Extracting nuclear scattering phase shifts from ab initio energy spectrum calculation

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In collaboration with Chan Gwak, Ragnar Stroberg, Petr Navratil, and Jason Holt;
In collaboration with J. Melendez, and R. Furnstahl

Outline

- Difficulty with continuum physics: a cluster-based EFT perspective
- Busch (BERW) formula relates two-cluster spectrum in a harmonic trap to the two-cluster scattering
- Improve the BERW formula
- How precise is the phase-shift extraction?: NN and N-alpha (toy model) systems
- Confront the reality: $\mathrm{n} -^{24} O$ and $\mathrm{n} - \alpha$
- Conclusion and outlook

Difficulty with continuum physics: an EFT perspective

- Nuclear structure calculation methods have been developed to study compact system
- When dealing with continuum/resonances, the large distance configuration (DOF) is hard to be included in these methods
- Meanwhile, cluster-based-EFT (known as Halo-EFT)/cluster-model decrease the "resolution" scale in their descriptions, and focus on the large-distance DOF
- How to combine the two methods? Here is another way different from RGM

Busch (BERW) formula: infrared extrapolation

V_s

Continuum

Trap them in $\frac{1}{2}M_N\omega_T r^2$potential

Bound State

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

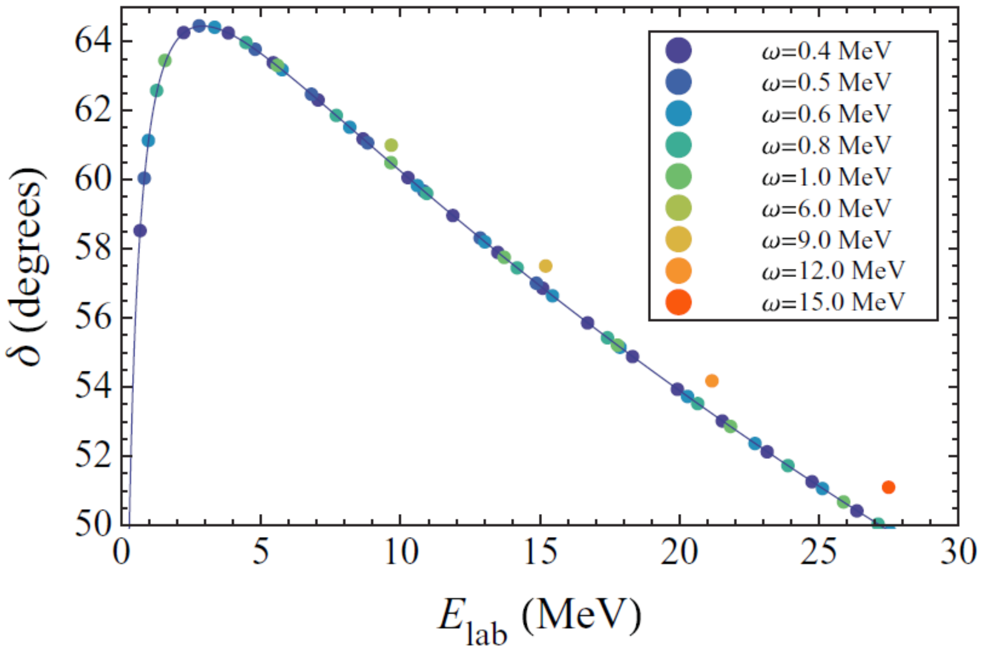
Ab initio

calculations

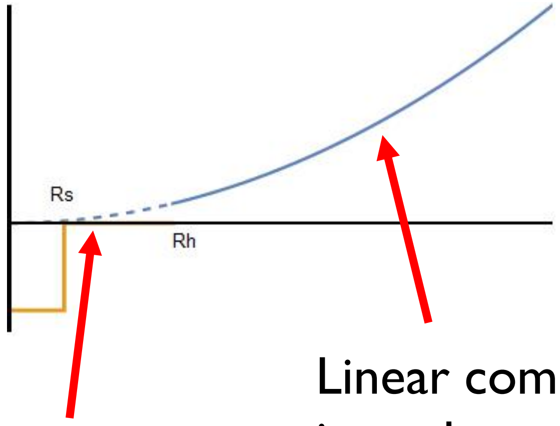
BERW formula's application in nuclear physics

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

Here: $E \equiv \frac{p^2}{2M_R}$ is the eigenenergy; Λ is a ref. scale



- T. Luu, M. Savage, A. Schwenk, and J. Vary, PRC (2010): N-N phase shift
- J. Rotureau, I. Stetcu, B.R. Barrett, and U. van Kolck, PRC (2012): N-D phase shift



Linear combination of regular and irregular oscillator wave functions

$\mathrm{Cos}\,\delta\, j_l + \mathrm{Sin}\,\delta\, n_l$

Improve BERW Formula (last year's talk)

$$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} C_{i,j}\left(\frac{b^{-4}}{\Lambda^4}\right)^i\left(\frac{p^2}{\Lambda^2}\right)^j = (-1)^{l+1}\left(\frac{4\,M_R\omega_T}{\Lambda^2}\right)^{l+1/2}\frac{\Gamma(\frac{3}{4}+\frac{l}{2}-\frac{E}{2\omega_T})}{\Gamma(\frac{1}{4}-\frac{l}{2}-\frac{E}{2\omega_T})}$$

$$\left(\frac{p^2}{\Lambda^2}\right)^{l+\frac{1}{2}} Cot\delta_l = \sum_{j=0}^{\infty} C_{i=0,j}\left(\frac{p^2}{\Lambda^2}\right)^j$$

- $b = \sqrt{\frac{1}{M_R\omega}}$
- Λ is the high momentum scale in this EFT, which treats all the interaction as short-ranged. Λ is NOT directly related to regulator. It is used as a reference scale to change otherwise dimensional full variables to dimensionless variables.
- C_{ij} should be O(1) if not fine tuned

A digression to Bayesian inference

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

Posterior distribution

Likelihood function

Prior distribution

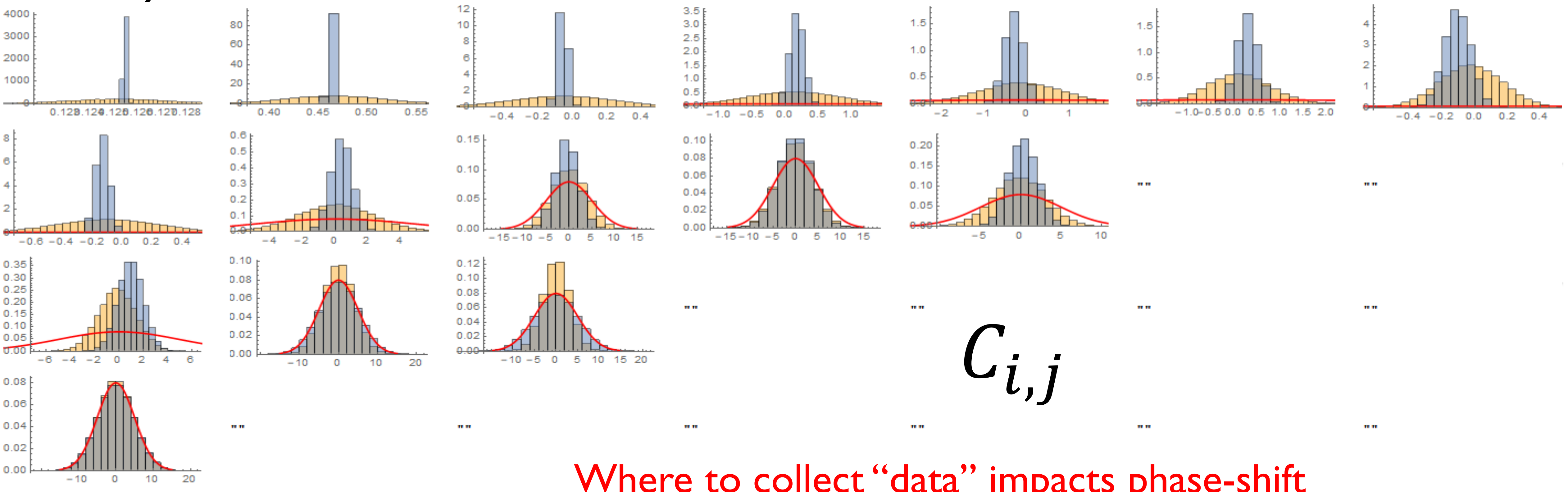
T: $\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} C_{i,j}\left(\frac{b^{-4}}{\Lambda^4}\right)^i\left(\frac{p^2}{\Lambda^2}\right)^j = (-1)^{l+1}\left(\frac{4\,M_R\omega_T}{\Lambda^2}\right)^{l+1/2}\frac{\Gamma(\frac{3}{4}+\frac{l}{2}-\frac{E}{2\omega_T})}{\Gamma(\frac{1}{4}-\frac{l}{2}-\frac{E}{2\omega_T})}$

Instead of trying different ω_T to map out the phase-shift curve, the unknown parameter vector $\boldsymbol{C}$ can be fixed against eigenenergy "data" and then predict phase shift

How precise can we extract phase shifts, optimistically speaking?

NN $^1S_0$ at N6LO assuming zero data error bar

The energy spectra are from the calculations by J. Vary et.al. [T. Luu, M. Savage, A. Schwenk, and J. Vary, PRC (2010)] and private communications with J. Vary (2018)

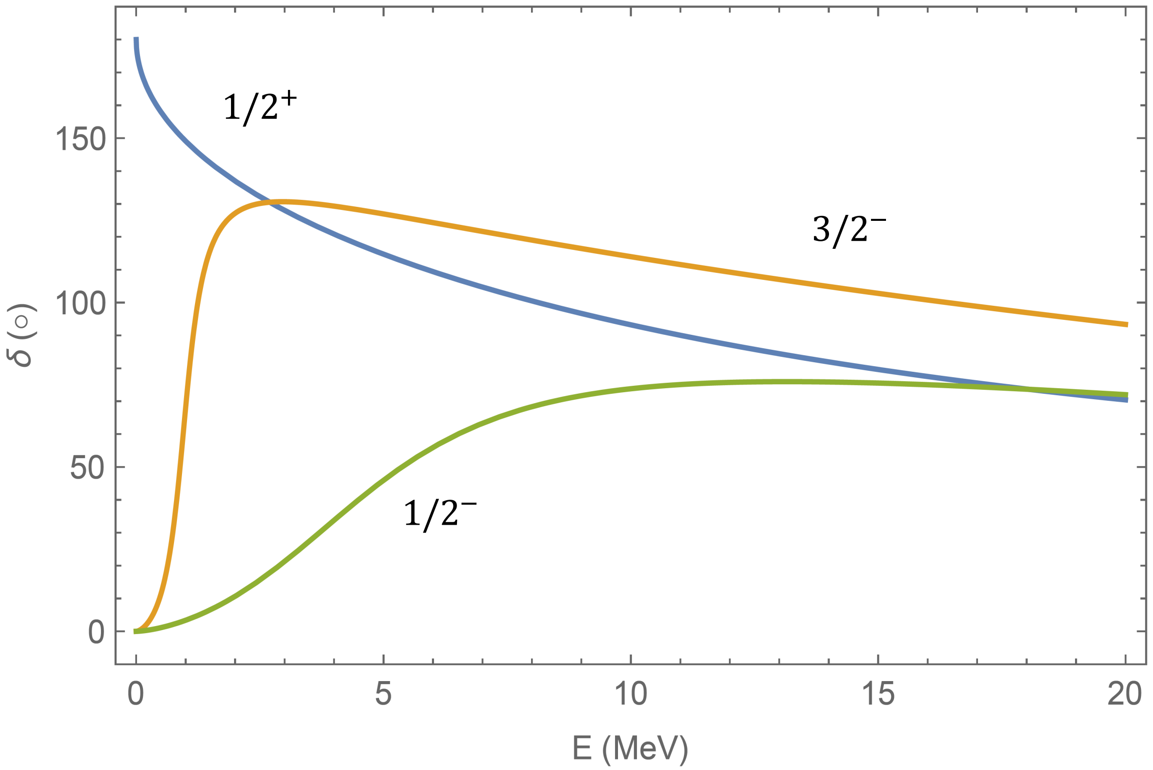


Where to collect "data" impacts phase-shift extraction, i.e., experimental design is relevant here!

n − α system

$$V_s(r) = \begin{cases} V_0(1+\beta \boldsymbol{L}\cdot\boldsymbol{\sigma}) & \text{when } r < r_c \\ 0 & \text{when } r > r_c \end{cases}$$

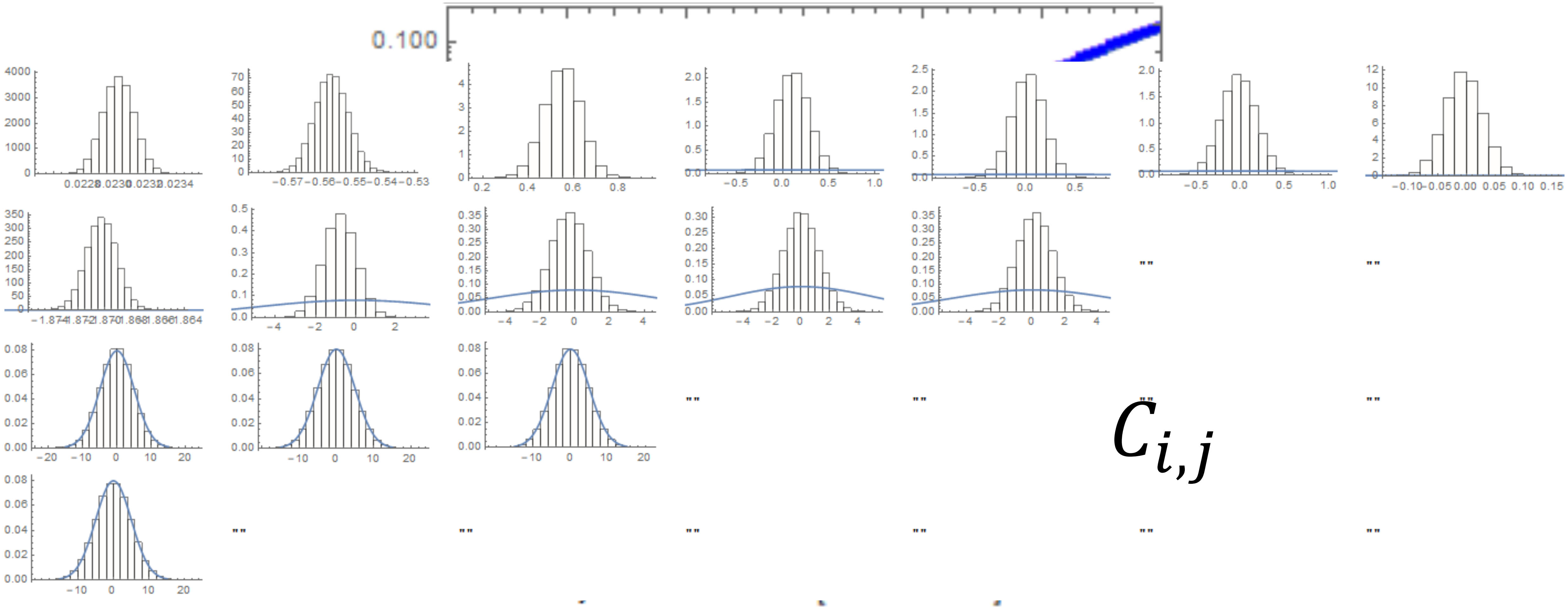
$V_0 = 33$ MeV
$\beta = 0.103,$
$r_c = 2.55$fm



Note $\Lambda = 200\ MeV$ from α excitation energy

S.Ali et.al., RMP **57,** 923 (1985)

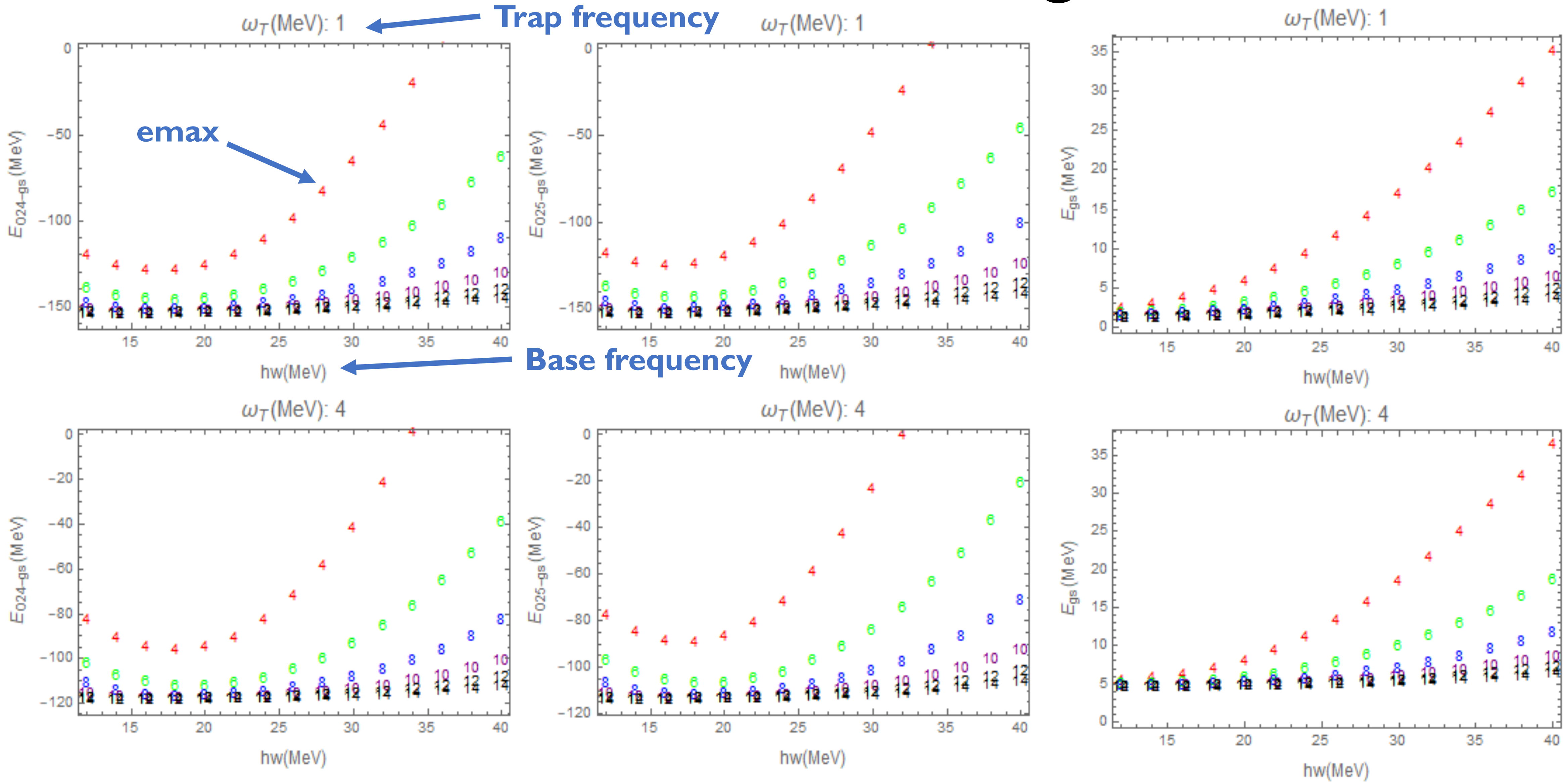
$3/2^{-}$ at N6LO assuming zero data error bar



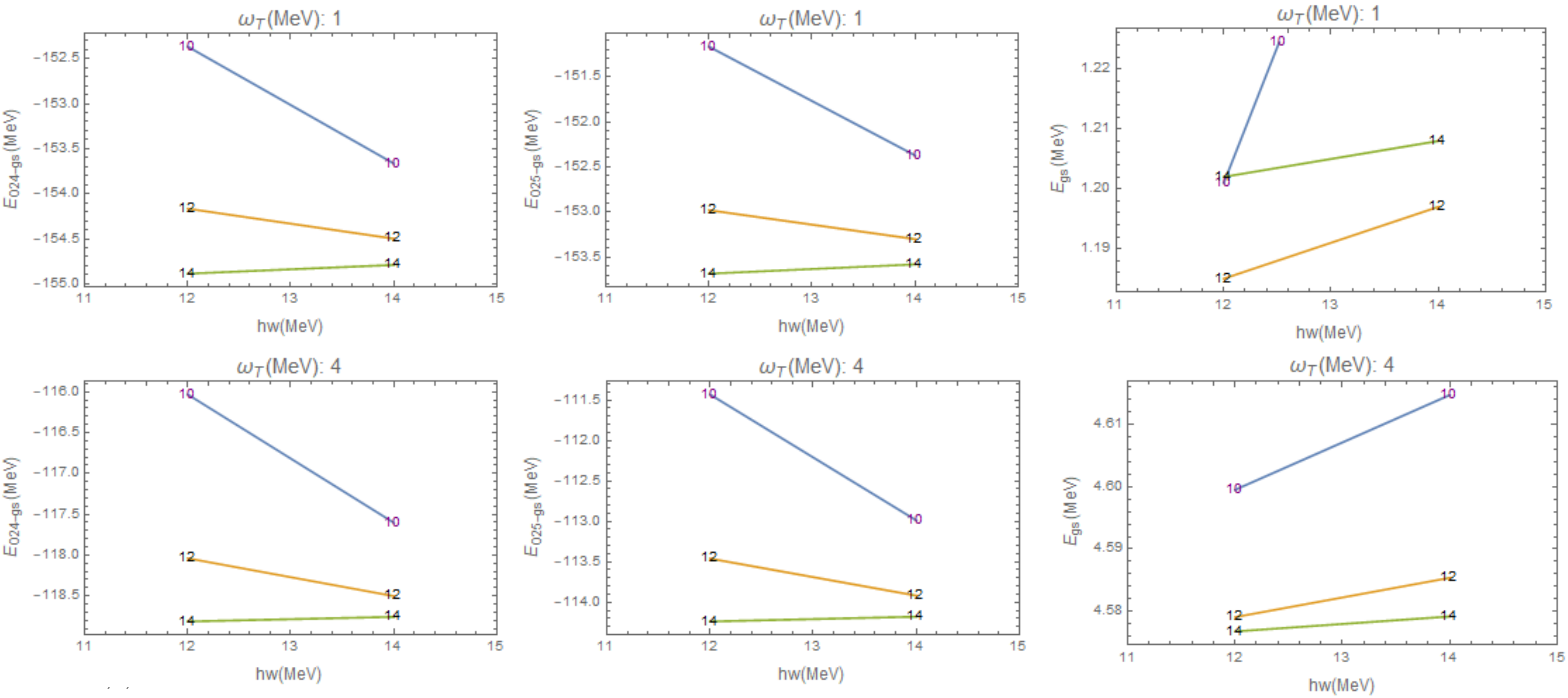
Confront the reality:
$n - {}^{24}O$ in 3/2+ channel (d wave)

In collaboration with the "IMSRG" group: Chan Gwak, Ragnar Stroberg, and Jason Holt

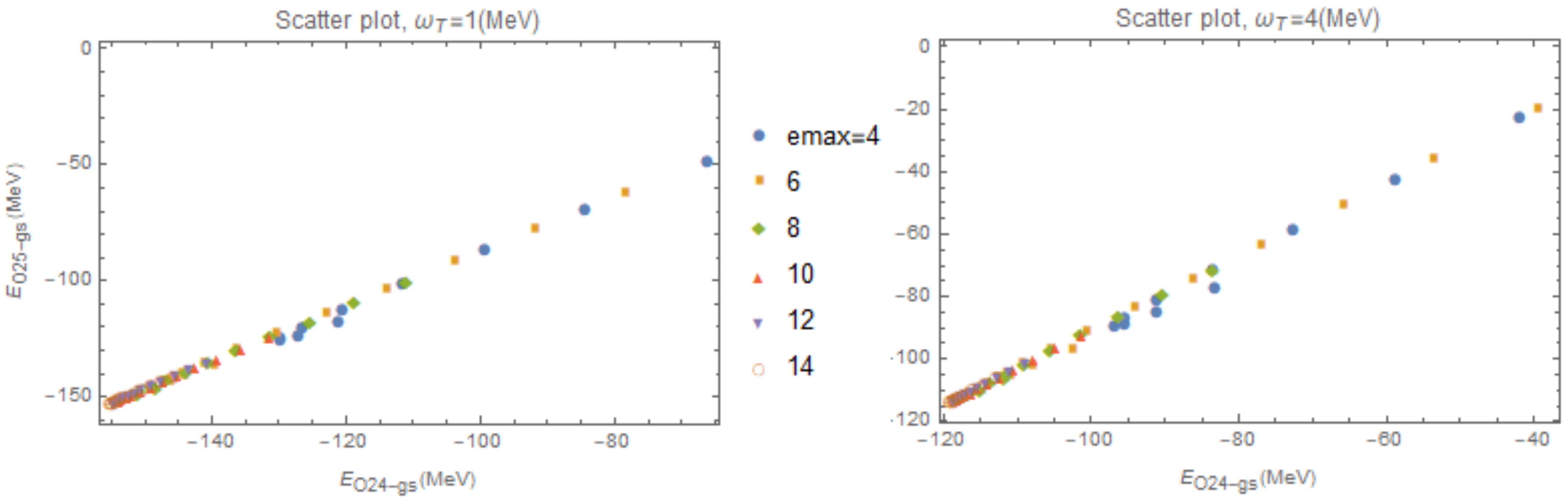
Raw “data” for ^{24}O and ^{25}O ground states



Look more closely

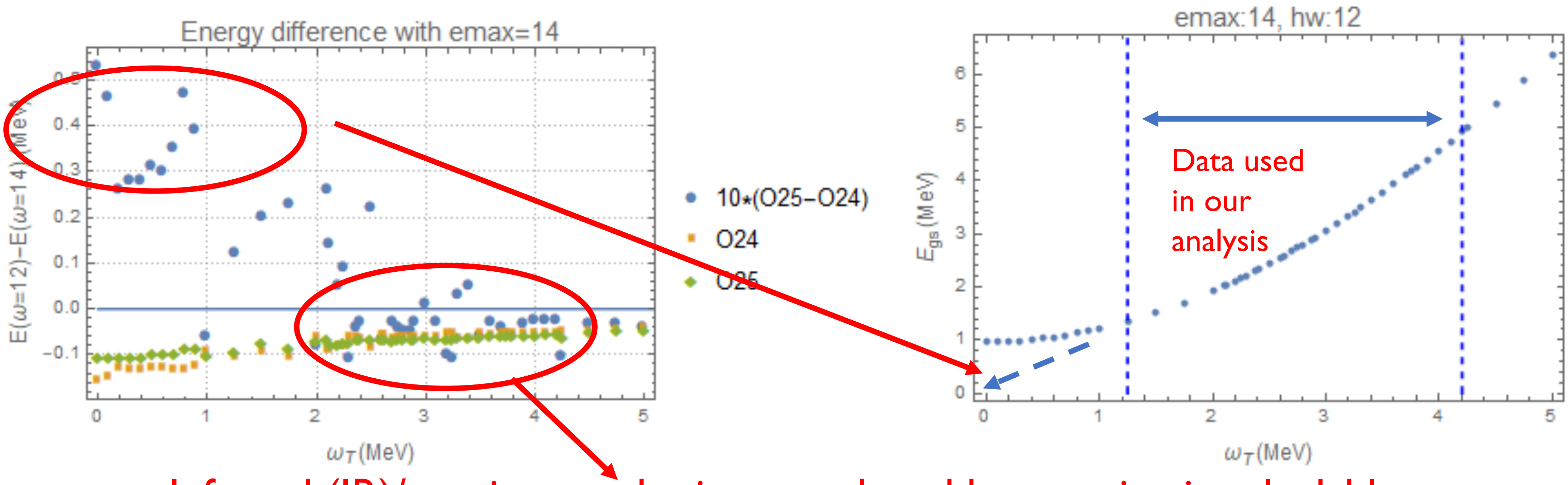


What is going on?



- For a given emax, different points have different hw from 12 to 40 MeV
- It suggests:
  1. O24 itself and the O24 in O25 in the same trap have similar ultraviolet (UV) error;
  2. the UV error dominates

Interesting correlation



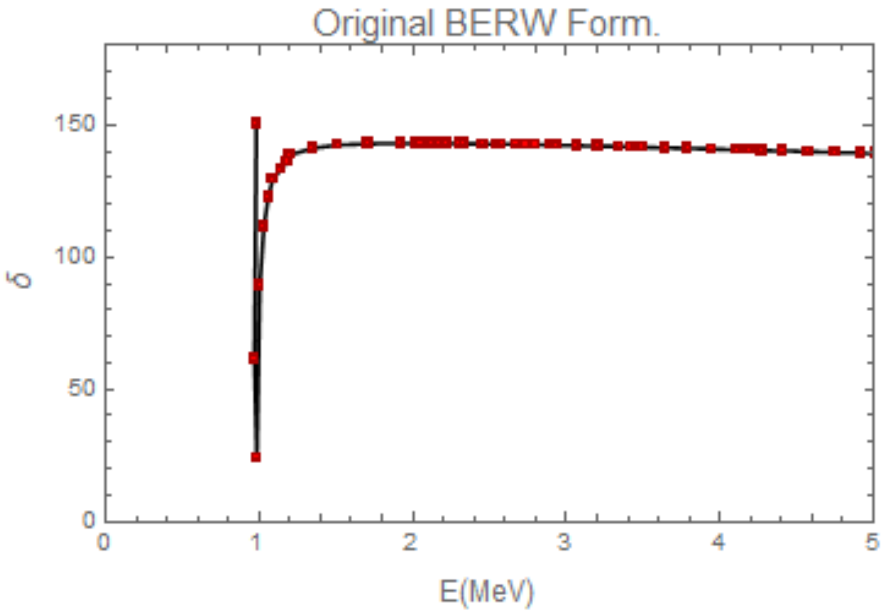
Infrared (IR)/continuum physics as reduced by trapping is calculable using current ab initio structure calculation !

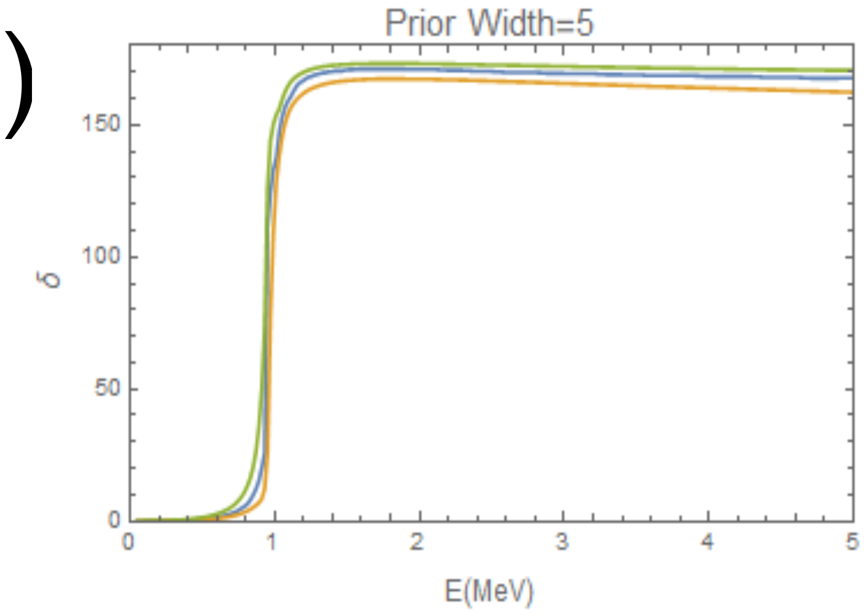
With R. Furnstahl and J. Melendez, we start studying the errors of ab initio output to give proper weight to these data to improve phase-shift analysis

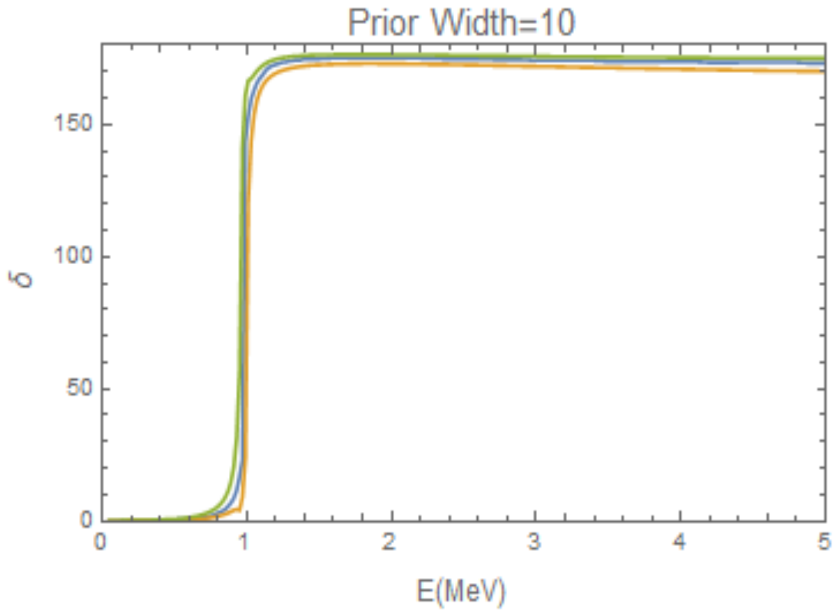
Preliminary results (N4LO)

$$\mathrm{pr}(\mathbf{C}|\mathrm{I}) \propto Exp[-\frac{\mathbf{C}^2}{2(PW)^2}]$$

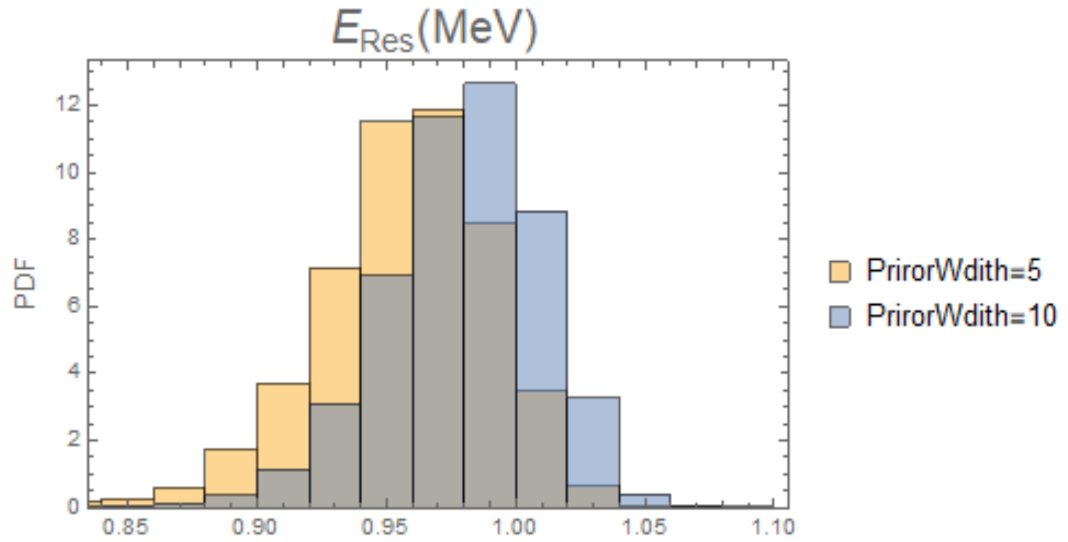
Note $\Lambda \approx 100\ MeV$
from O24's excitation energy

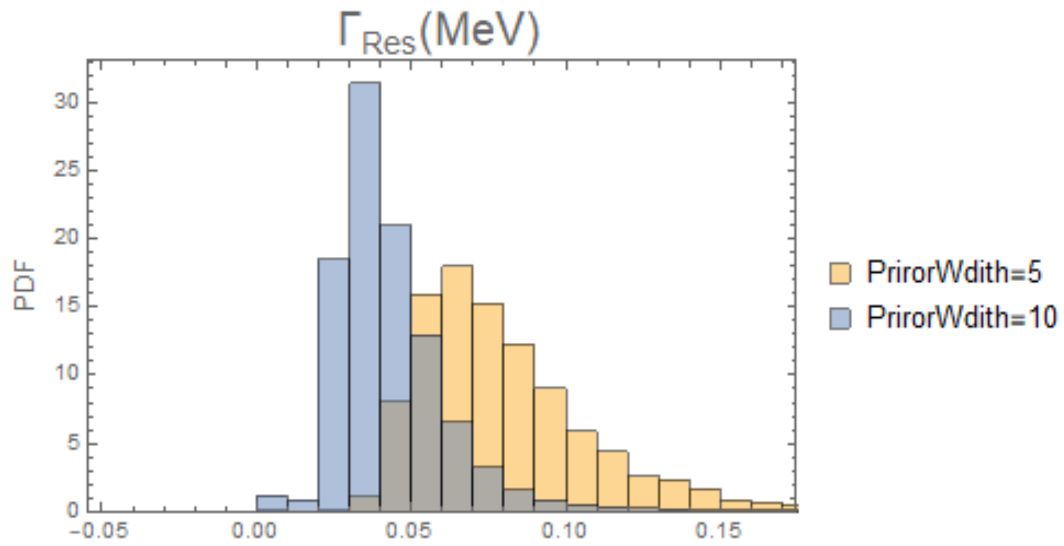


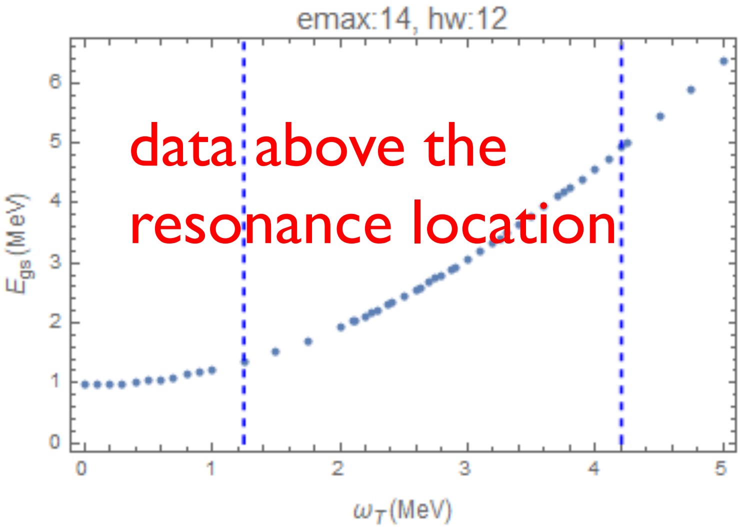




3/2+ resonance properties







$$E_{Res} = 0.959 - 0.029 + 0.036\, MeV\ (PW = 5)$$
$$0.983 - 0.029 + 0.033\ \ MeV (PW = 10\ )$$

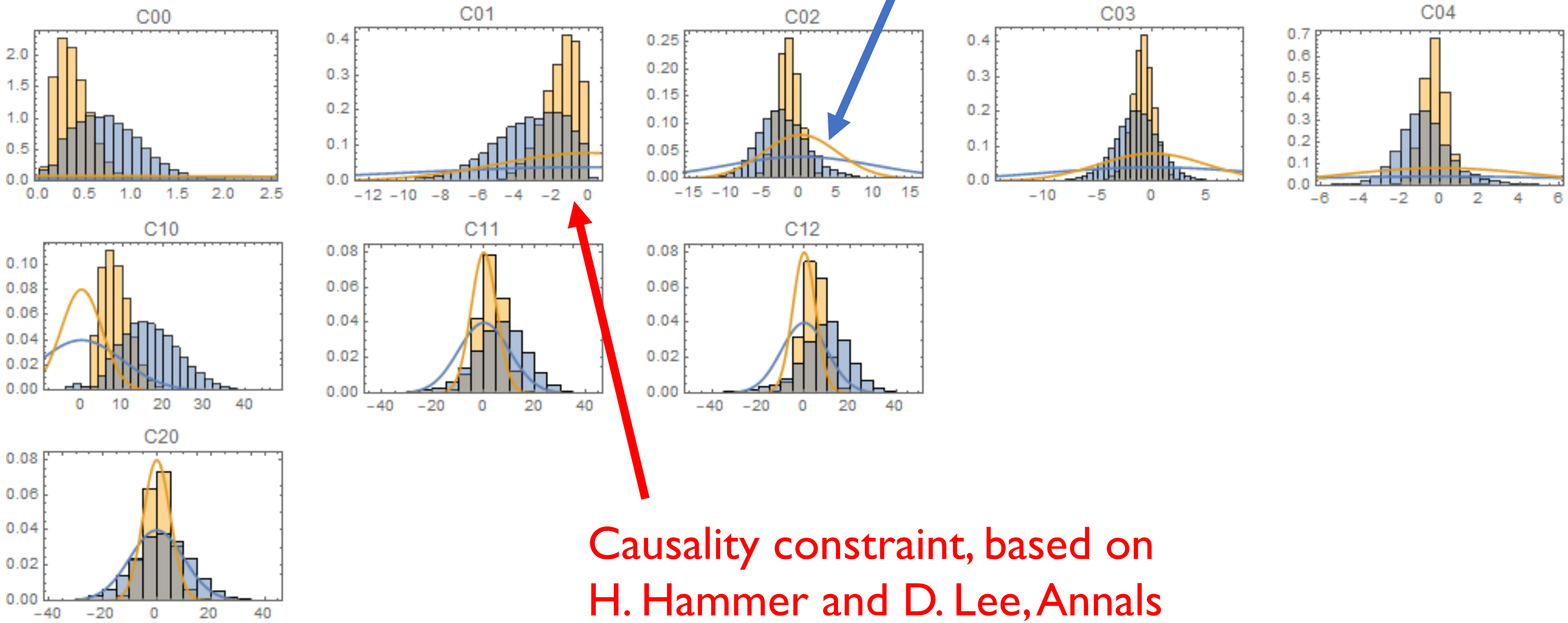
$$\Gamma_{Res} = 65.1 - 18.4 + 28.5\, keV\ (PW = 5)$$
$$33.8 - 9.9 + 17.2\, keV\ (PW = 10)$$

$$E_{Res} \approx 0.75\, MeV, \Gamma_{Res} \approx 90\, keV\ \ PRC.96.054322(2017)$$

The IR/continuum physics information in the erroneous eigen-energies can be recovered and translated to the scattering phase shift

C’s distributions

Two different PWs

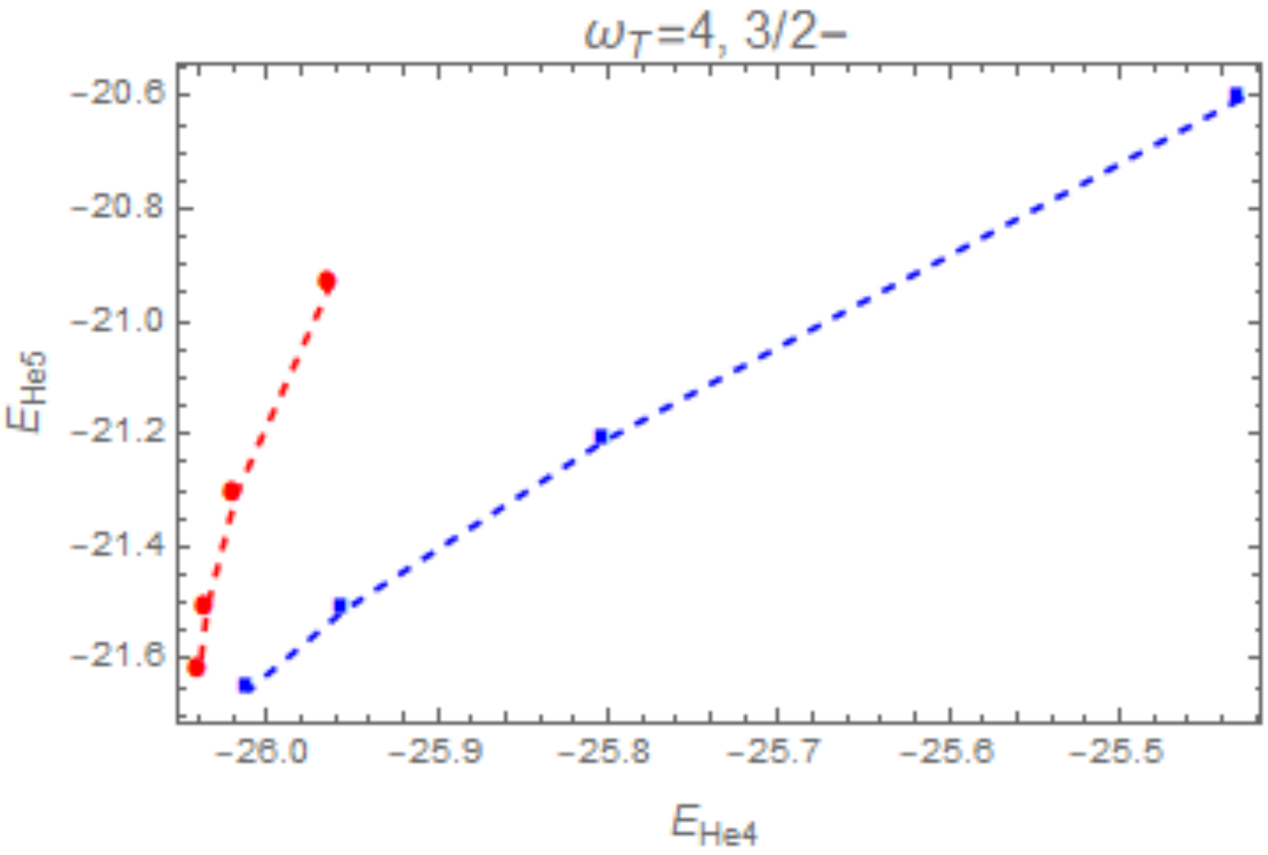


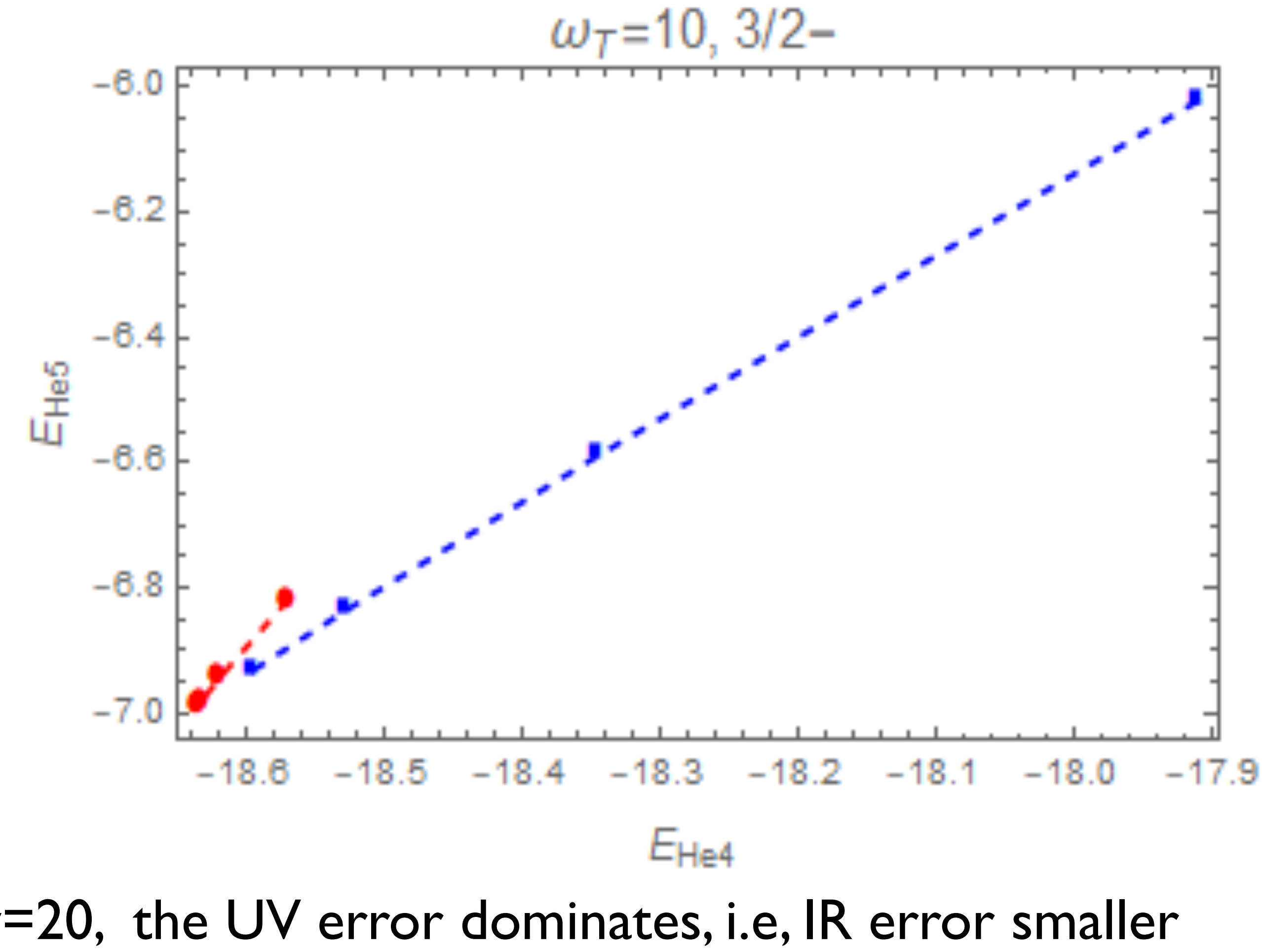
Causality constraint, based on H. Hammer and D. Lee, Annals of Physics 325, 2212 (2010)

Confront the reality:
$\mathrm{n} - \alpha$ in resonance and non-resonance channels

In collaboration Petr Navratil

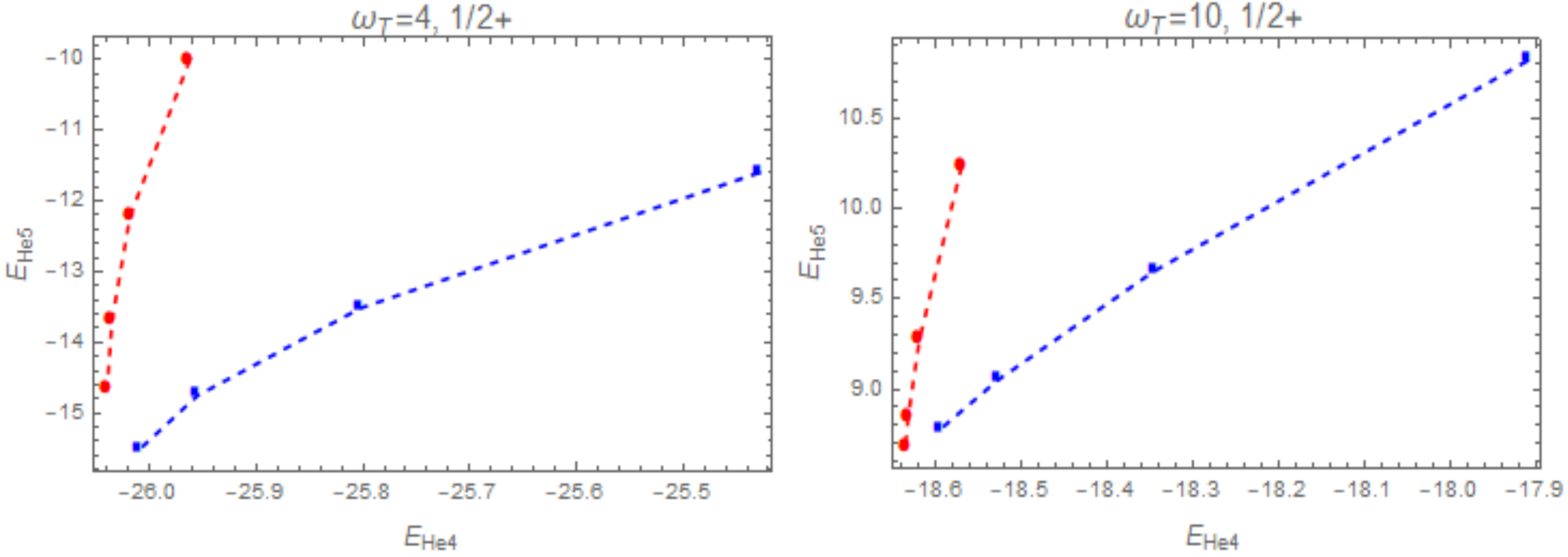
Large hw vs Low hw: hw=28, 20 MeV with Nmax 10 to 16





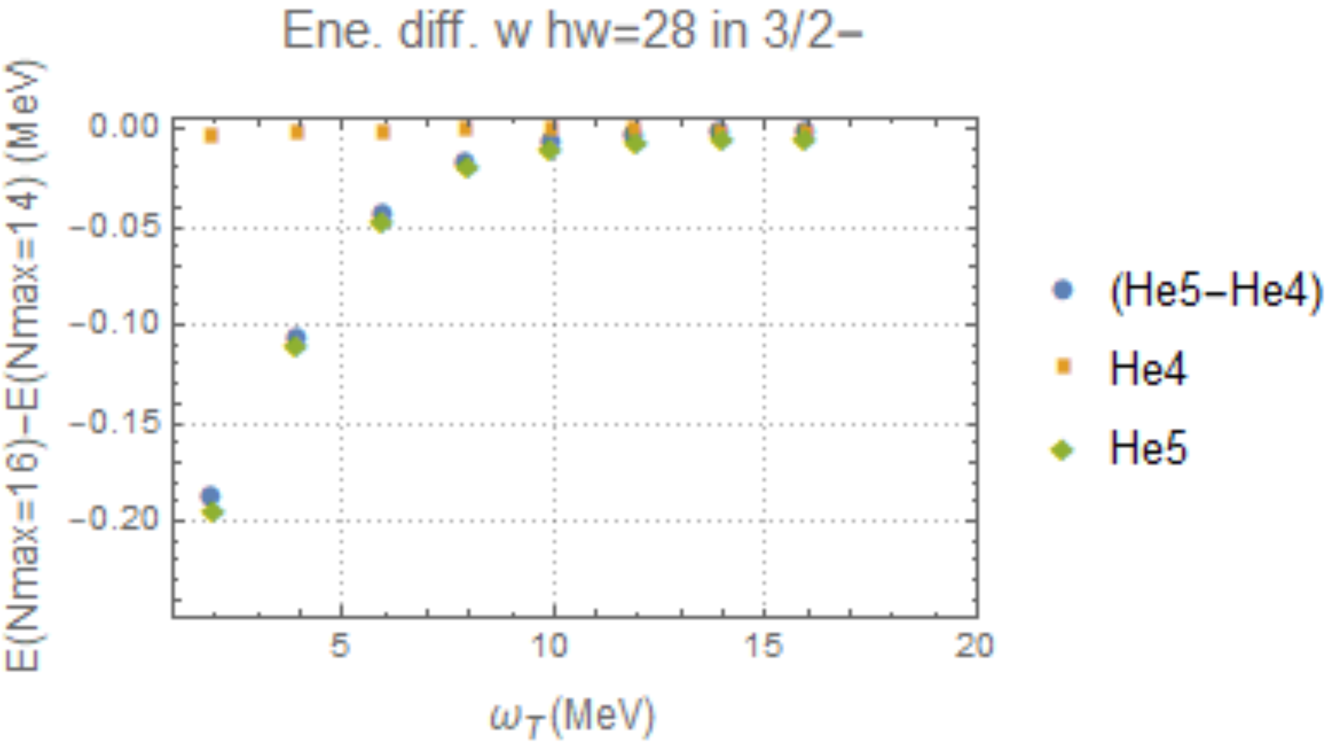
- With hw=20, the UV error dominates, i.e, IR error smaller
- With hw=28, the IR error dominates

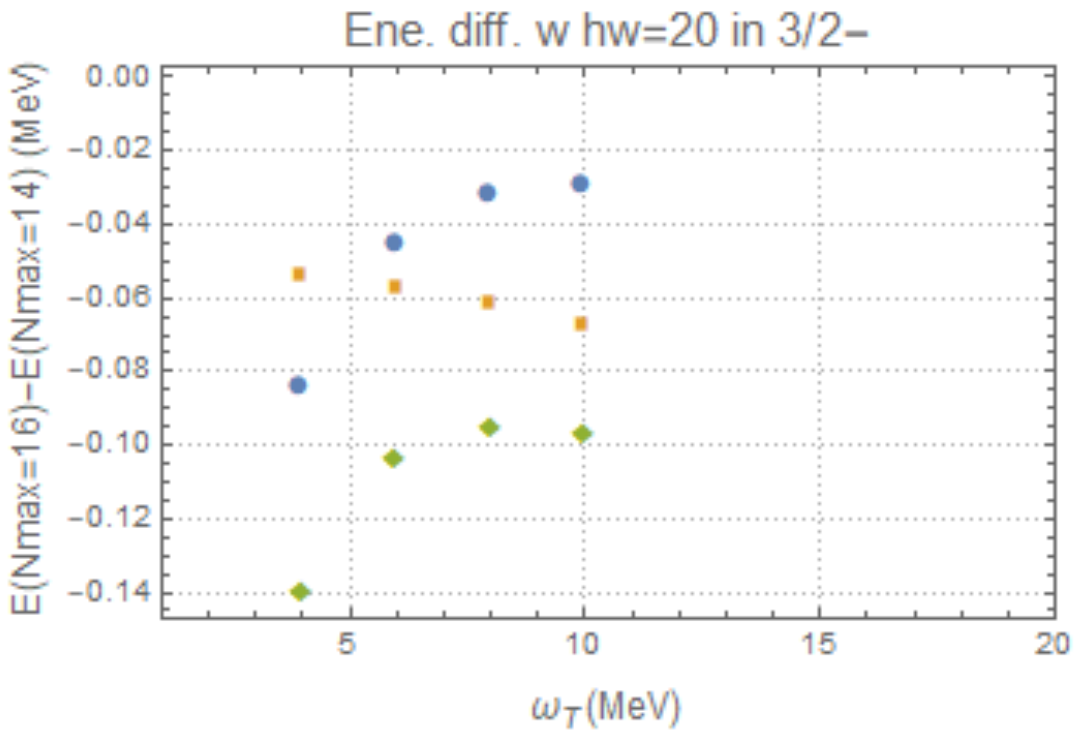
Large hw vs Low hw: hw =28, 20 MeV with Nmax 10 to 16



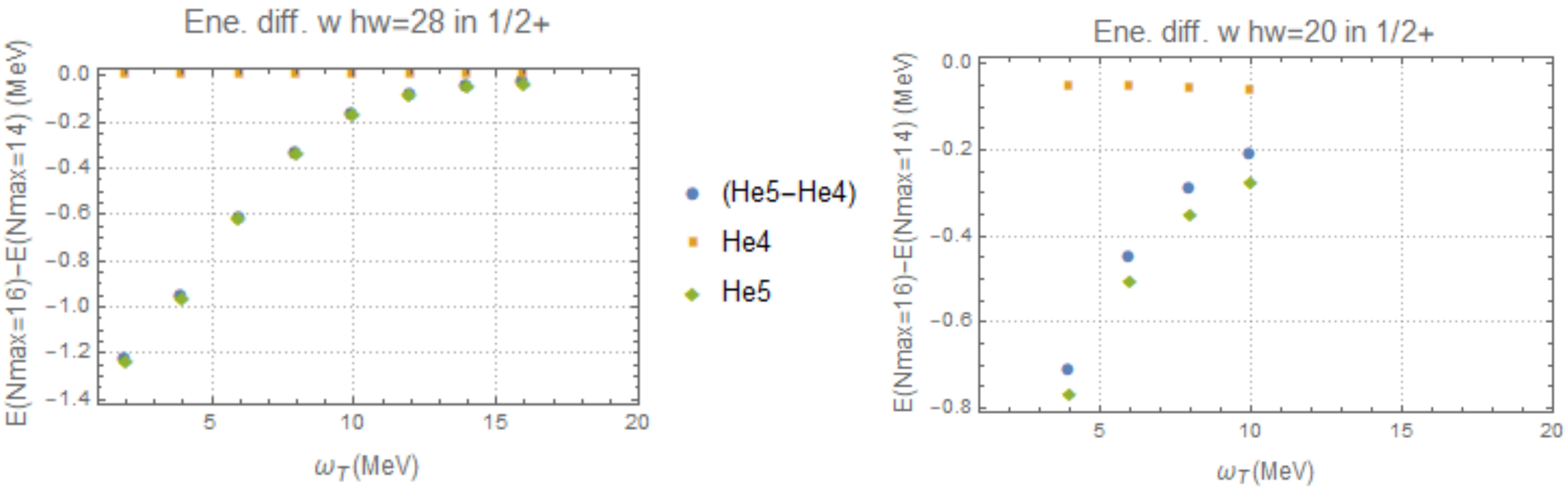
- Similar trend as in resonance channel
- However compare the s-wave (nonres) to p-wave, for the same trap, the IR size expands
- Tightening trap reduces IR physics

Look at difference between Nmax=16 and Nmax=14, fixing hw



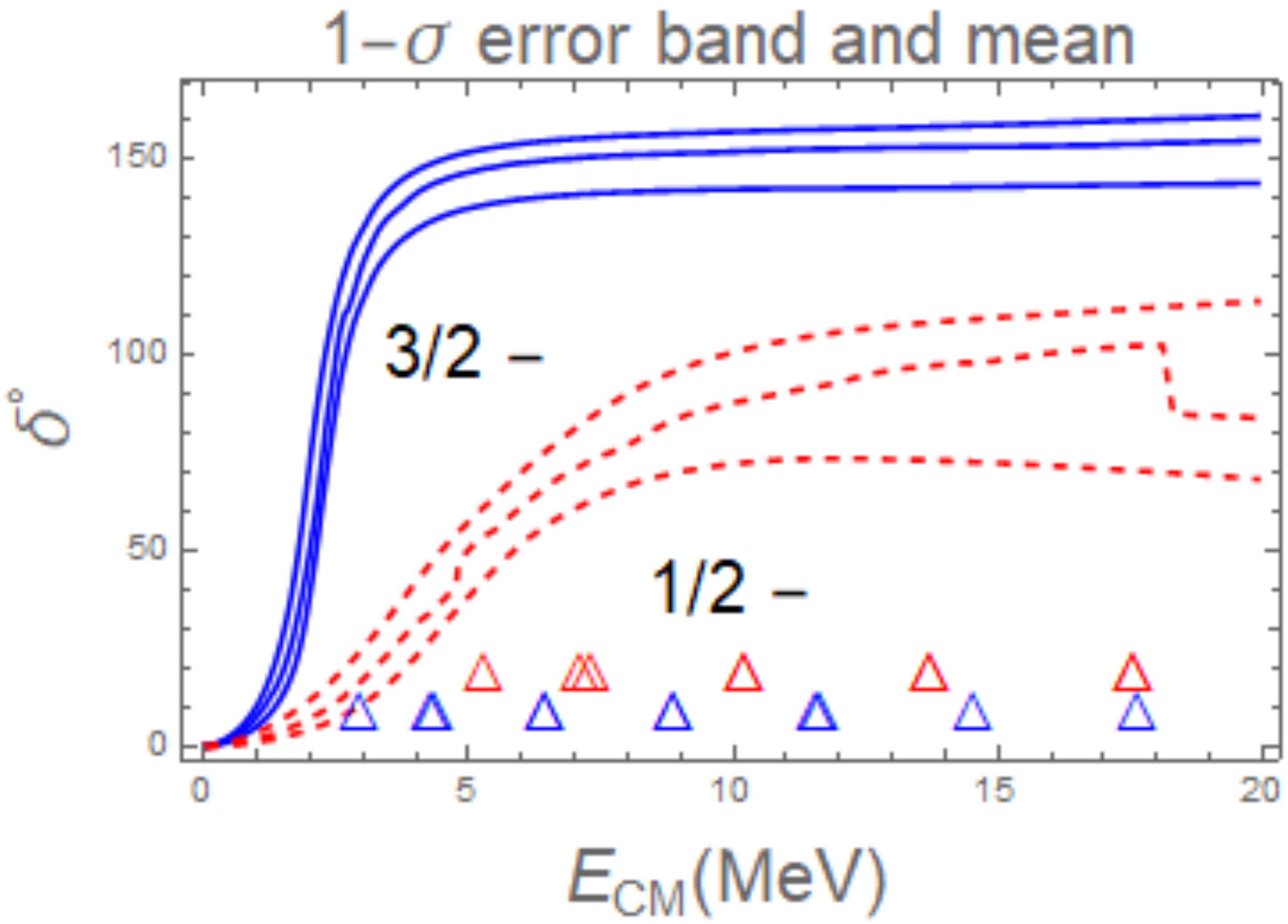


Look at difference between Nmax=16 and Nmax=14, fixing hw

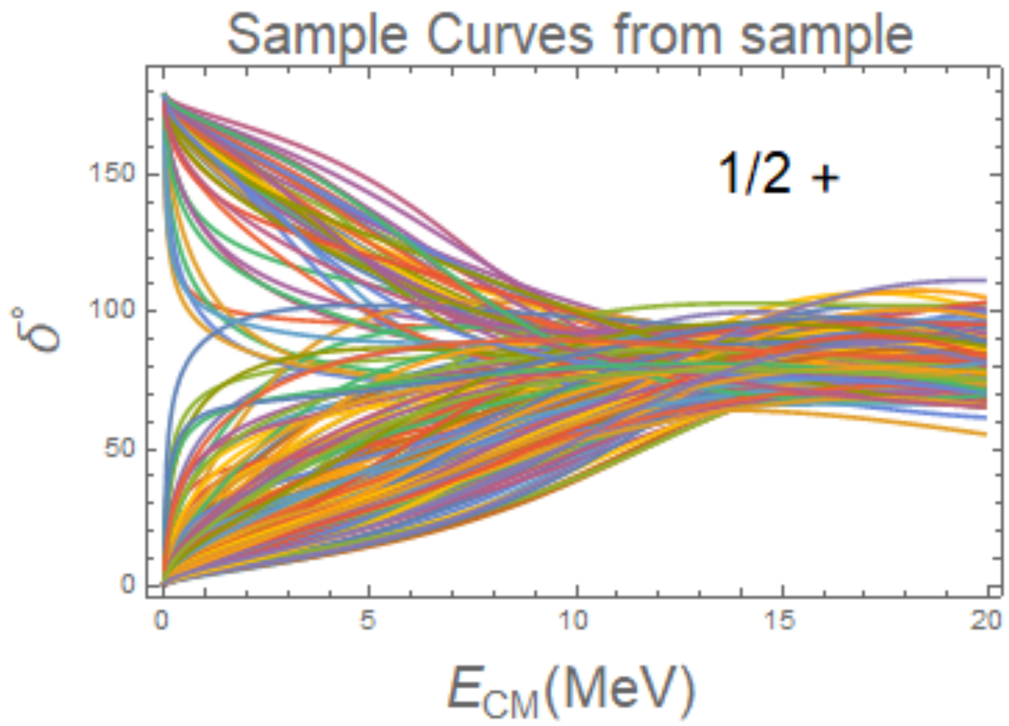


Take advantage of the UV error correlation, focus computational resource on the IR physics.

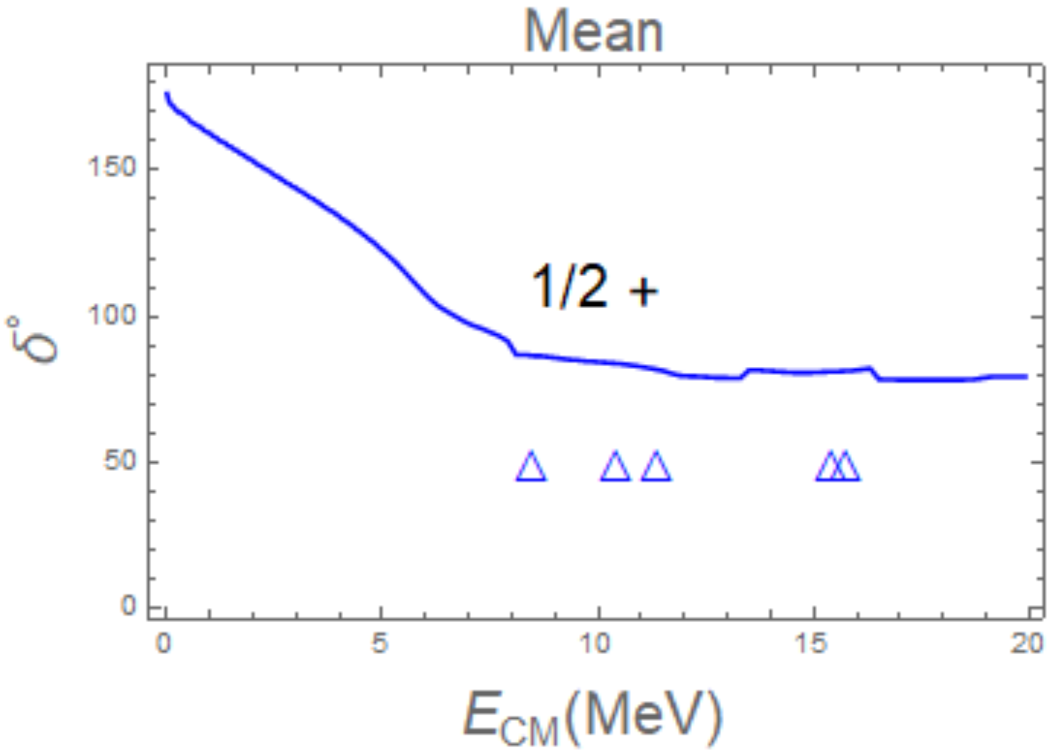
Very preliminary results (N4LO)



Very preliminary results (N4LO) given limited data so-far



Require positive effective range

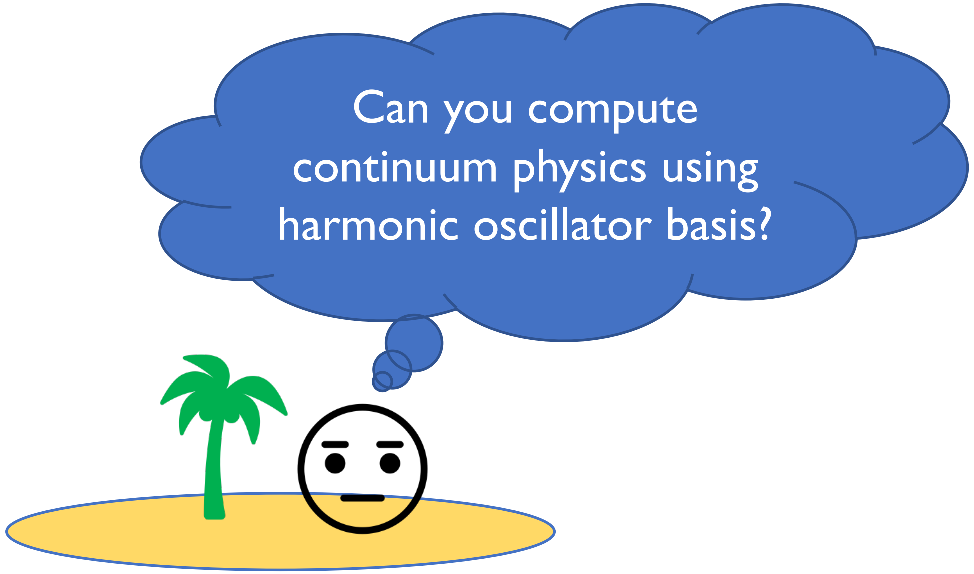


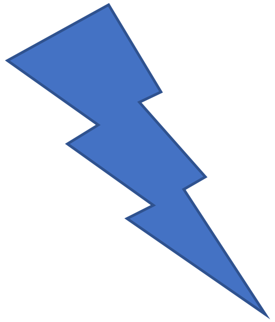
Summary

- The improved BERW formula can be used to infer scattering from structure calculation:
  - precision calculation for NN system
  - In $\mathrm{n} - ^{24}O$ d-wave scattering in 3/2+ channel, a narrow resonance is extracted with 10s keV error (so perhaps 1keV-precision prediction of threshold is not a dream!)
  - In $\mathrm{n} - \alpha$ p-wave scatterings, resonances are seen
  - In $\mathrm{n} - \alpha$ s-wave scattering, no resonance is seen, in agreement with previous studies. The method is not limited to studying resonance
- The error analysis (including correlation) of the ab initio output is interesting and important
- In retrospect:
  - the continuum phys. can be computed reliably even using just harmonic osc. basis. However this requires proper set up of "expt." and choice of "observable" to "measure". Trapping system reduces the continuum phys.---but not eliminating it--to a level that can be handled by current ab initio structure method
  - the minimum requirement on the structure calculation suggests the applicability of this approach for studying larger systems. Meanwhile, the ab initio output adds another dimension to the information source for studying scattering and reaction in the framework of cluster theory. This is to echo the point made in the last year's FRIB Theory alliance workshop in June: *need to find a way to bridge structure and reaction studies*

Outlook

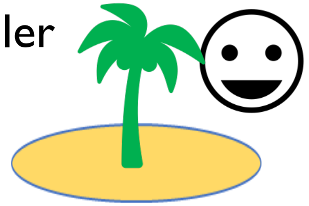
- Will soon study carbon isotopes
- Better "data", better "experimental" design, better analysis (PW, Λ) →better phase shift
- Consider generalizing it to study two-cluster reactions and three-cluster systems
- Consider the connection between this method and the infrared extrapolation used in structure calculation





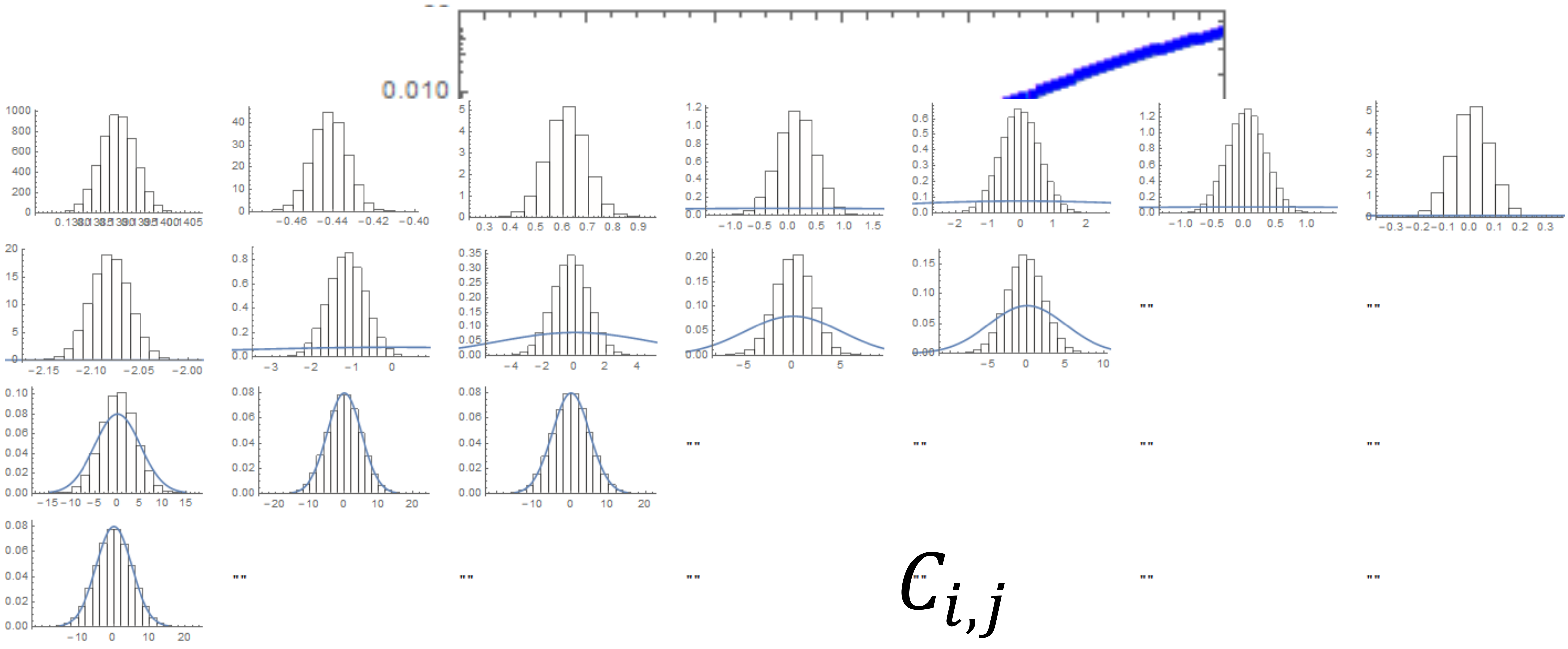
Nuts! Only possible at infinite Hilbert space! Or work for Petr!

You can do it here, if you make systems smaller



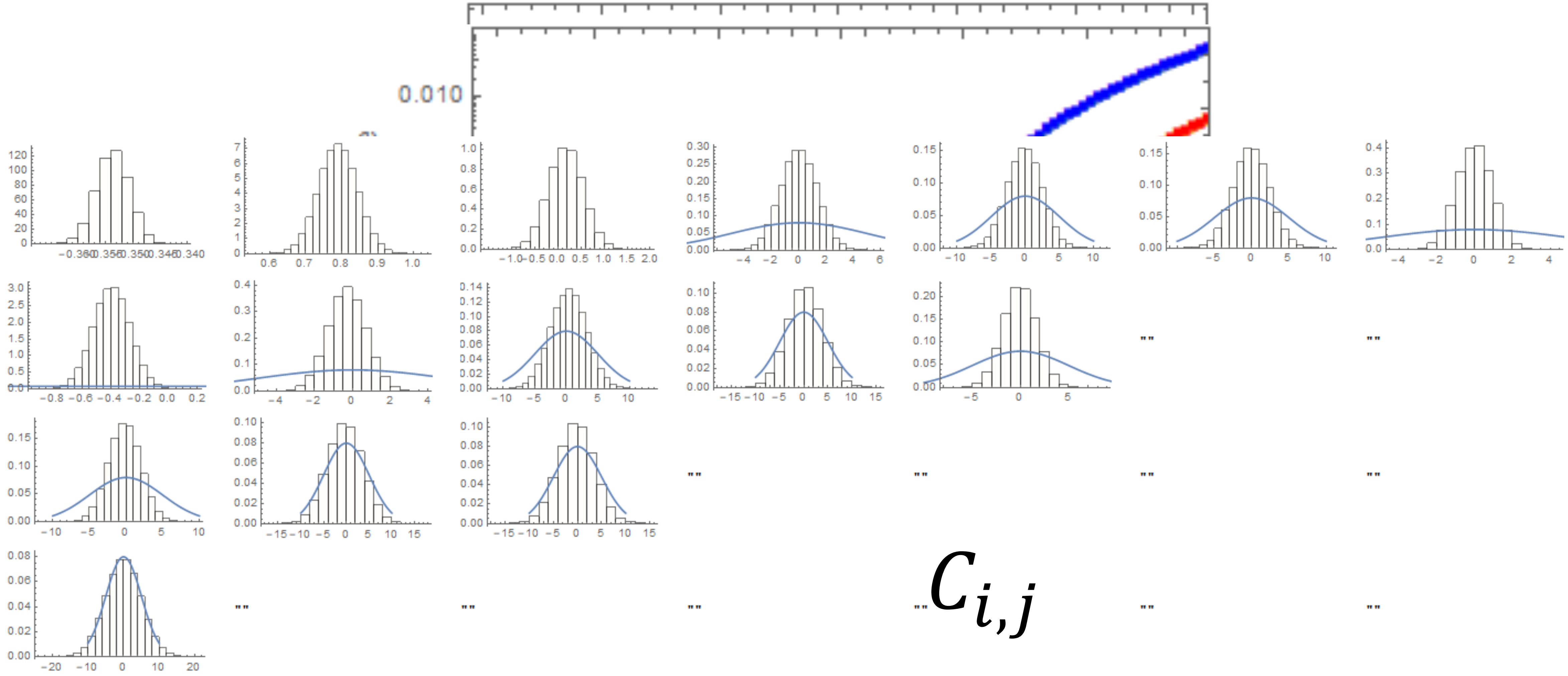
Back up

$1/2^-$ at N6LO



$C_{i,j}$

1/2$^+$ at N6LO



$C_{i,j}$