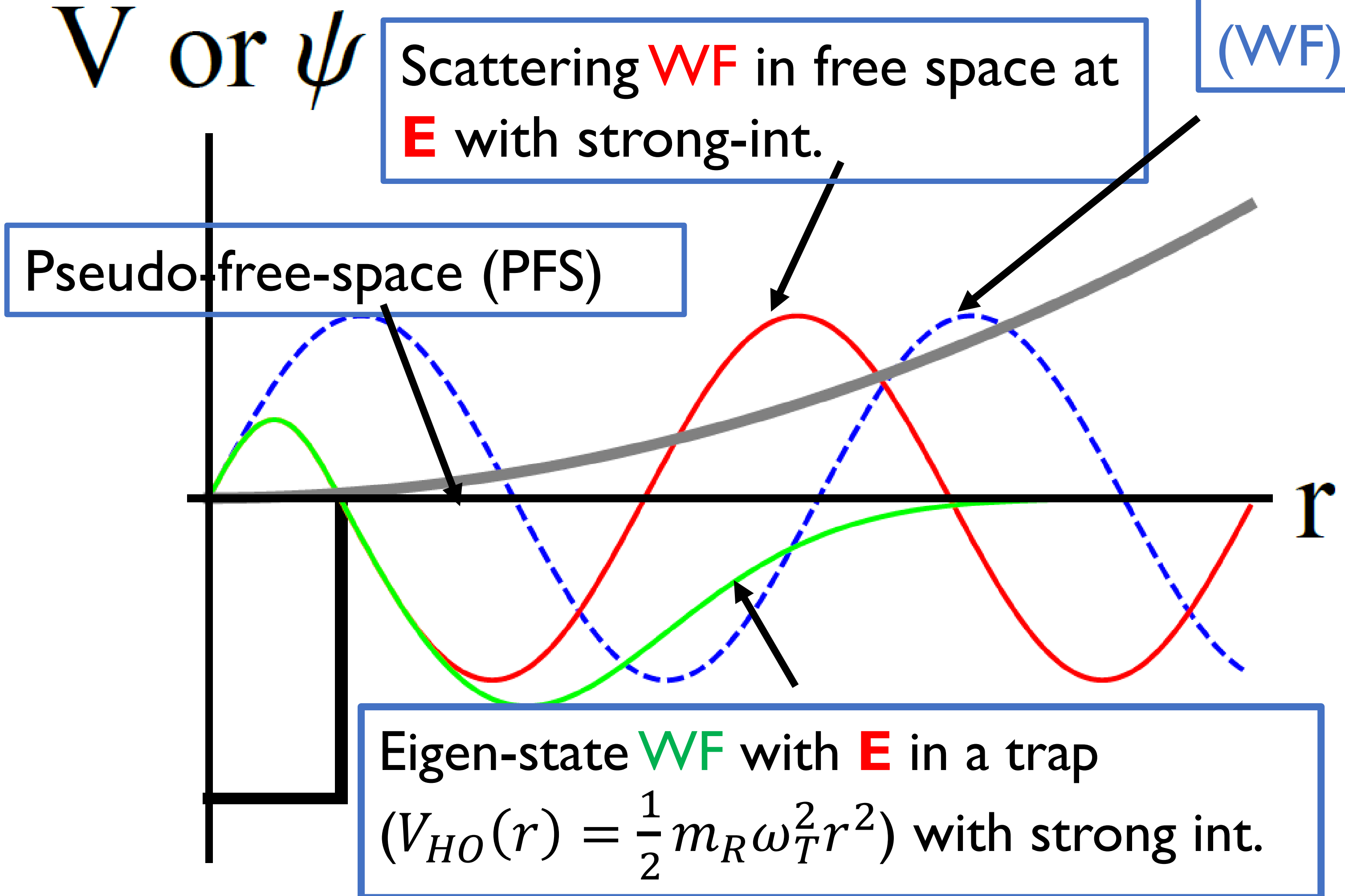
$$(E, \omega_T) \rightarrow \delta_l(E)$$

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).

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

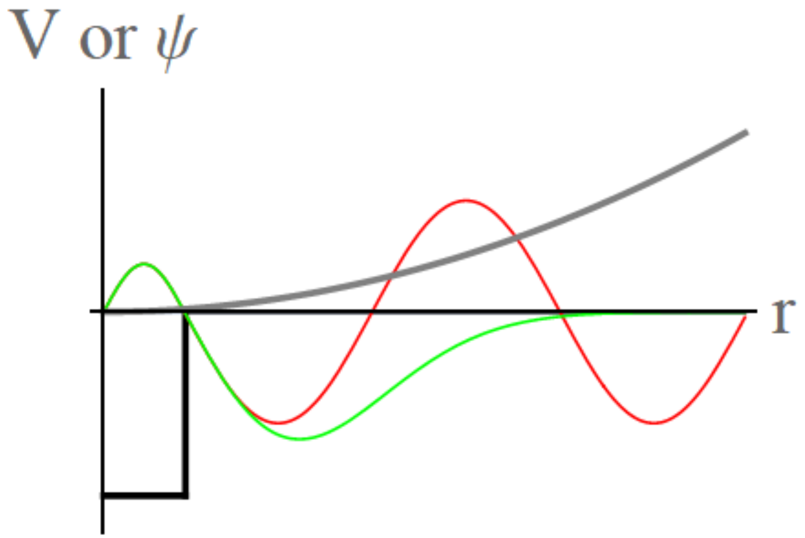
Suppose we know the eigen-energy (E) of the system in a trap for s-wave.



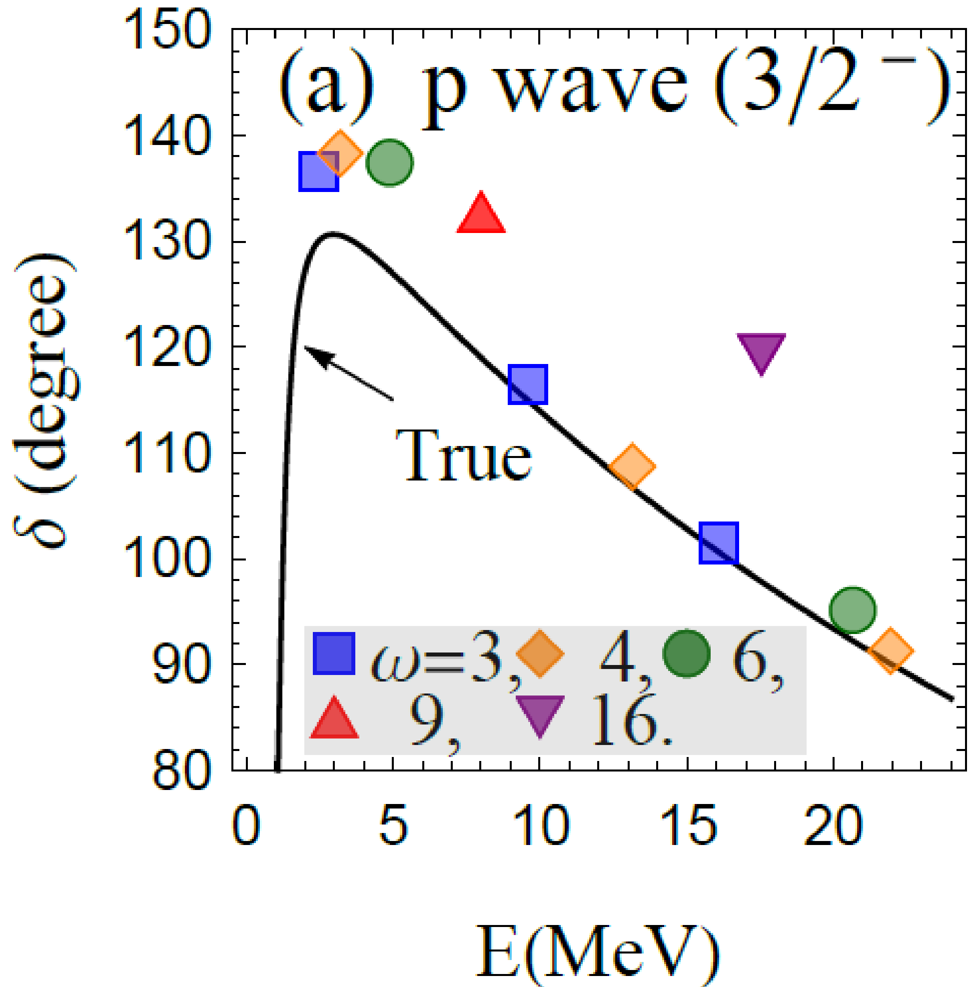
- The full WF dies off in a gaussian form. We can integrate Schrodinger equation from large distance inward, and get WF at PSF (i.e, WF determined by **E** and ω_T): $\left[-\frac{\partial_R^2}{2m_R} + V_{HO}(r)\right]\psi(r) = E\psi(r)$
- At PFS, at lowest order (or shallow trap limit, $\omega_T \to 0$), the full WF is close to the scattering WF with strong interaction: $\cos\delta\, j_0 + \sin\delta\, n_0$
- Matching them gives BERW formula
- **BERW: left side → strong int.;**
  right side→ (bound. cond.) long-dis. physics

XZ, 1905.05275.

BERW formula: the UV-defect



$n-\alpha$ two-body potential model



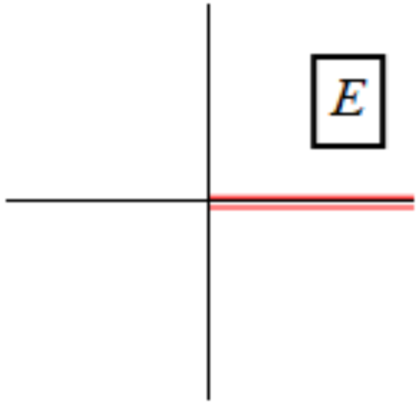
- However, PFS is not real free space.
- And how to separate the IR-physics (boundary condition) and the strong-interaction physics?
- Effective field theory (EFT) separates IR and UV in scattering amplitude

Cure the BERW formula with the UV-defect

- T-matrix in free space

$$S_l = e^{2i\delta_l} \rightarrow T_l \sim \frac{S_l - 1}{2i}$$

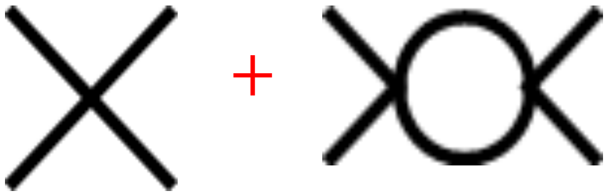
$$T(E) \sim \frac{1}{p^{2l+1} cot\delta_l - U(E)}$$



- Non-analyticity from IR physics: $U(E) = ip^{2l+1}$ (note $ip = \sqrt{-E}$)
- Analytical expansion from UV physics, i.e., effective range expansion (ERE):

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

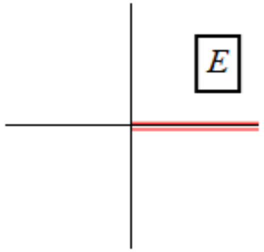
- EFT derivation :

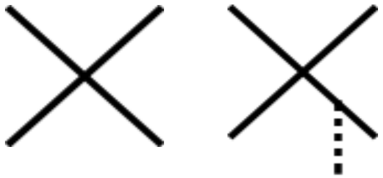


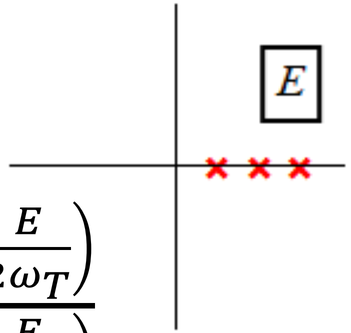
$+ \cdots$

Cure the BERW formula with the UV-defect

- In a harmonic trap: $U(E) = ip^{2l+1}$



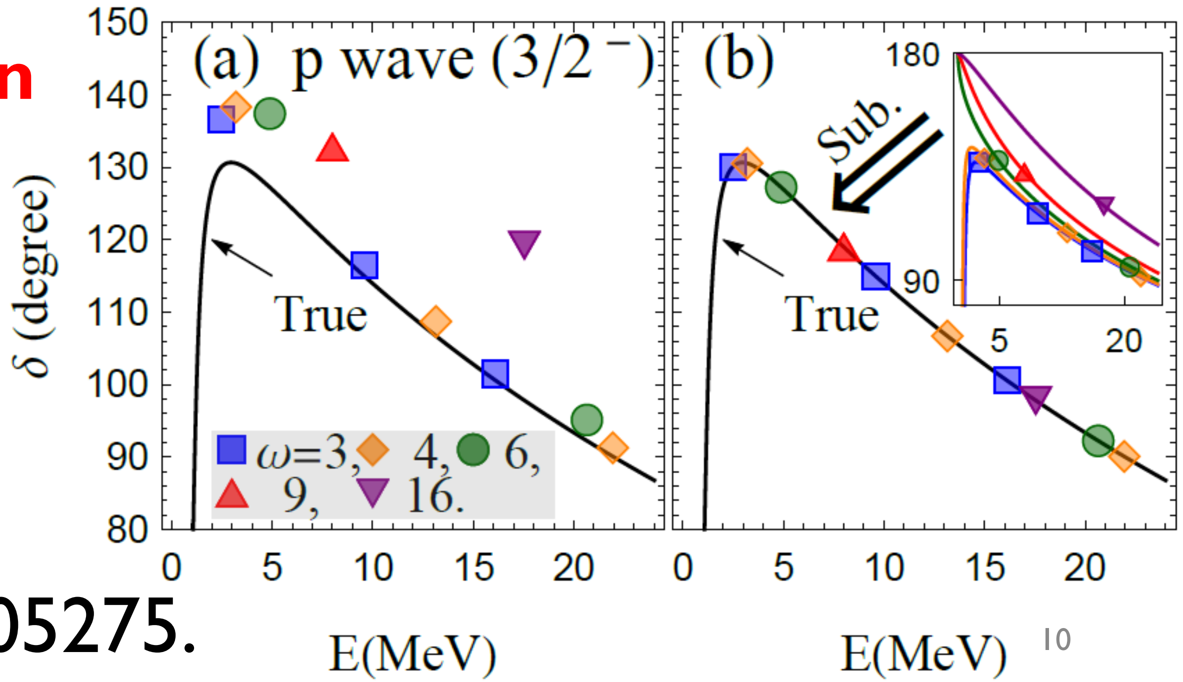

+ **loop diags :** $U(E) = (-1)^{l+1}(4\, M_R\omega_T)^{l+\frac{1}{2}} \frac{\Gamma\left(\frac{3}{4}+\frac{l}{2}-\frac{E}{2\omega_T}\right)}{\Gamma\left(\frac{1}{4}-\frac{l}{2}-\frac{E}{2\omega_T}\right)}$



- **Generalized ERE and quantization conditions**

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

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



XZ, 1905.05275.

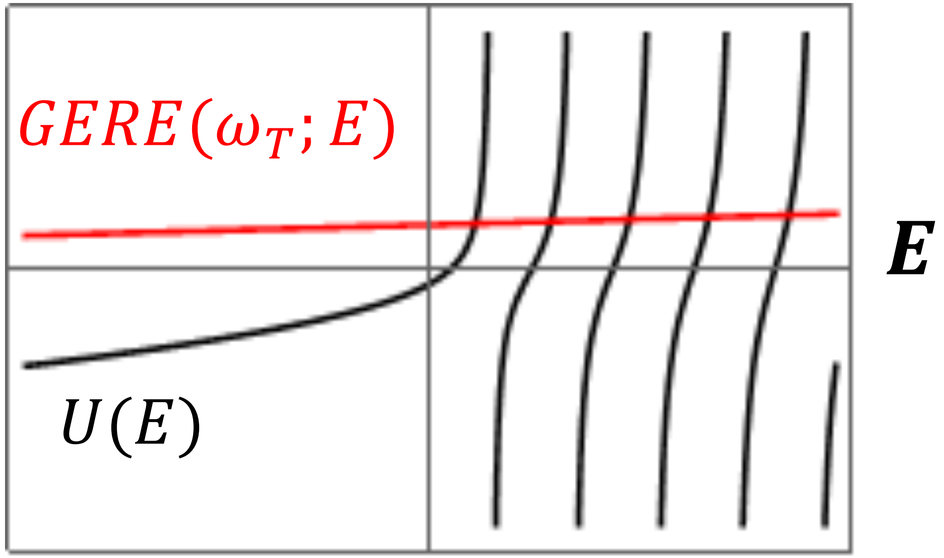
The perfect computer expt. (no errors!)

Quantization conditions:

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

$$U(E) = (-1)^{l+1}(4\,M_R\omega_T)^{l+\frac{1}{2}}\frac{\Gamma\left(\frac{3}{4}+\frac{l}{2}-\frac{E}{2\omega_T}\right)}{\Gamma\left(\frac{1}{4}-\frac{l}{2}-\frac{E}{2\omega_T}\right)}$$

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



C n

Trap them within ab initio calculations

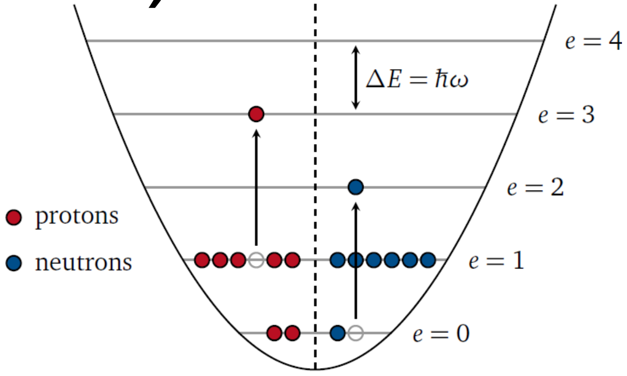
Bound State

U(E) at E

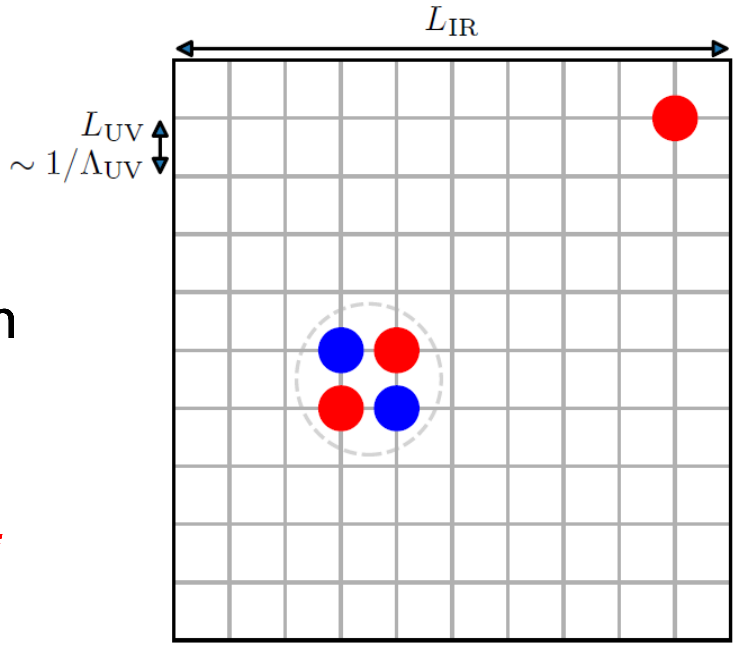
Fit them using GERE expansion

$C_{i=0,j}$ gives phase shift as func. of E

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



- Working with ab initio groups using harmonic-oscillator-wave-function as basis: NCSM and IMSRG
  - NCSM requires the total energy below $N_{max}\,\omega$ (ω as basis frequency)
  - IMSRG requires single particle energy below $e_{max}\,\omega$
- Regulators modify both IR and UV physics→ systematic errors
- To model the IR error? → modify U function with truncation on relative motion
- To model the UV impact→ the extracted GERE parameters $C_{i,j}$ becomes $C_{i,j}(\Lambda_{uv})$. $\boldsymbol{C_{i,j}(\infty)}$ **(Cont. limit), predicts reality**

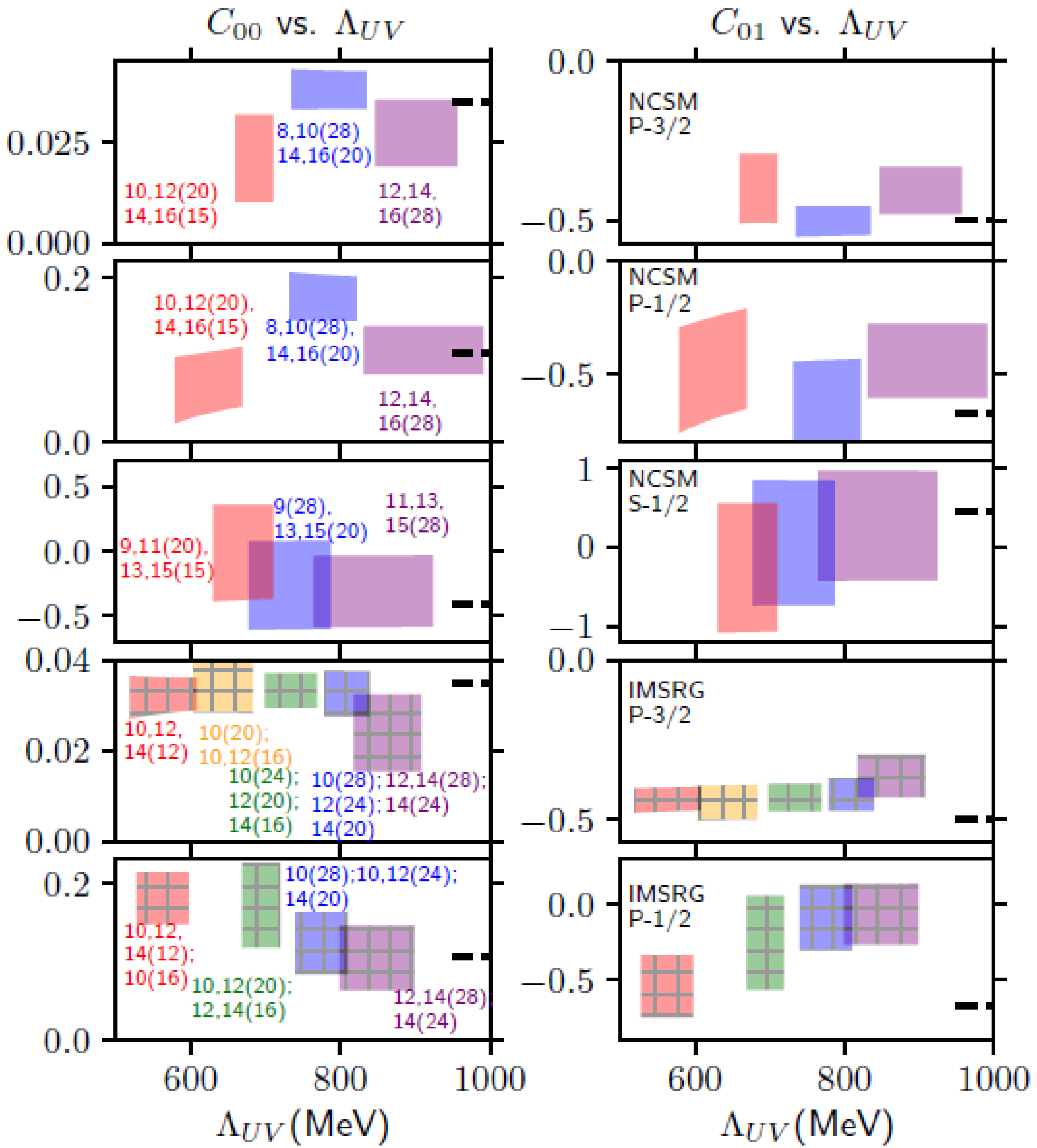


Before error analysis, let's first see results

Two sets of results based on NCSM and IMSRG output

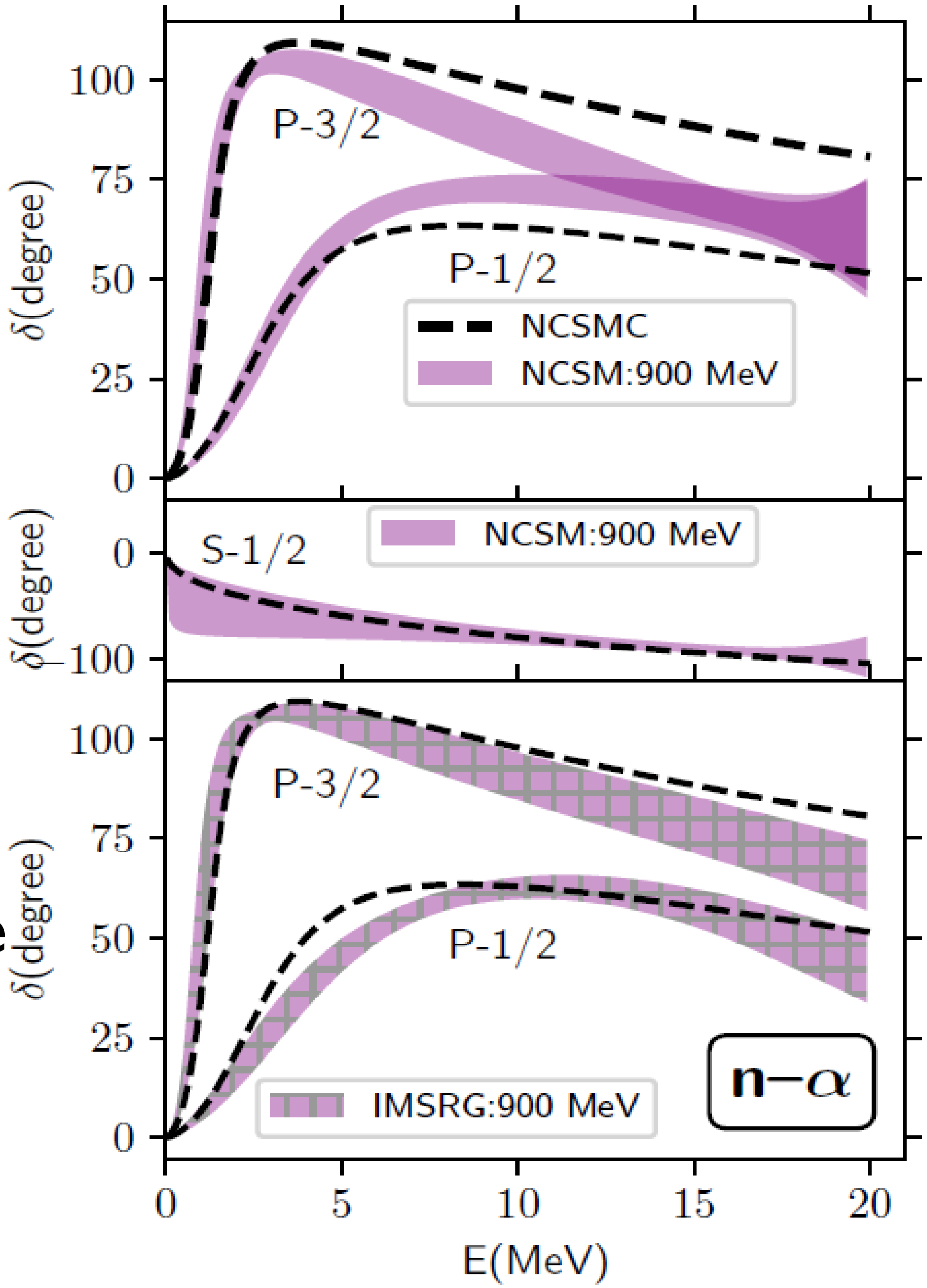
n-α scatterings in s and p waves

- $C_{i,j}(\Lambda_{uv})$ are the GERE parameters (dimensionless).
- **The error band partially comes from IR-error, while the UV-error (not in the band) approaches zero with large Λ_{uv}**
- Different data sets (using different Nmax and ω) are grouped in different Λ_{UV} bins.
- The parameters are extracted independently among these bins.
- Smooth Λ_{UV}-dependence, a signal that the IR physics is under control

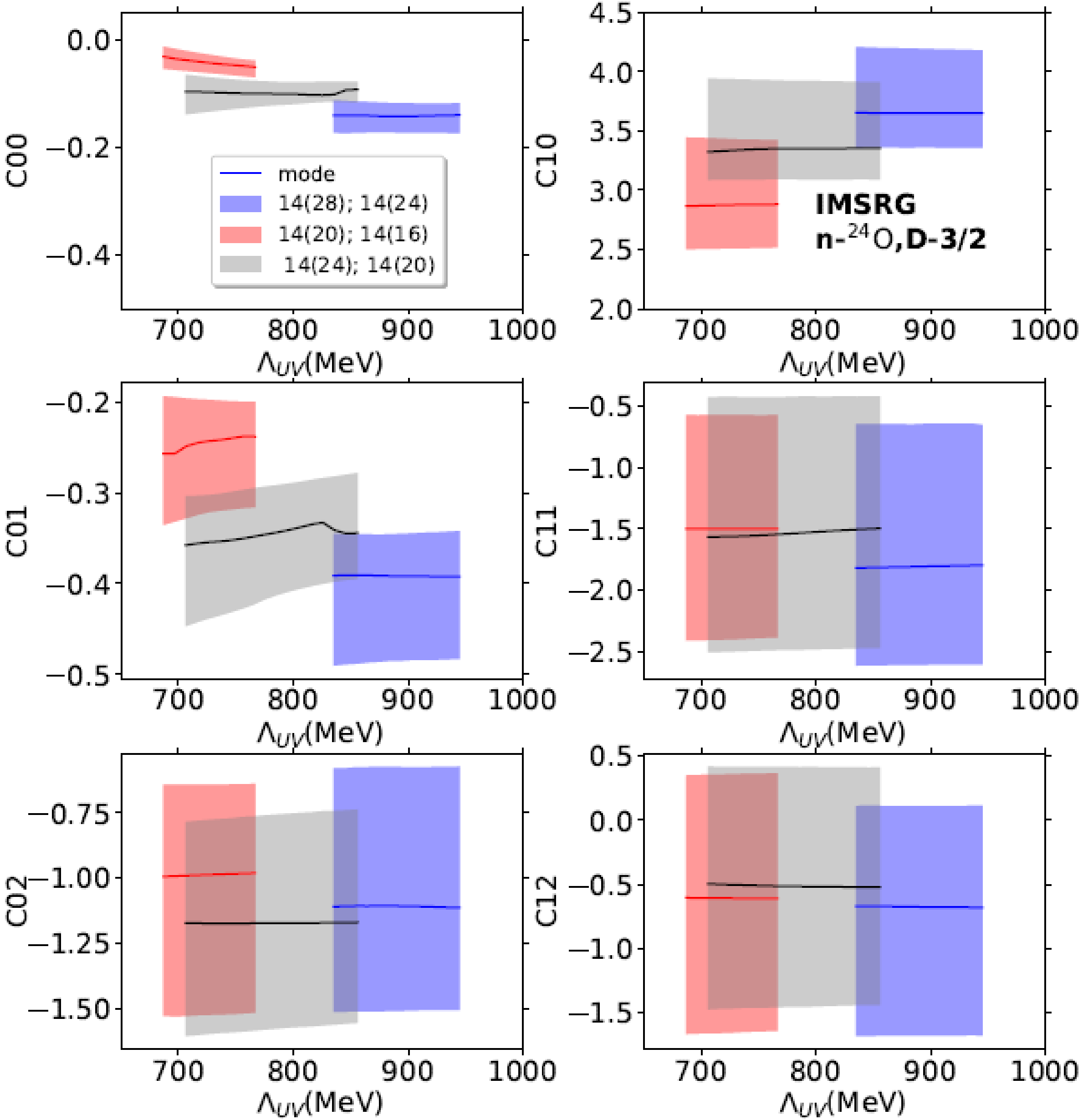


n-α scatterings in s and p waves

- The NCSM extraction agrees with Petr's direct phase-shift calculation below 5 MeV with **high** Λ_{UV}
- The IMSRG p-3/2 agrees with Petr's direct calculation, but p-1/2 is somewhat different
- Since we model both UV and IR physics components, we can use most (Nmax/emax, ω) results and extract phase-shifts. This is like LQCD producing results at different Lattice spacing.

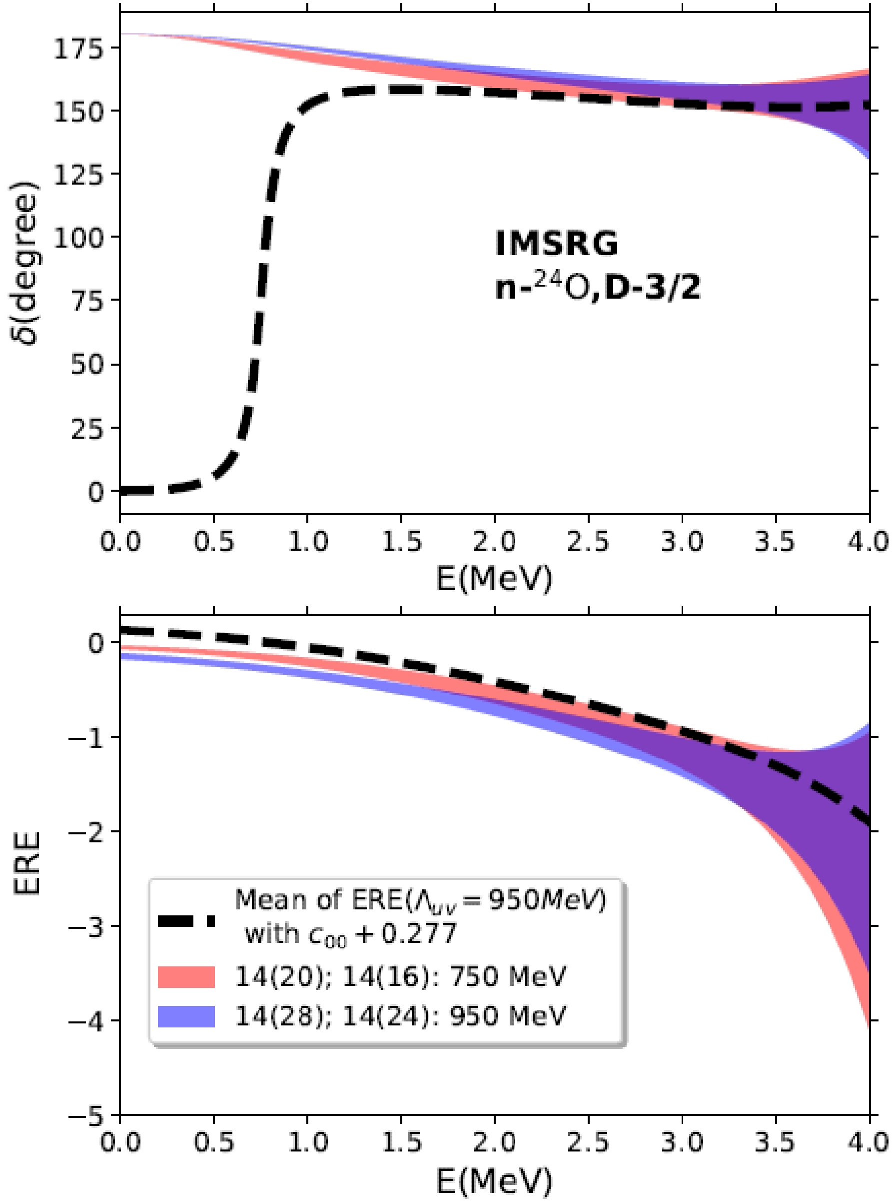


Analyze O24 and O25 energies from IMSRG and extract n-O24 scattering in d-3/2 channel



- C00 decreases with increasing Λ_{UV} **(smooth evolution:** C00~0.1, NOT 10 or 0.001)
- C01 and C10 have also some UV dependence
- Approaching to the continuum limit, no resonance behavior in scattering
- If C00 were positive, the resonance shows up **(NOT the prediction of the used nucleon interaction)**

Analyze O24 and O25 energies from IMSRG and extract n-O24 scattering in d-3/2 channel

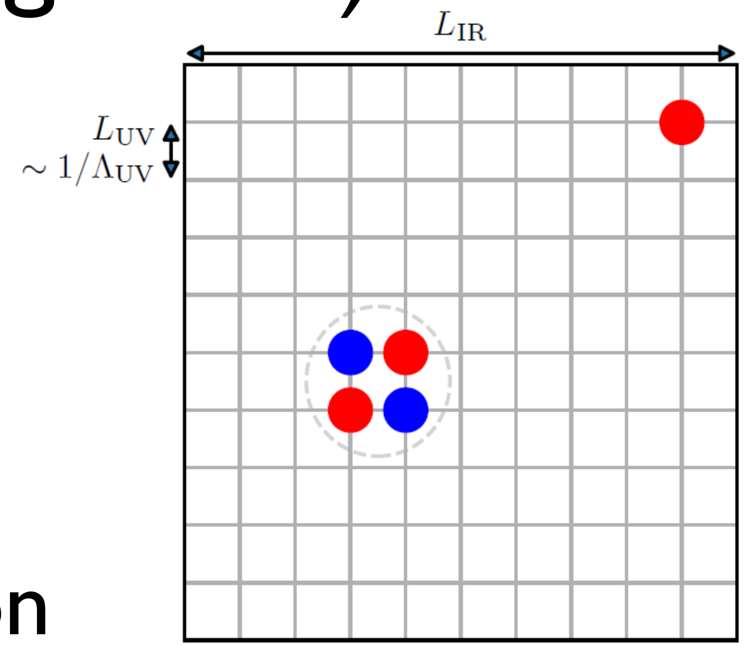


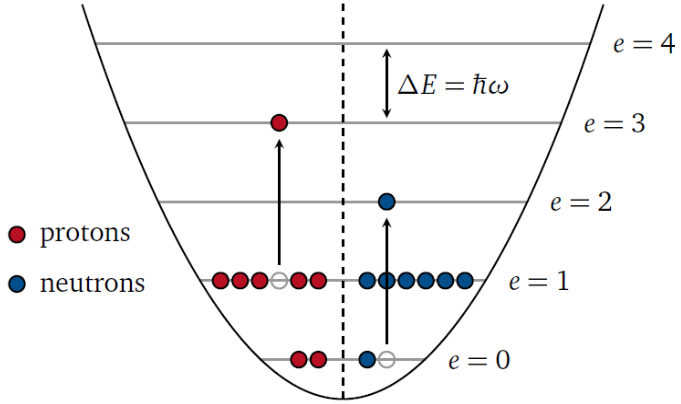
- Studying ERE at **E<0 region** predicts a low-energy bound state with 75% prob., the BE is -1.4 ± 0.54 MeV **(the property of the NN force)**
- The method should also be used to compute BE of shallow bound state (drip-line nuclei),
- Use the mean value of Cs(900 MeV) and increase C00 by about 0.28→a resonance (dashed curve) at 0.75 MeV and width of135 keV (similar to the expt. info): tuning nucleon interaction could improve the prediction

Here comes the messy part

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

- They modify both IR and UV physics → systematic errors (tiny stochastic errors)
- To model the IR error? → modify U function with truncation on relative motion
- To model the UV impact → the extracted GERE parameters $C_{i,j}$ becomes $C_{i,j}(\Lambda_{uv})$





Model the IR-error

With n_Λ truncating number of excitation quanta in terms of $\boldsymbol{\omega}$:

$$U = (-1)^{l+1}\left(\frac{2}{xb_T}\right)^{2l+1}\frac{\Gamma(l+3/2)}{\Gamma(\frac{1}{2}-l\,)}\frac{\Gamma(n_\Lambda+2)}{\Gamma(n_\Lambda+l+5/2)}\frac{{}_2F_1\left(n_E+1,-n_\Lambda-l-\frac{3}{2},-l+\frac{1}{2},x^2\right)}{{}_2F_1\left(n_E+l+\frac{3}{2},-n_\Lambda-1,l+\frac{3}{2},x^2\,\right)}$$

- $n_E = \frac{E}{2\omega_T}-\frac{l}{2}-\frac{3}{4};\, b_T = \frac{1}{\sqrt{m_R\omega_T}},\, b = \frac{1}{\sqrt{m_R\omega}}\,,\, x = \frac{2\,b_T b}{b_T^2+b^2}$
- **The U depends on truncation parameters. It models the IR-error**
- **It approaches the U(E) in the continuum limit (zero IR-error) with $\boldsymbol{\omega \to \omega_T}$ or $\boldsymbol{n_\Lambda \to \infty}$**

Access the UV-error (besides series truncation error in GERE)

Use the following as interpolator over a small Λ_{uv} bin (less than 100 MeV). $C_{i,j,0}$ $C_{i,j,1}$ and Q are fitting parameters

$$C_{i,j}(\Lambda_{uv}) = C_{i,j,0} + C_{i,j,1}\left(\frac{Q}{\Lambda_{uv}}\right)^2$$

Another error

For example, the n-alpha data:

He-5 (He-4) mass tabulated in terms of Nmax5 (Nmax4), ω, and ω_T

$$E(N_{\max 5}, \omega, \omega_T) = E_{He5}(N_{\max 5}, \omega, \omega_T) - E_{He4}(N_{\max 4}, \omega, \omega_T)$$

For IR-error: $n_\Lambda = n_\Lambda(N_{max,5})$

A digression to Bayesian inference

$$\mathrm{pr}(\mathbf{C},\mathbf{d}|D,T,I) \propto \mathrm{pr}(D|\mathbf{C},d,T,I)\mathrm{pr}(\mathbf{C},\mathbf{d}|I)$$

Posterior distribution

Likelihood function

Prior distribution

C are the GERE parameters; **d** are the other parameters describing the IR and UV error

A few thoughts on the connection to other approaches and its potential application in quantum computing

	Generalized Luscher	Luscher in Lattice calculations	Single-State HORSE (Harmonic Oscillator Representation of Scattering Eqs)
IR regulator	Trap	Large volume	Effective cavity in the Nmax truncations
UV regulator	Nominal Λ_{UV}	Lattice spacing	Λ_{UV}?
IR-UV explictly coupled?	Yes, so we need a model to extract them	Decoupled	Yes
IR-error	Use effective Nmax or emax for relative motion to access this error	Imbedded in MC sampling: the calculation can not handle arbitrarily large volume, i.e., there is error related to IR physics in sampling. (what is the signal for that error?)	?
Error types	Mostly systematic, except the rounding errors	Stochastic error in sampling	?

In our approach, if the base frequency approaches trap frequency, the IR-error would disappear. While doing so, to reduce the UV error, Nmax/emax has to be increased significantly. So perhaps quantum computer is one way to go.

Summary

- The Luscher method used in LQCD is generalized to work with ab initio nuclear structure methods (NCSM and IMSRG)
- The extracted n-α phase-shifts are compatible with the existing ab initio results using the same nucleon interaction
- The n- O24 scattering calculation demonstrates the method's capability to study systems heavier (it is based on bound-state spectrum calculation)
- The UV and IR physics are correctly modeled → results from different regulators are consistent (smooth UV-scale dependence)
- We now report results as function of UV scale, a practice common in Lattice methods (Lattice QCD, NLEFT), but not in other ab intio calculations

U(E) in the finite model space (H.O. basis, NCSM)

Approaches approx. to a fuzzy cavity limit, with $L = \sqrt{2(2n_\Lambda + l + \frac{3}{2} + 2)}\, b$, in a non-trivial way ($\Lambda = \sqrt{2(2n_\Lambda + l + \frac{3}{2} + 2)}\,/b$)

- In a "cavity" for relative motion with radius L

$$U = p^{2l+1} \frac{y_l(Lp)}{j_l(Lp)} \leftarrow < i \left| V_s \frac{1}{E - H_0} V_s \right| i >$$

- In Nmax truncation scheme for two-body relative motion ("U for the un-trapped and the truncated"):

$$U = \frac{(-1)^{l+1}}{b^{2l+1}} \frac{\Gamma(l+3/2)}{\Gamma(\frac{1}{2}-l)} \frac{\Gamma(n_\Lambda+2)}{\Gamma(n_\Lambda+l+5/2)} \frac{M\left(-n_\Lambda-l-\frac{3}{2}, -l+\frac{1}{2}, p^2 b^2\right)}{M\left(-n_\Lambda-1, l+\frac{3}{2}, p^2 b^2\right)} \leftarrow < i \left| V_s \hat{P} \frac{1}{E - H_0} \hat{P} V_s \right| i >$$

$H_0 \rightarrow H_{\omega_T}$

  - $\hat{P} = \hat{P}(N_\Lambda, \omega) = \sum_{n=0}^{n_\Lambda} |HO_n >< HO_n| = \sum_{\mu=0}^{n_\Lambda} |DVR_\mu >< DVR_\mu|\,; N_{max} = 2n_\Lambda + l$
  - $b = 1/\sqrt{m_R \omega}$ (ω is base freq.)

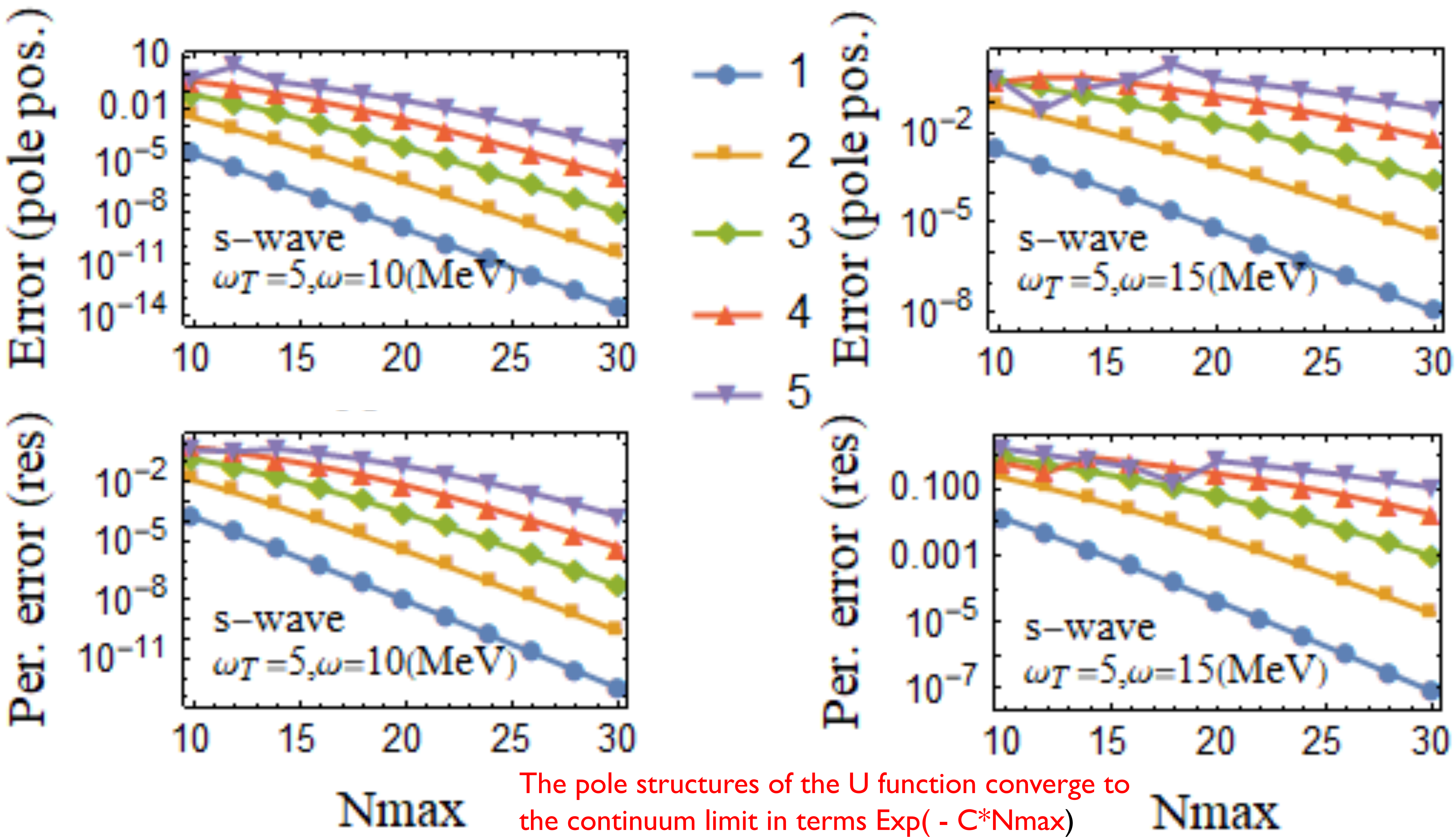
Approaches to above when $\omega_T \rightarrow 0$, also to the continuum limit properly when $\omega \rightarrow \omega_T$ or $n_\Lambda \rightarrow \infty$

- Now with the trapping potential, with ω_T frequency ("U for the trapped and truncated")

$$U = (-1)^{l+1} \left(\frac{2}{x b_T}\right)^{2l+1} \frac{\Gamma(l+3/2)}{\Gamma(\frac{1}{2}-l)} \frac{\Gamma(n_\Lambda+2)}{\Gamma(n_\Lambda+l+5/2)} \frac{{}_2F_1\left(n_E+1, -n_\Lambda-l-\frac{3}{2}, -l+\frac{1}{2}, x^2\right)}{{}_2F_1\left(n_E+l+\frac{3}{2}, -n_\Lambda-1, l+\frac{3}{2}, x^2\right)}$$

  - $n_E = \frac{E}{2\omega_T} - \frac{l}{2} - \frac{3}{4}$; $b_T = \frac{1}{\sqrt{m_R \omega_T}}$, $x = \frac{2\, b_T b}{b_T^2 + b^2}$
  - the low−energy pole position of this function is very interesting:

$$n + O\left((n_\Lambda+1)^{d+\frac{1}{2}} e^{-\frac{(n_\Lambda+1)}{2}\eta^2}\right), \text{ with } d < 0, \eta \sim -\sqrt{-2\,Log(1-x^2)}$$



The pole structures of the U function converge to the continuum limit in terms Exp(- C*Nmax)

Outlook

- Need to understand the origin of the parameters modeling errors in our "data" analysis in terms of microscopic picture
- Explore other observables
- To compute reactions, need to study coupled-channel problem within traps. EFT provide one way to approach this problem
- From the angle of computer experiment, other existing models used in nuclear experiments (potential model and R-matrix), could also be used in data analysis. The important steps involve understanding the theory error of the model and the computer-experiment's error (UV and IR modification within the ab initio calculation)

In retrospect

- In the harmonic-oscillator-basis structure calculations, the clustering physics already exists, i.e., the basis can handle continuum physics with the help of a trap

- The key is to understand properly the IR physics/condition in terms of clusters.

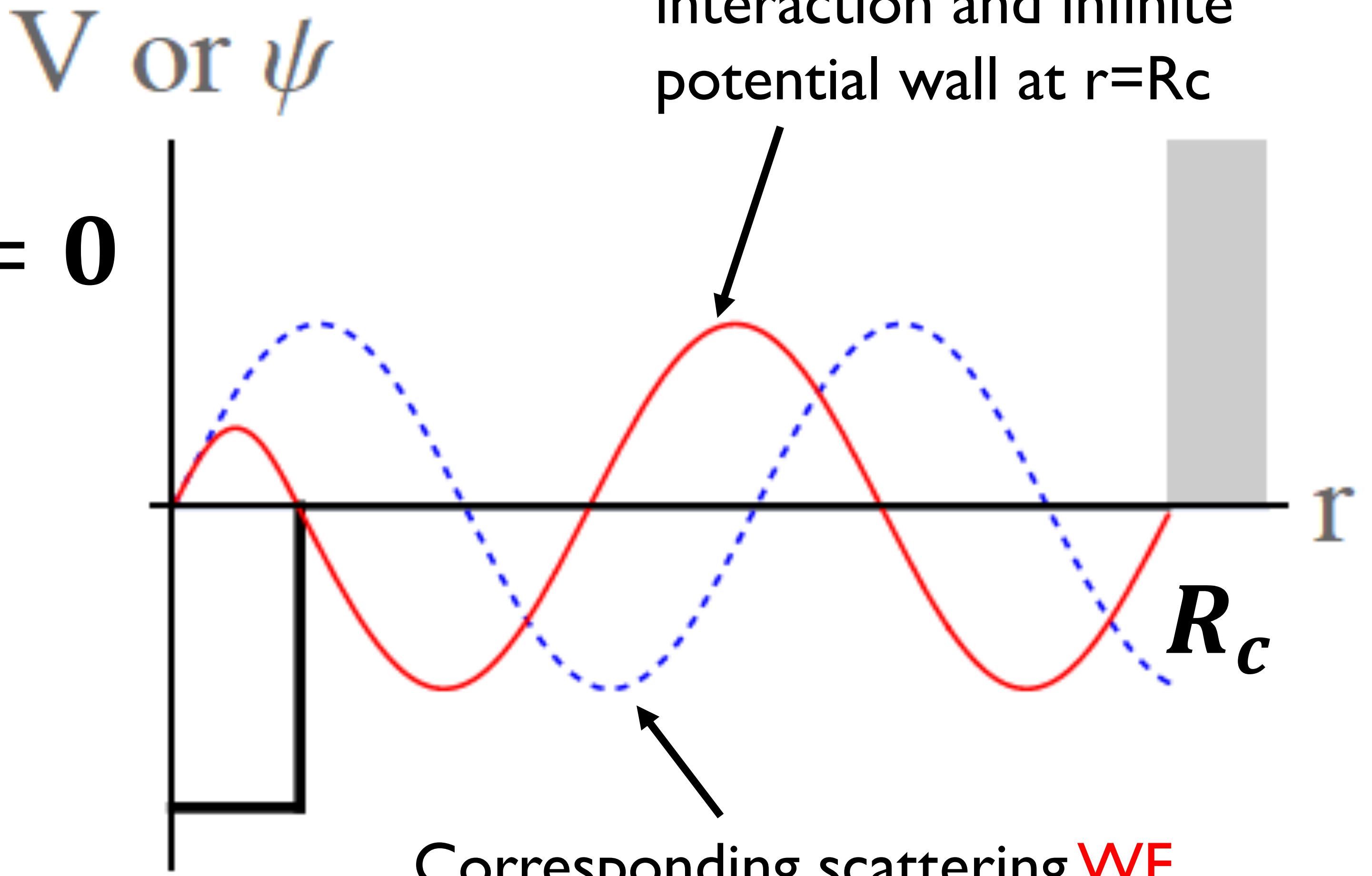
- Our IR is dictated by the trap. Truncation leads to IR error and approaches to zero in the continuum limit

Cavity boundary condition (for relative motion)

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

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

Discrete eigen-energies for system in a cavity gives the phase shift at those energies

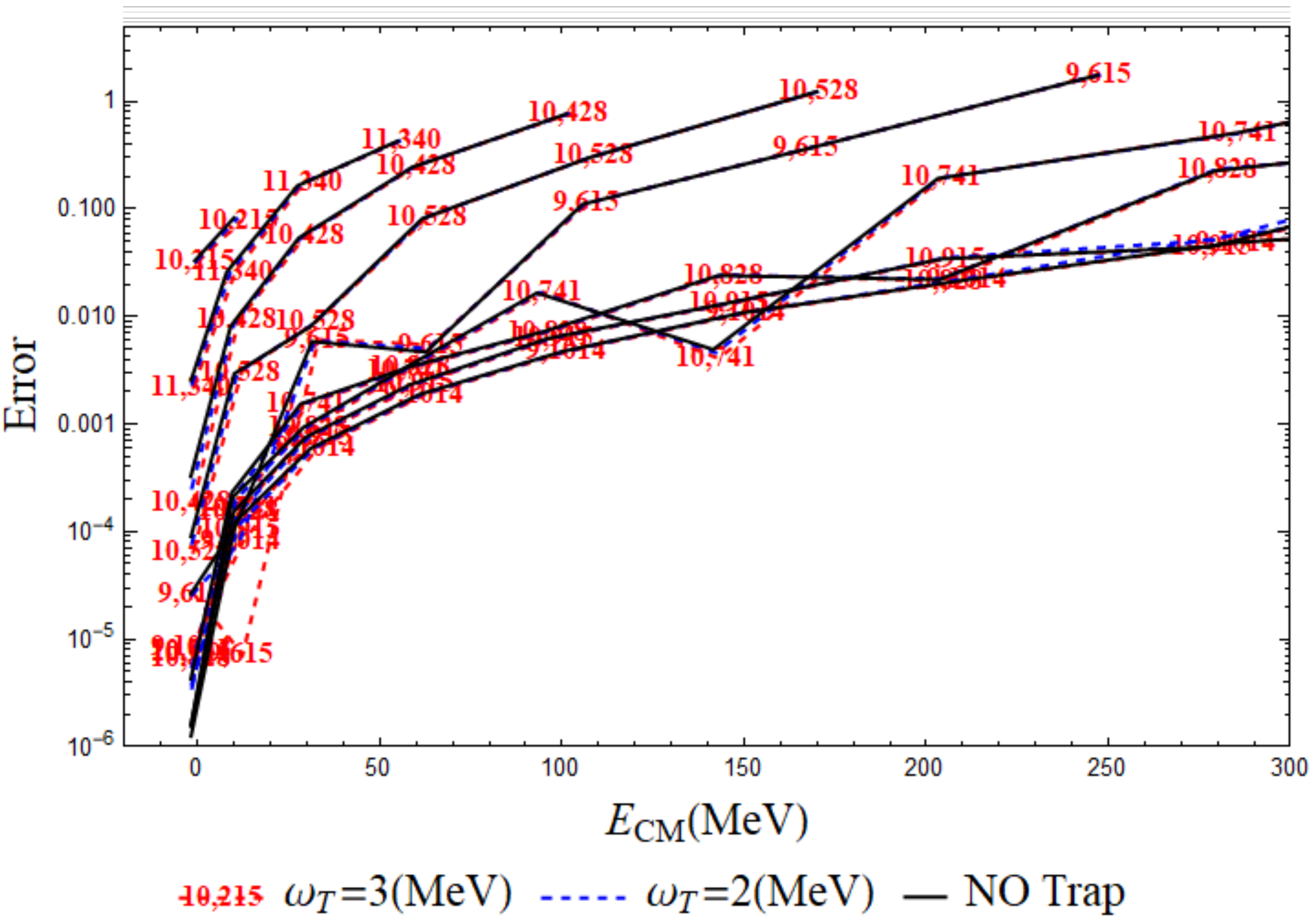


However trapping nucleons in harmonic potential well is better suited for harmonic-oscillator-basis calculations

- Reduces degrees of freedom (DOF) → make ab initio calculations feasible
- The center of mass (CM) and internal DOF are **decoupled**
- Cavity boundary condition requires high energy modes (CM-internal-decoupling is violated in cavity)
- Lattice regulator breaks rotational invariance

There is a "universal" formula for two-cluster system at low energy→ BERW (Busch) formula $(E, \omega_T) \rightarrow \delta_l(E)$

- NN model:(G)ERE extractions for the s-wave, for both trapped and non-trapped system.
- The markers are **L and Λ** as defined before
- UV error scales as $1/L\Lambda^3$ at leading order
- Different IR modification is disentangled from UV error
- The UV error can be reduced by improving potential's UV behavior
- This also suggests that if NN is optimized, adding further trap doesn't require further optimization



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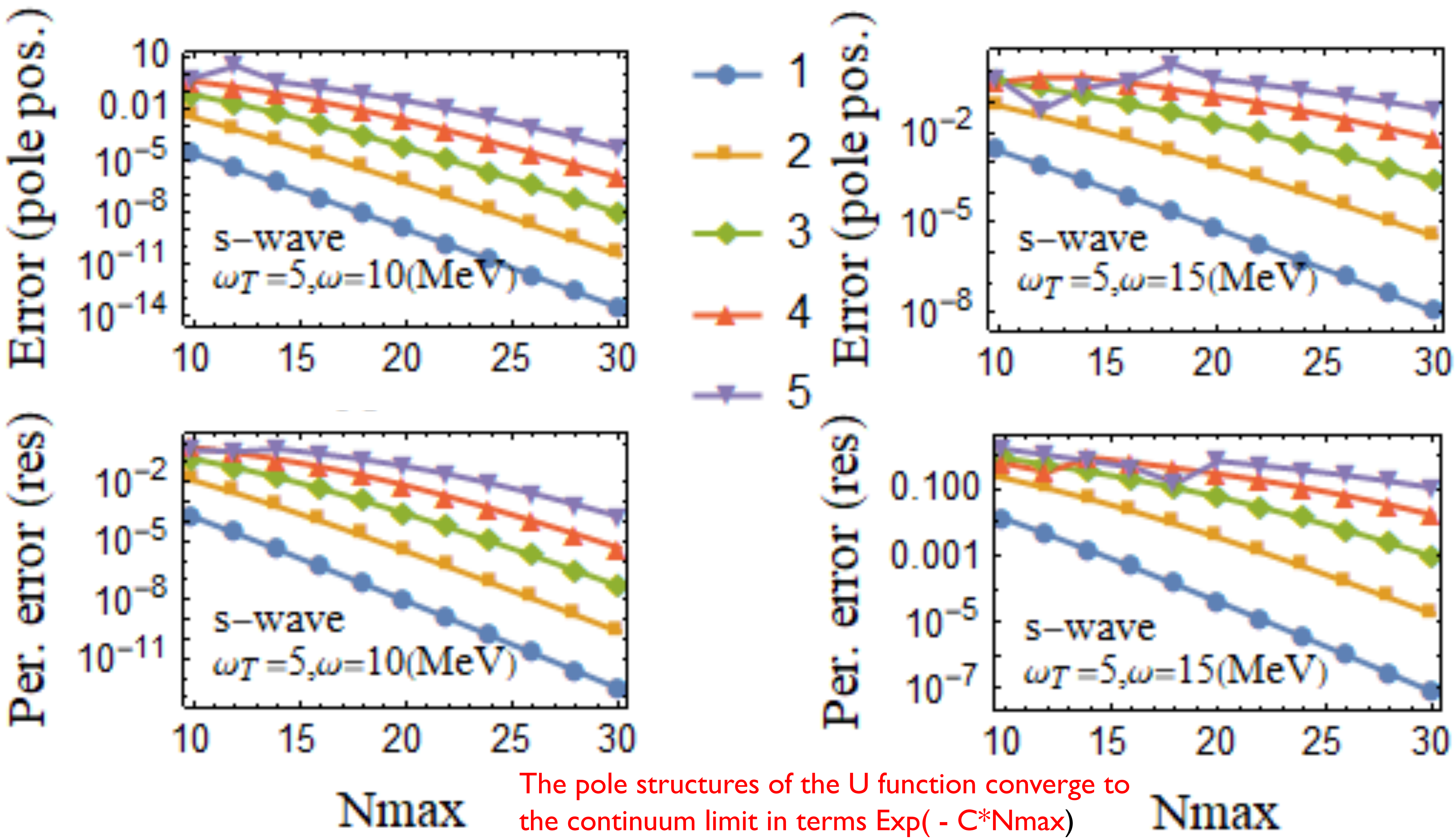
Approaches to above when $\omega_T \rightarrow 0$, also to the continuum limit properly when $\omega \rightarrow \omega_T$ or $n_\Lambda \rightarrow \infty$

- Now with the trapping potential, with ω_T frequency ("U for the trapped and truncated")

$$U = (-1)^{l+1}\left(\frac{2}{xb_T}\right)^{2l+1}\frac{\Gamma(l+3/2)}{\Gamma(\frac{1}{2}-l\,)}\frac{\Gamma(n_\Lambda+2)}{\Gamma(n_\Lambda+l+5/2)}\frac{{}_2F_1\left(n_E+1,-n_\Lambda-l-\frac{3}{2},-l+\frac{1}{2},x^2\right)}{{}_2F_1\left(n_E+l+\frac{3}{2},-n_\Lambda-1,l+\frac{3}{2},x^2\right)}$$

- $n_E = \frac{E}{2\omega_T} - \frac{l}{2} - \frac{3}{4}; b_T = \frac{1}{\sqrt{m_R\omega_T}}, x = \frac{2\,b_T b}{b_T^2+b^2}$
- the low−energy pole position of this function is very interesting:

$$n + O\left((n_\Lambda+1)^{d+\frac{1}{2}}e^{-\frac{(n_\Lambda+1)}{2}\eta^2}\right),\ \text{with } d < 0, \eta \sim -\sqrt{-2\,Log(1-x^2)}$$

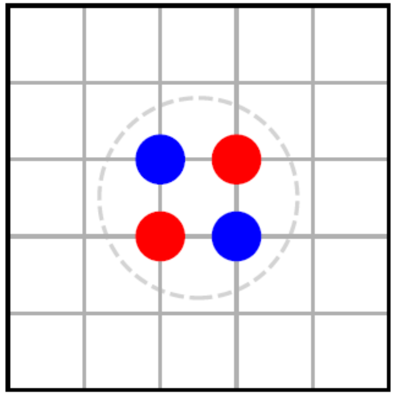


The pole structures of the U function converge to the continuum limit in terms Exp(- C*Nmax)

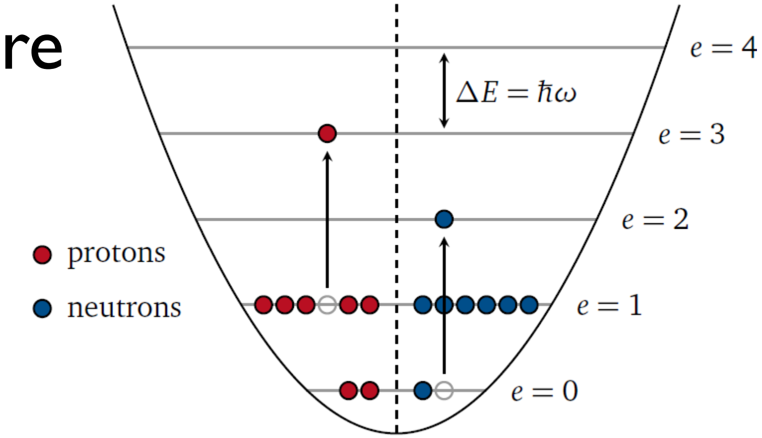
Useful references:

- Cavity boundary condition: E.g., R. J. Furnstahl, S. N. More, and T. Papenbrock (2014)
- Discrete Variable Representation (DVR): S. Binder, A. Ekstrom, G. Hagen, T. Papenbrock, and K. A. Wendt (2016)
- Many-body extrapolation: K. A. Wendt, C. Forssen, T. Papenbrock, and D. Saaf (2015)
- J-matrix derivation **(known as HORSE or SS-HORSE in nuclear physics for extracting phase-shift from energy spectrum):** A. M. Shirokov, A. I. Mazur, I. A. Mazur, and J. P. Vary (2016); A. M. Shirokov, A. I. Mazur, I. A. Mazur, E. A. Mazur, I. J. Shin, Y. Kim, L. D. Blokhintsev, and J. P. Vary (2018)

Ab initio calculations of bound nuclei

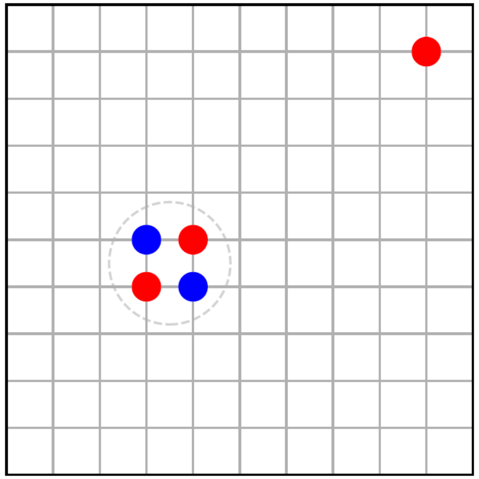


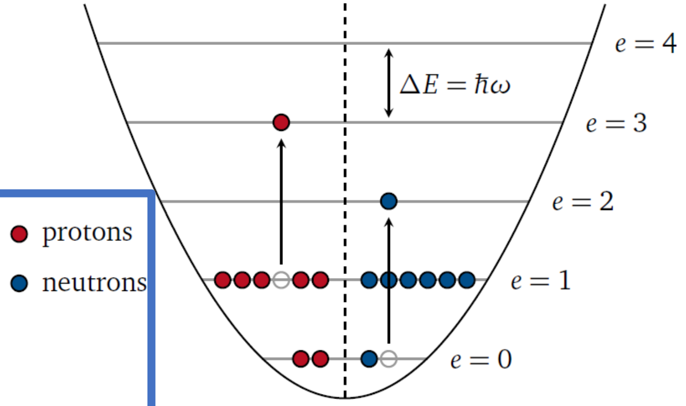
- Count degrees of freedom (DOF): nucleons' space locations (& internal DOF). Treating differently:
  - Green's function MC, nuclear lattice effective field theory (NLEFT), as well as lattice QCD (LQCD)
  - Basis method, e.g. Hamiltonian diagonalization in no-core shell model (NCSM) and in-medium similarity renormalization group (IMSRG), and coupled-cluster



Ab initio calculations of scattering/reactions

- For scattering/reactions, all the nucleons must be treated in the same way→ too many DOF. Then options are
  - NCSM+continuum
  - Gamow shell-model
  - Ab initio optical potential
  - Compute energies by MC-sampling of important configurations **at finite volume**: NLEFT, GFMC, LQCD





- **Finite volume reduces DOF. So is trapping!**
- **And eigen-energies give phase shift.**
- Regulators also in other calculations (e.g., Geant simulation)

Trapping nucleons in ab-initio spectrum calculations

V_s

Continuum

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

Bound State

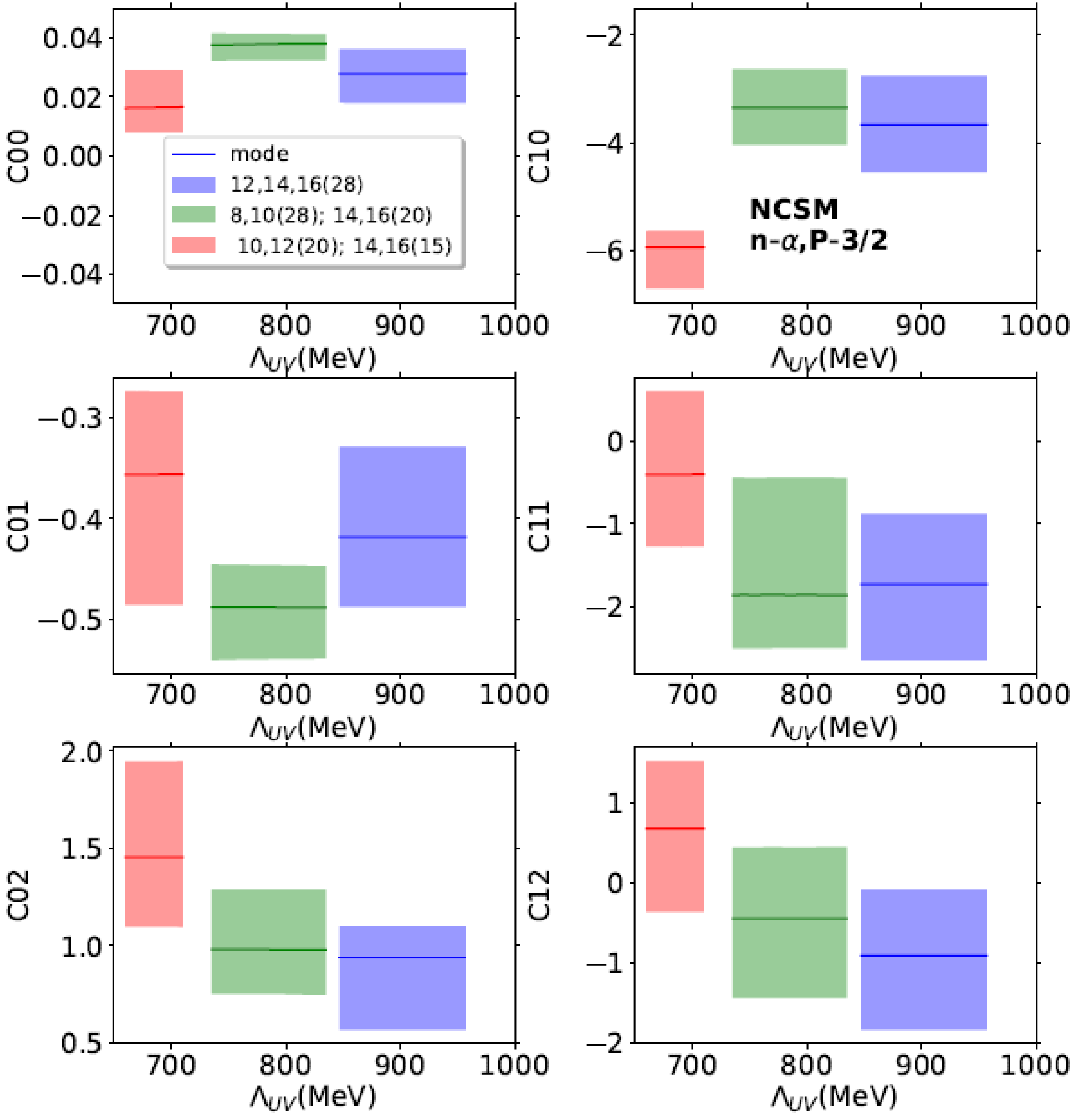
Constrain EFT (or model on V_s) and use it to compute scattering and reaction

There is a "universal" formula for two-cluster system at low energy→ BERW (Busch) formula

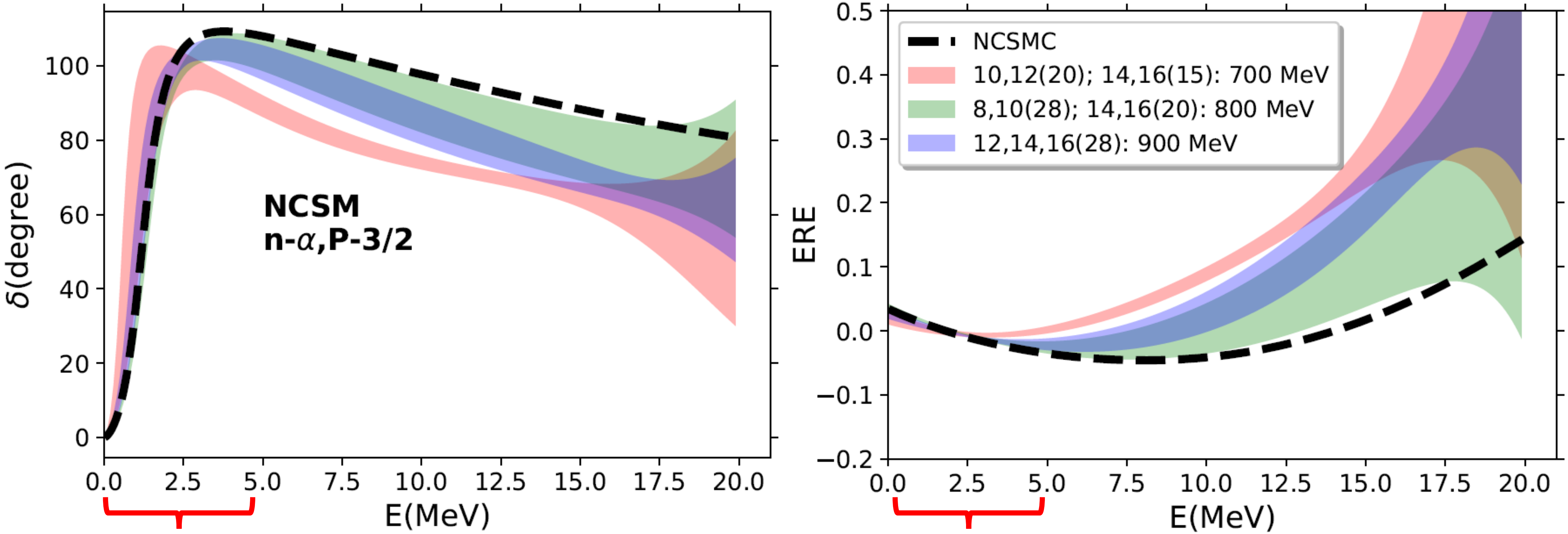
$$(E, \omega_T) \rightarrow \delta_l(E)$$

Analyze He4 and He5 energies from NCSM and extract n-α scattering in P-3/2 channel

- $C_{i,j}(\Lambda_{uv})$ are the GERE parameters (dimensionless).
- **The error band partially comes from IR-error, while the UV-error (not in the band) approaches zero with large Λ_{uv}**
- Different data sets (using different Nmax and ω) are grouped in different Λ_{UV} bins.
- The parameters are extracted independently among these bins.
- Smooth Λ_{UV}-dependence, a signal that the IR physics is under control

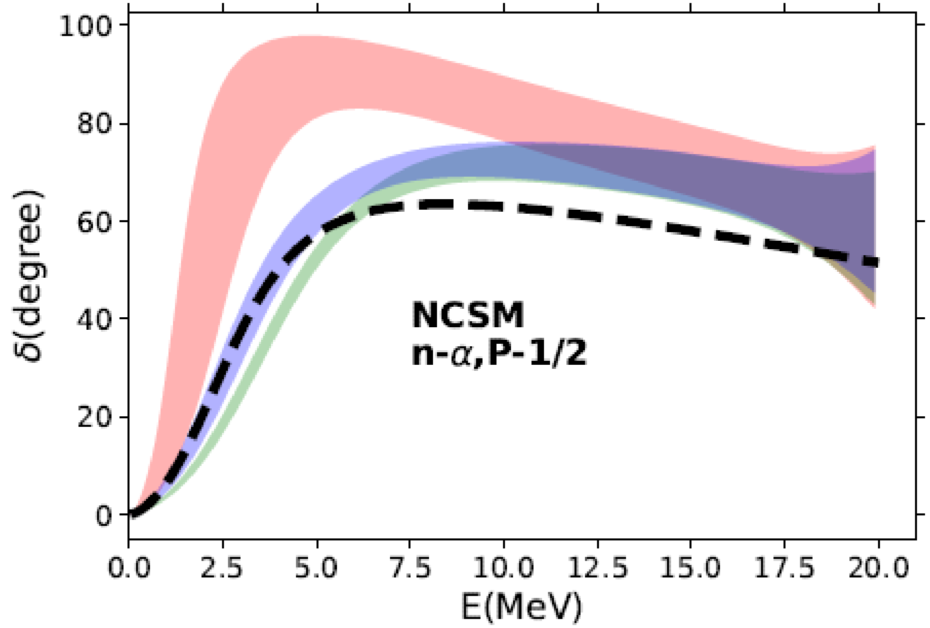


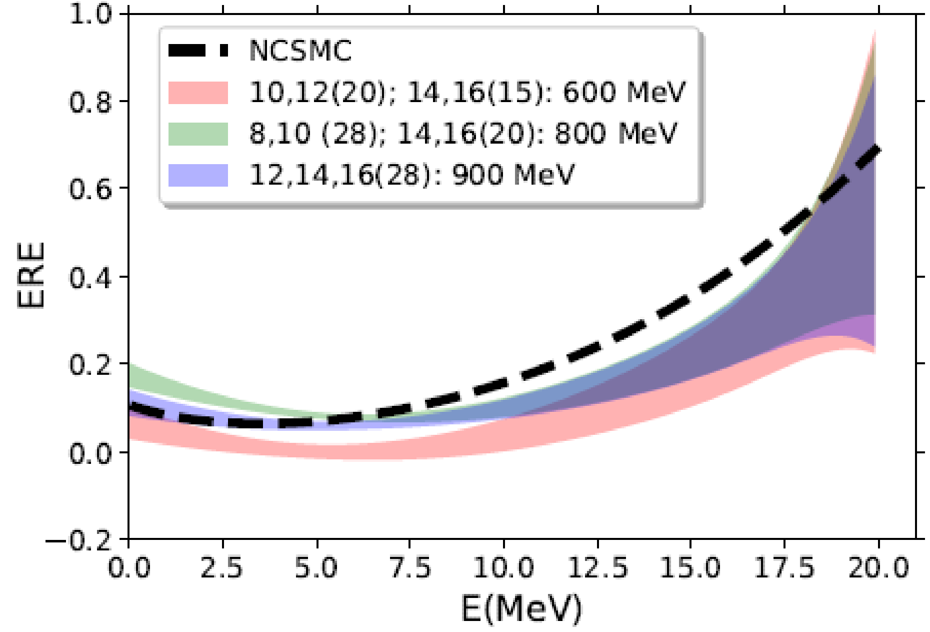
Analyze He4 and He5 energies from NCSM and extract n-α scattering in P-3/2 channel

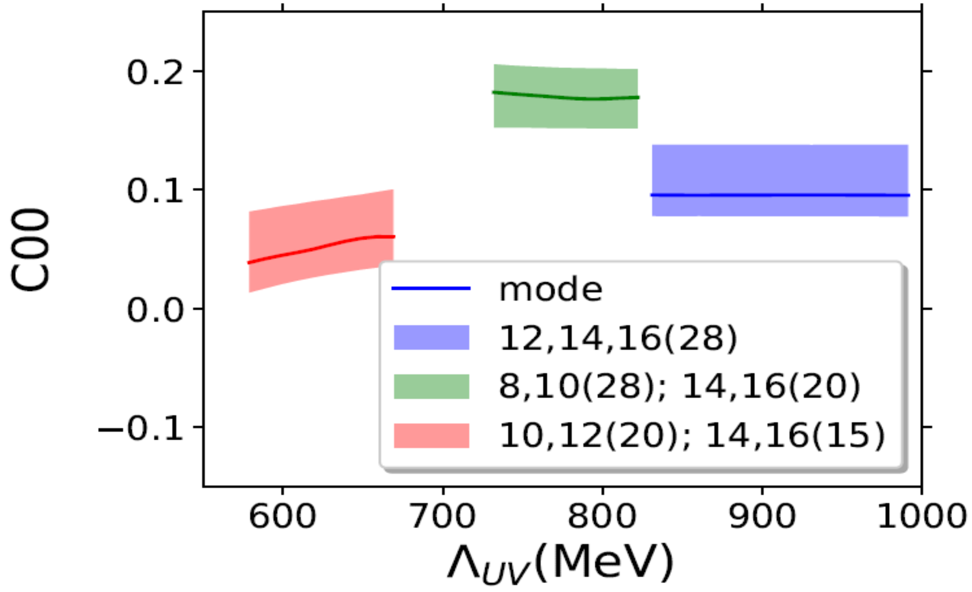


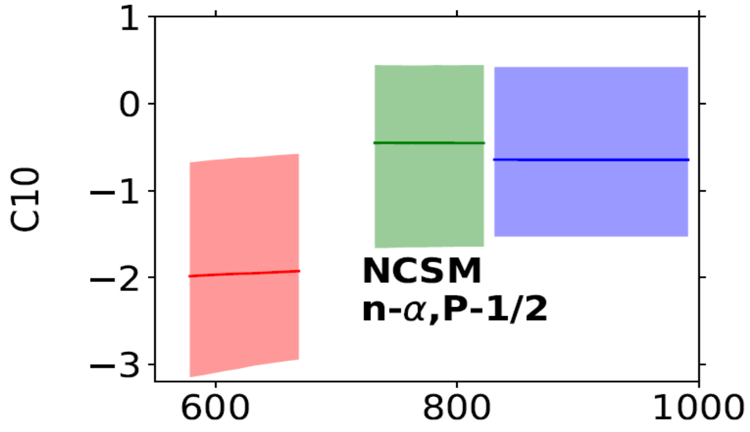
- Lowering Λ_{UV} has a trend to turn a resonance to bound state (also seen in p-½ channel)
- The extraction agrees with Petr's direct phase-shift calculation below 5 MeV with **high** Λ_{UV}
- Since we model both UV and IR physics components, we can use most (Nmax, ω) results and extract phase-shifts. This is like LQCD producing results at different Lattice spacing.

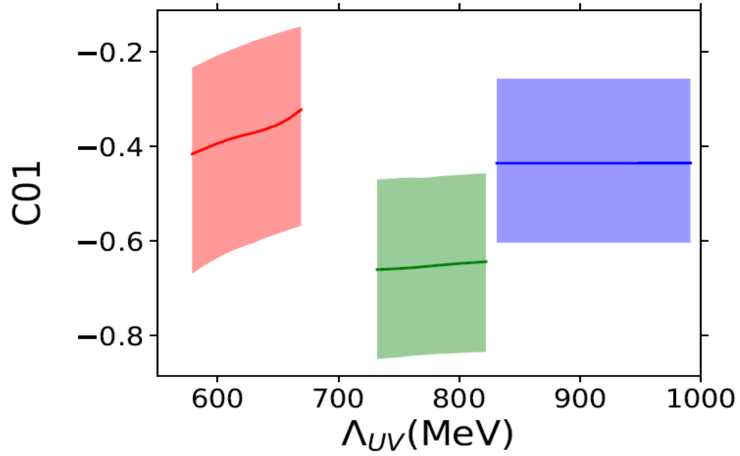
n-α in P-1/2 channel from NCSM





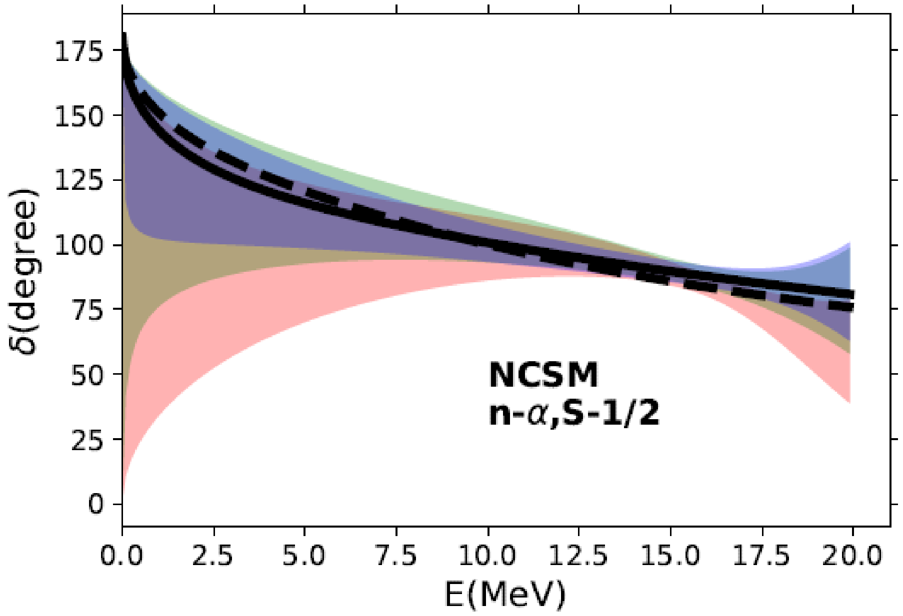


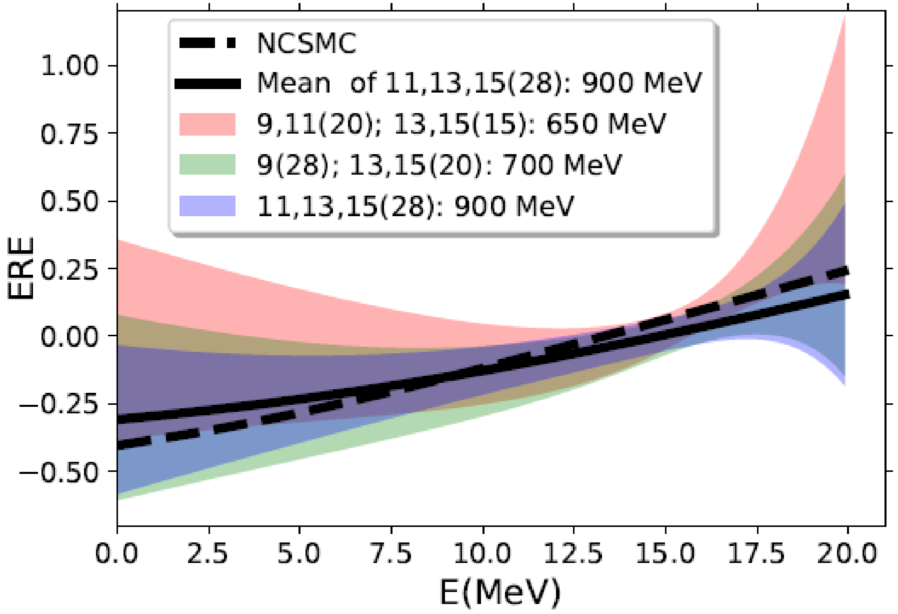


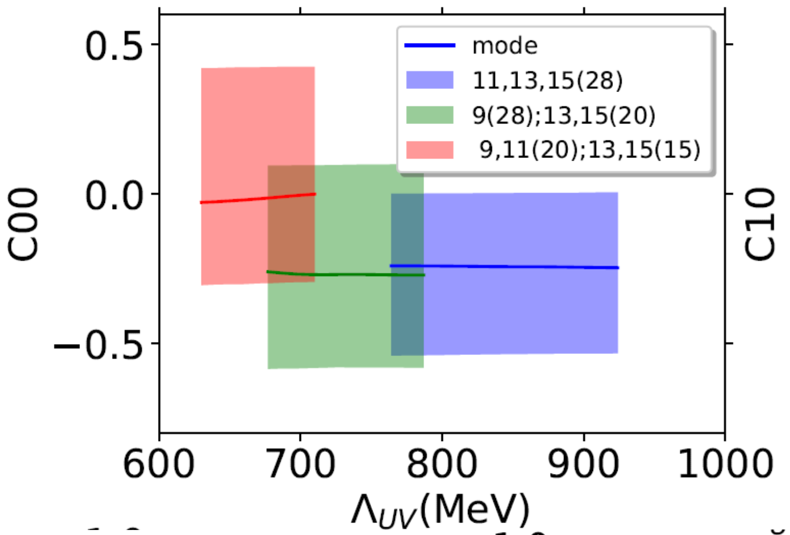


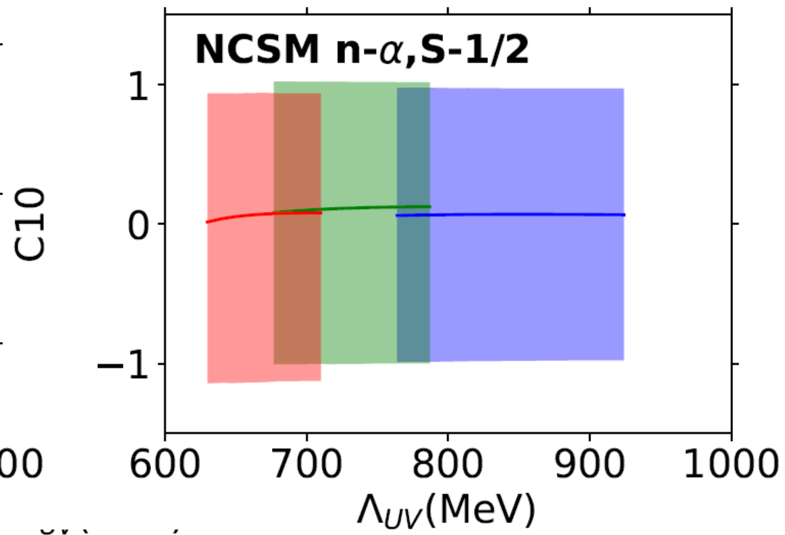
Similar conclusions can be drawn as in P-3/2

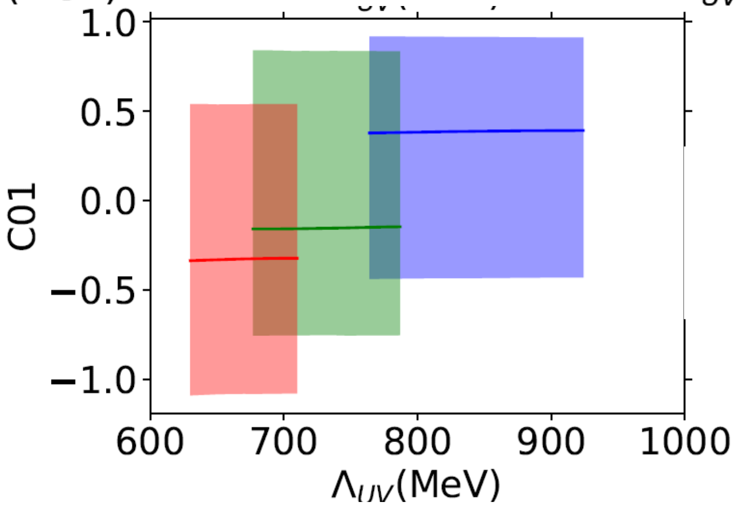
n-α in S-1/2 channel from NCSM





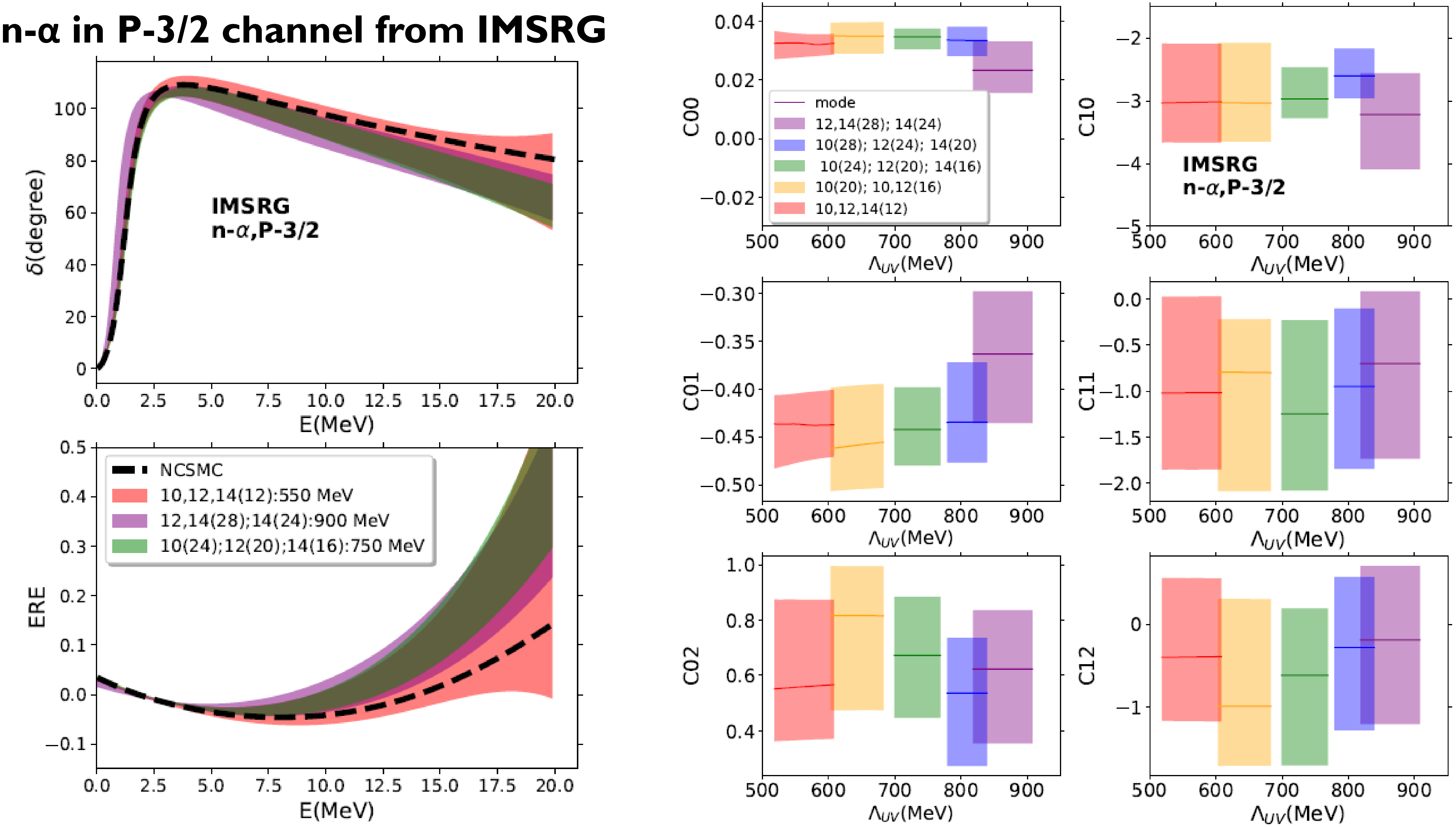






- Less data
- Mean values agree with NCSMC quite well

n-α in P-3/2 channel from IMSRG



n-α in P-1/2 channel from IMSRG