Scattering Applications with the Ab Initio No Core Shell Model

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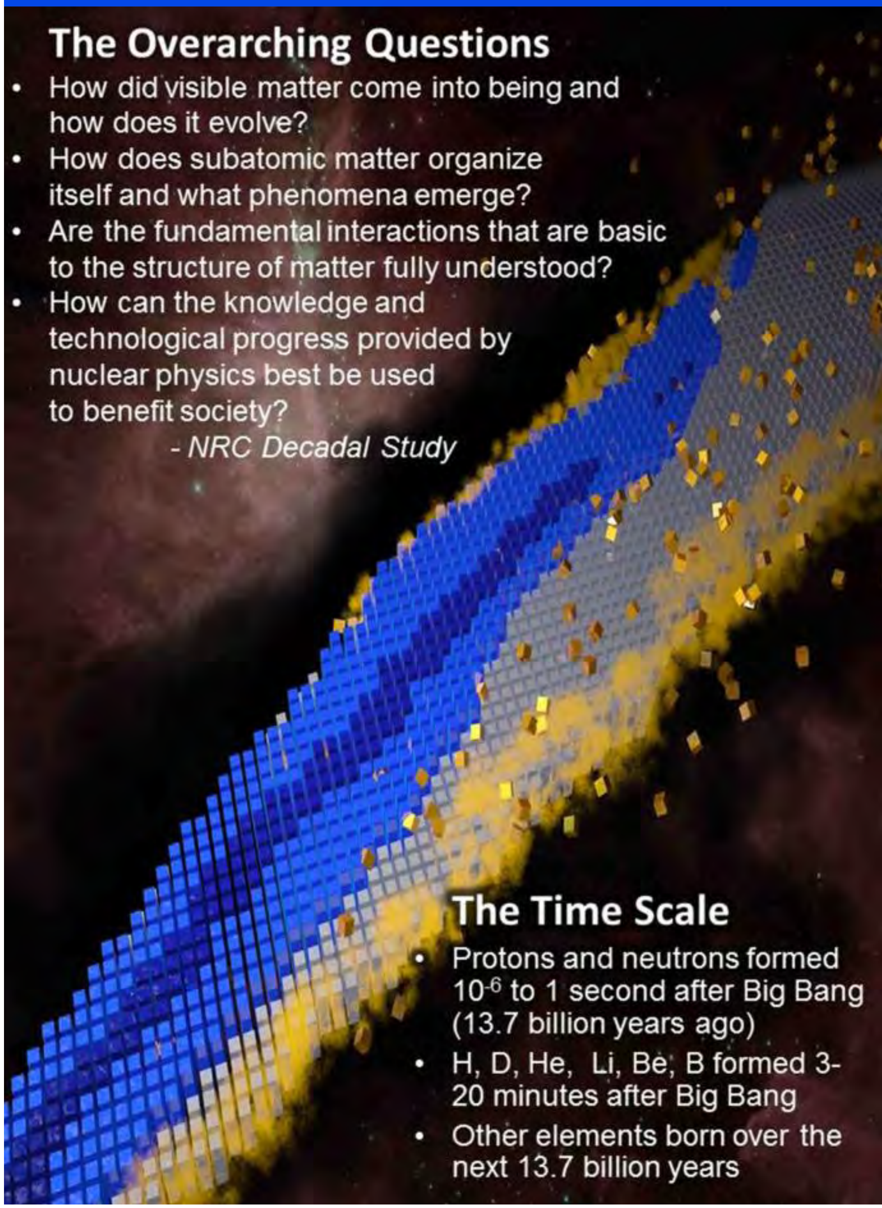
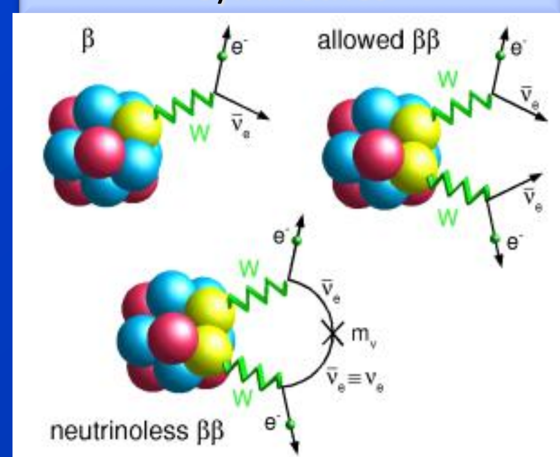


LENPIC

Topical Collaboration on Neutrinos and Fundamental Symmetries



Scattering Applications with the Ab Initio No-Core Shell Model
Two Approaches

"SS-HORSE"

Single State – Harmonic Oscillator Representation of Scattering Equations

For elastic scattering resonances – can be broad resonances

^{7}He (n + ^{6}He channel)

Tetraneutron (democratic decay)

"tBF"

Time-dependent Basis Function

For elastic and inelastic scattering

Sub-barrier Coulomb dissociation of deuteron by ^{208}Pb

Common features:

Employ NCSM results for bound and unbound states

Non-perturbative treatment of scattering without phenomenological optical potentials

Can employ chiral EFT interactions (strong and EM) in scattering applications

Systematically improvable

General idea of the HORSE formalism

"Harmonic Oscillator Representation of Scattering Equations"

$$T \;+\; V$$

NCSM with:

$\lambda(N,\hbar\Omega)$ & $\Lambda(N,\hbar\Omega)$

Infinite set of algebraic equations in HO basis of relative motion:

$$\sum_{n'=0}^{N}\left(T^{l}_{nn'}+V^{l}_{nn'}-\delta_{nn'}E\right)a_{n'l}(E)=0. \qquad n\le N-1$$

Matching condition at $n = N$

$$\sum_{n'=0}^{N}\left(T^{l}_{Nn'}+V^{l}_{Nn'}-\delta_{Nn'}E\right)a_{n'l}(E)+T^{l}_{N,N+1}a_{N+1,l}(E)=0. \quad n\le N-1$$

Then for $n\ge N+1$

$$\sum_{n'=0}^{\infty}\left(T^{l}_{nn'}-\delta_{nn'}E\right)a_{n'l}(E)=0,\ \text{which produces:}$$

$$T^{l}_{n,n-1}a_{n-1,l}(E)+\left(T^{l}_{nn}-E\right)a_{nl}(E)+T^{l}_{n,n+1}a_{n+1,l}(E)=0.$$

"think outside the box"=> T

Arises as a natural extension of NCSM where both potential and kinetic energies are truncated

This is an exactly solvable algebraic problem!

Single-State HORSE (SS-HORSE)

$$\sum_{n'=0}^{N} H^{l}_{nn'} \langle n' | \lambda \rangle = E_\lambda \langle n | \lambda \rangle, \qquad n \le N$$

$$(H-E)^{-1}_{nn'} \equiv -G_{nn'} = \sum_{\lambda'=0}^{N} \frac{\langle n|\lambda'\rangle\langle\lambda'|n'\rangle}{E_{\lambda'}-E}$$

Standard HORSE

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN} T^{l}_{N,N+1} S_{N+1,l}(E)}{C_{Nl}(E) - G_{NN} T^{l}_{N,N+1} C_{N+1,l}(E)}. \quad \text{Also, S-matrix} = \mathrm{S}(G_{NN})$$

Suppose $E = E_{\lambda'}$ ⟵ Single-State HORSE

$$\tan\delta(E_\lambda) = \frac{S_{N+1,l}(E_\lambda)}{C_{N+1,l}(E_\lambda)} = (-1)^l q^{2l+1} \Gamma(-l+\tfrac{1}{2}) \frac{L^{l+1/2}_{(N-l)/2}(q^2)}{\Phi(-N/2 - l/2 - 1/2, -l+1/2; q^2)}$$

where $L^{l+1/2}_{(N-l)/2}$ are associated Laguerre polynomials, Φ are confluent hyper-

geometric functions and $q = \sqrt{\dfrac{2E_\lambda}{\hbar\Omega}}$.

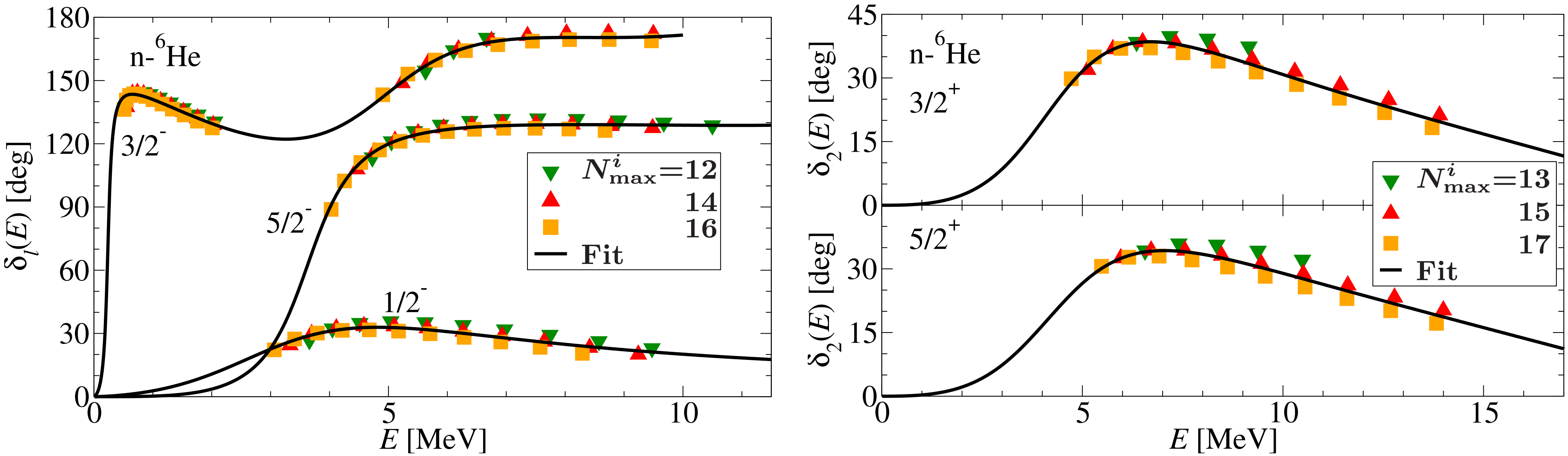
E_λ are (obtained from) eigenvalues of the NCSM (for given $\hbar\Omega$ and N_{max}). Once a scattering channel is defined (sets the continuum energy scale) the phase shift is calculated. Ananlog of Lüscher's method for a plane-wave basis.

A.M. Shirokov, A.I. Mazur, I.A. Mazur and J.P. Vary, PRC 94, 064320 (2016); arXiv:1608.05885

Resonances in Exotic ^{7}He Nucleus within the No-Core Shell Model

I. A. Mazur,[1,2] A. M. Shirokov,[2,3,4] I. J. Shin,[5] A. I. Mazur,[2] Y. Kim,[5] P. Maris,[4] and J. P. Vary[4]

arXiv: 2001.08898



Once the converged phase shifts are obtained via SS-HORSE, proceed to analyze:
Phase shifts -> S-matrix -> complex poles of the S-matrix

Use the spread of the phase shifts to determine resonance uncertainties.

Experiments: stripping/pickup reactions, IAS studies, one neutron knockout from ^{8}He

SS-HORSE (Daejeon16) agrees with Experiment, GSM and NCSMC for two resonances

TABLE II: Energies E_r (relative to the $n+{}^6$He threshold) and widths of resonant states in ^{7}He nucleus. Our estimate of the uncertainties of the quoted results are presented in parentheses. The available results of the GSM calculations [24] in the *psdf* valence space and of the NCSMC calculations [25], [26] with SRG-evolved N^{3}LO chiral NN force together with experimental data are shown for comparison. All values are in MeV.

		This work	GSM	NCSMC	Experiment		
						[20]	
	E_r^1	0.24(6)	0.39	0.71		0.430(3)	
$3/2^-$	Γ^1	0.11(2)	0.178	0.30		0.182(5)	
	E_r^2	4.9(3)					
	Γ^2	3.1(3)					
					[21]	[22]	[23]
$1/2^-$	E_r	2.7(4)		2.39	3.0(5)	3.5	1.0(1)
	Γ	4.3(3)		2.89	2	10	0.75(8)
						[19]	
$5/2^-$	E_r	3.63(18)	3.47(2)	3.13		3.36(9)	
	Γ	1.36(3)	2.3(3)	1.07		1.99(17)	
$3/2^+$	E_r	4.1(3)					
	Γ	4.4(5)					
$5/2^+$	E_r	4.2(5)					
	Γ	5.0(5)					

SS-HORSE (Daejeon16) predicts 4 more resonances (1/2- ~ NCSMC) that could help explain conflicting Experiments

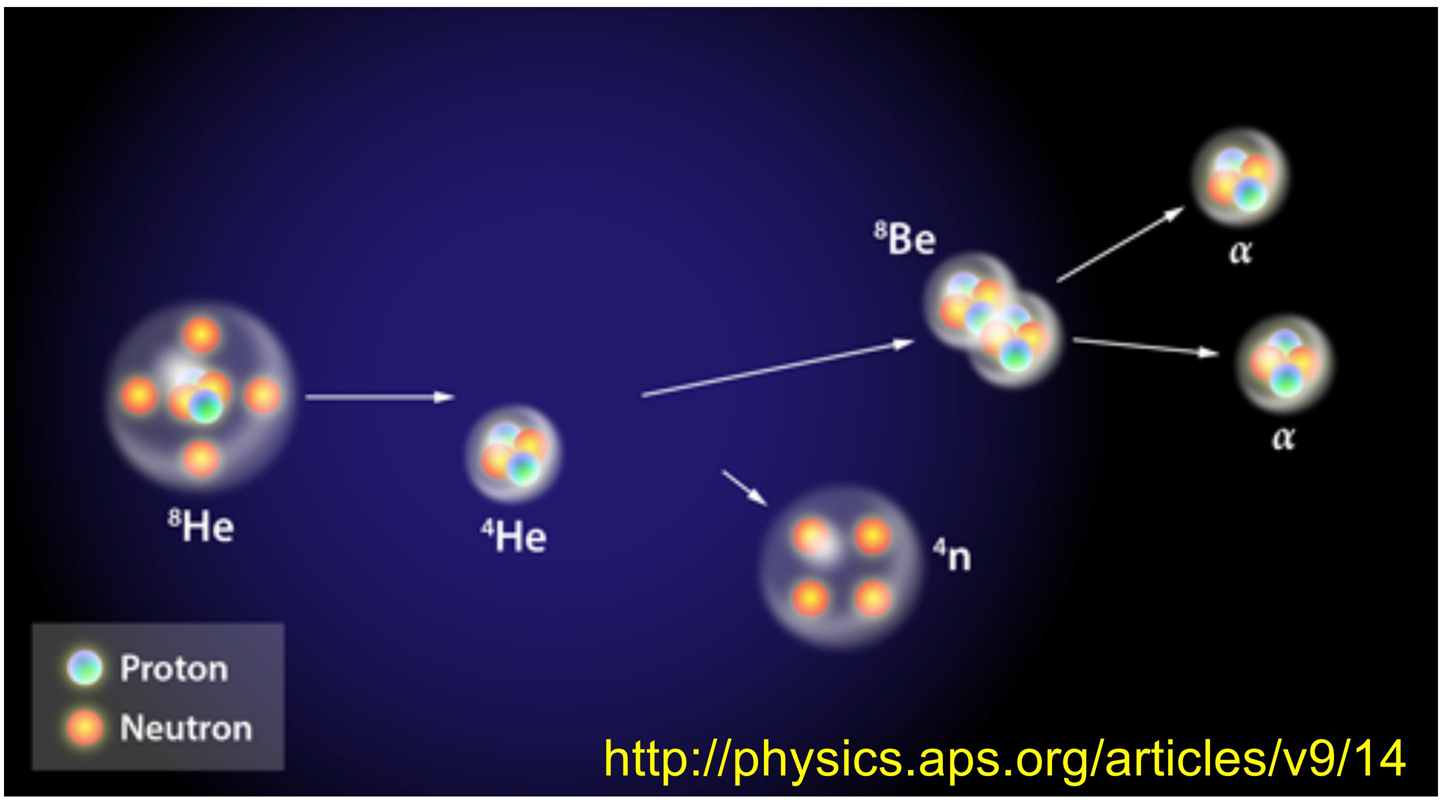
I.A. Mazur, et al., arXiv: 2001.08898

PHYSICAL REVIEW LETTERS

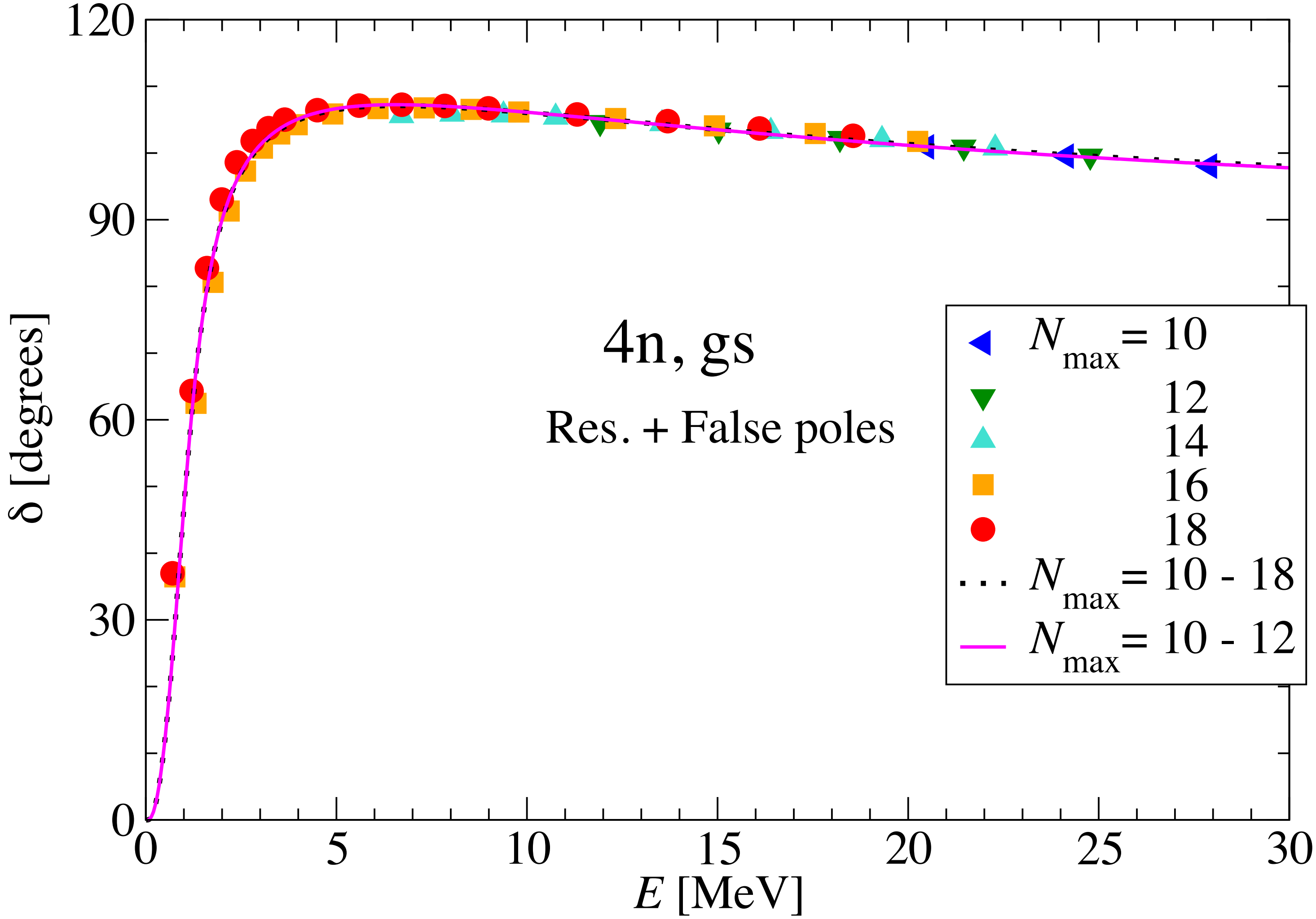
Candidate Resonant Tetraneutron State Populated by the $^{4}\mathrm{He}(^{8}\mathrm{He}, ^{8}\mathrm{Be})$ Reaction

K. Kisamori *et al.*

Phys. Rev. Lett. **116**, 052501 – Published 3 February 2016



Tetraneutron, JISP16



N_{max} =10-12 resonance params:
E_r = 844 keV, Γ = 1.378 MeV,
E_{false} = -55 keV.

vs

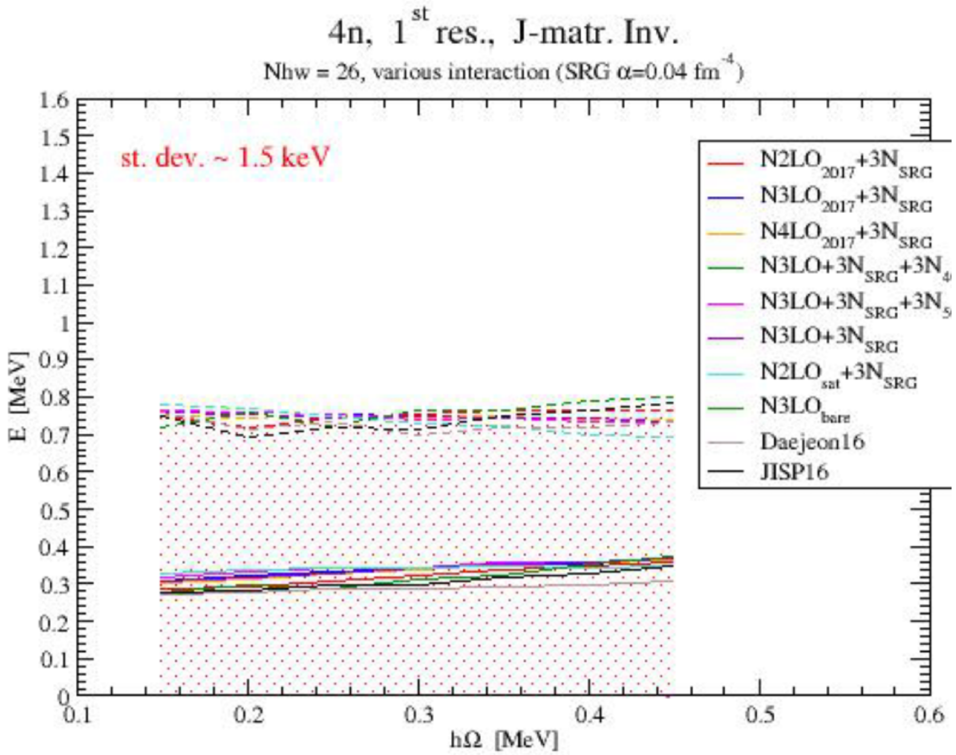
N_{max} =10-18 resonance params:
E_r = 844 keV, Γ = 1.377 MeV,
E_{false} = -55 keV.

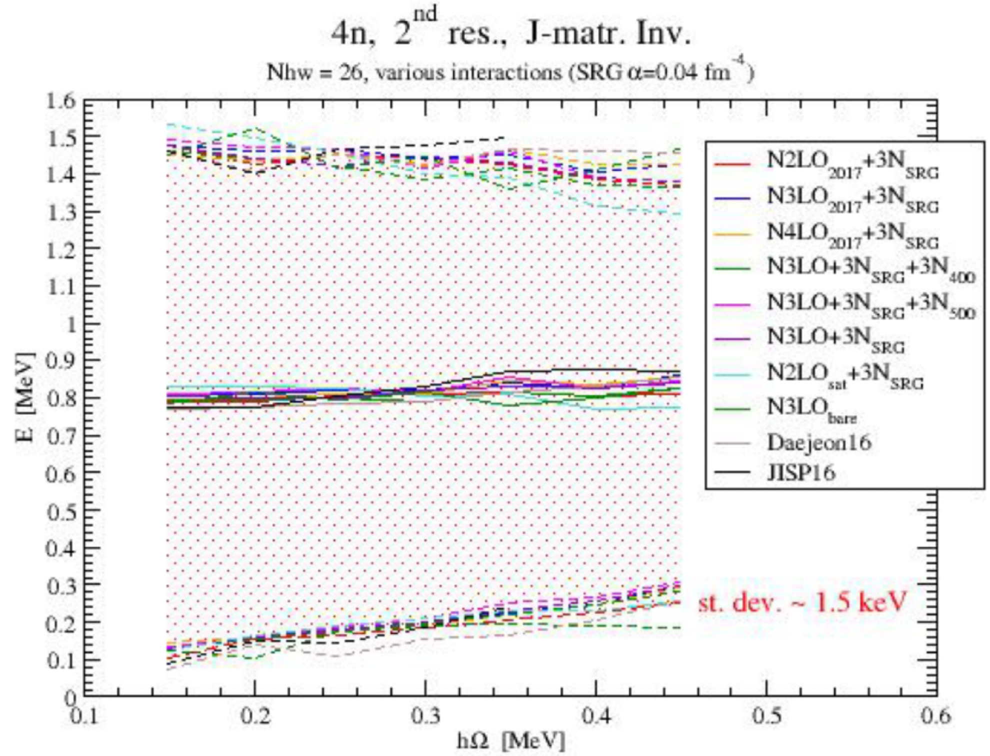
Tetraneutron:

Interaction	JISP16, Ref. [16]	Daejeon16	Idaho N3LO, SRG $\Lambda = 1.5\ \text{fm}^{-1}$	Idaho N3LO, SRG $\Lambda = 2.0\ \text{fm}^{-1}$	Idaho N3LO
a (MeV$^{\frac{1}{2}}$)	0.701	0.749	0.613	0.662	—
b^2 (MeV)	1.09	1.28	0.970	1.07	—
c (MeV$^{-\frac{5}{2}}$)	-27.0	-16.2	-31.6	-28.1	4960
d (MeV^{-4})	0.281	0.717	0.720	0.776	2330
E_r (MeV)	0.844	0.997	0.783	0.846	—
Γ (MeV)	1.38	1.60	1.15	1.29	—
E_f (keV)	-54.9	-63.4	-52.1	-54.5	—
$\|E_v\|$ (keV)	—	—	—	—	15.2
Ξ (keV)	43.8	47.9	29.0	31.7	19.4

JISP16 results: A. M. Shirokov, G. Papadimitriou, A. I. Mazur, I. A. Mazur, R. Roth, and J. P. Vary, Phys. Rev. Lett. 117, 182502 (2016);
Other results: A. I. Mazur, A. M. Shirokov, I. A. Mazur, L. D. Blokhintsev, Y. Kim, I. J. Shin, and J. P. Vary, Phys. At. Nucl. 82, 537 (2019); I. A. Mazur, A. M. Shirokov, A. I. Mazur, I. J. Shin, Y. Kim, P. Maris, and J. P. Vary, Phys. Part. Nucl., 50 , 537 (2019).

Newer tetraneutron results of Darmstadt group working in larger spaces (S. Alexa, et al, **preliminary**)





$E \approx 0.3\ \mathrm{MeV}, \Gamma \approx 0.85\ \mathrm{MeV}$

$E \approx 0.8\ \mathrm{MeV}, \Gamma \approx 1.3\ \mathrm{MeV}$

Before we had with JISP16:

E_r = 186 keV, Γ = 815 keV

E_r = 844 keV, Γ = 1.378 MeV,
E_{false} = -55 keV

Motivations for tBF

Can one study nuclear elastic and inelastic scattering non-perturbatively as an entangled/coherent state?

This could enable promising avenues of research to

- ❖ Probe *ab initio* nuclear structure results with strong external and time-dependent Coulomb + nuclear forces
- ❖ Use ab initio scattering amplitudes to compare with experimental cross section data
- ❖ Investigate "forbidden" transitions resulting from non-perturbative processes – sensitivity to EFT?
- ❖ Search for emergent phenomena – coherent non-perturbative processes (eka-resonances, resonant charge exchange, . . .)

Scattering with the time-dependent basis function (tBF) approach

1. *Ab initio* structure calculation

$$H_0|\beta_i\rangle = E_i|\beta_i\rangle$$

$$H_0 = T_{rel} + V$$

$$\{|\beta_1\rangle, |\beta_2\rangle, \cdots, |\beta_n\rangle\}$$

2. Time-dependent

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

$$H(t) = T_{rel} + V + V_I(t)$$

- State vector becomes amplitudes
- Operators become matrices

- Natural extension of the NCSM
- Non perturbative
- *Ab initio*
- Full quantal coherence

$V_I(t)$

- Weijie Du, Peng Yin, Yang Li, Guangyao Chen, Wei Zuo, Xingbo Zhao, and James P. Vary, *Phys. Rev. C* **97**, 064620 (2018);
- Weijie Du, Peng Yin, Guangyao Chen, Xingbo Zhao, and James P. Vary, *in Proceedings of the International Conference "Nuclear Theory in the Supercomputing Era–2016" (NTSE-2016), Khabarovsk, Russia, September 19–23,* 2016.
- Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, arXiv:1910.10586

We solve the time-dependent Schrödinger equation in the basis rep.

- Equation of motion of the scattering in the interaction picture is

$$i\frac{\partial}{\partial t}|\psi;t\rangle_I = V_I(t)\ |\psi;t\rangle_I$$

- Formal solution

$$|\psi;\ t\rangle_I = U_I(t;t_0)|\psi;\ t_0\rangle_I$$

$$U_I(t;t_0) = \hat{T}\left\{\exp\left[-i\int_{t_0}^{t} V_I(t')\ dt'\right]\right\}$$

- Within the basis rep., the state vector of the system under scattering is the superposition of the bases

initial value problem

$$|\psi;\ t\rangle_I = \sum_{j=1}^{n} A_j^I(t)|\beta_j\rangle$$

$$|\psi;\ t_0\rangle_I \equiv |\beta_i\rangle$$

or any initial state expressed as a superposition of NCSM states

- The transition amplitude is

$$A_{i\rightarrow j}^I(t) \equiv A_j^I(t) = \langle\beta_j|U_I(t;t_0)|\beta_i\rangle$$

Numerical solution of the time-evolution operator: Multi-Step Differencing (MSD)

- MSD for the evolution:

MSD2

$$
\begin{aligned}
|\psi;t+\delta t\rangle_I &= e^{-iV_I(t)\delta t}|\psi;t\rangle_I = (1 - iV_I(t)\delta t + O(iV_I(t)\delta t)^2)|\psi;t\rangle_I \\
|\psi;t-\delta t\rangle_I &= e^{iV_I(t)\delta t}|\psi;t\rangle_I = (1 + iV_I(t)\delta t + O(iV_I(t)\delta t)^2)|\psi;t\rangle_I
\end{aligned}
$$

$$
|\psi;t+\delta t\rangle_I = |\psi;t-\delta t\rangle_I - 2iV_I(t)\delta t|\psi;t\rangle_I + O(iV_I(t)\delta t)^3)|\psi;t\rangle_I
$$

- MSD is an explicit method – it does not evaluate matrix inversions
- MSD2 is accurate up to $(\delta t)^3$
- MSD4 is accurate up to $(\delta t)^4$, however less efficient
- We employ MSD2 for better numerical stability and efficiency

[T. Iitaka, Phys. Rev. E 49 4684 (1994)]

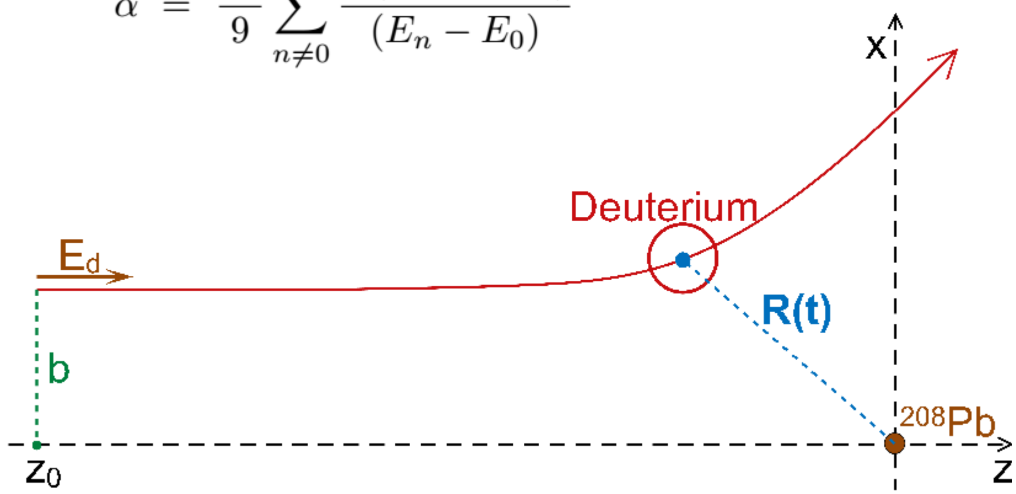
d+^{208}Pb scattering below Coulomb barrier

Solve EOM for CM motion in external field:

$$V_{\text{pot}} = V_{\text{c}} + V_{\text{pol}}$$

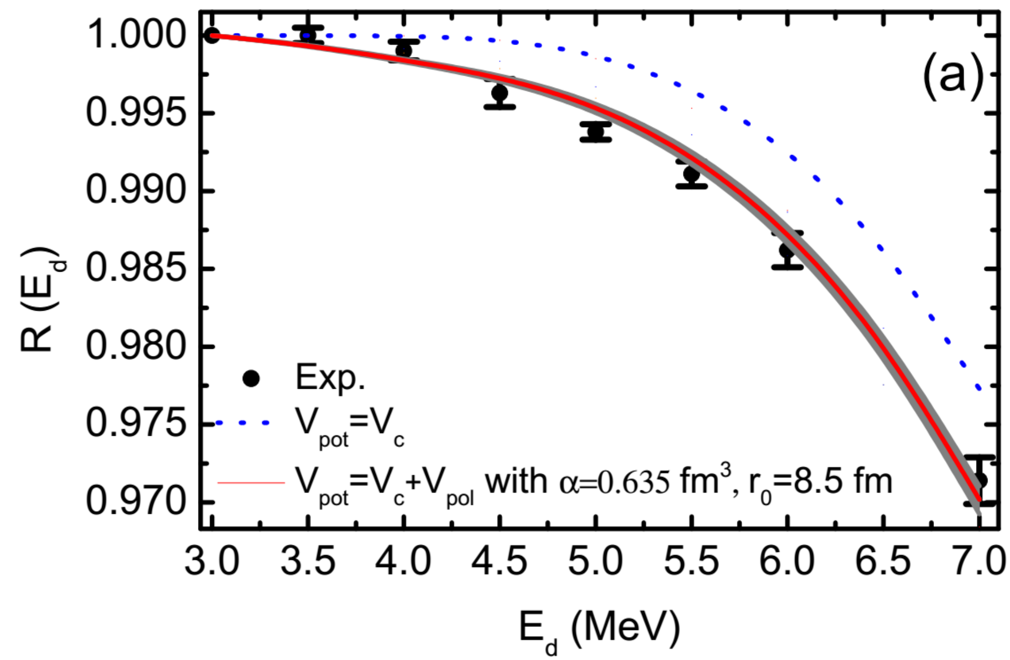
$$V_{pol} = -\frac{1}{2}\alpha Z^2 e^2 \frac{1}{(r^2 + r_0^2)^2}$$

$$\alpha = \frac{8\pi}{9} \sum_{n \neq 0} \frac{B(E1; 0 \to n)}{(E_n - E_0)}$$



$V_I(t) =$ time-dependent electric dipole field acting on np relative coordinates

$$R(E_d) = \frac{\sigma(E_d = 3\ \mathrm{MeV}, \theta_1 = 60^\circ)}{\sigma(E_d = 3\ \mathrm{MeV}, \theta_2 = 150^\circ)} \frac{\sigma(E_d, \theta_2 = 150^\circ)}{\sigma(E_d, \theta_1 = 60^\circ)}$$

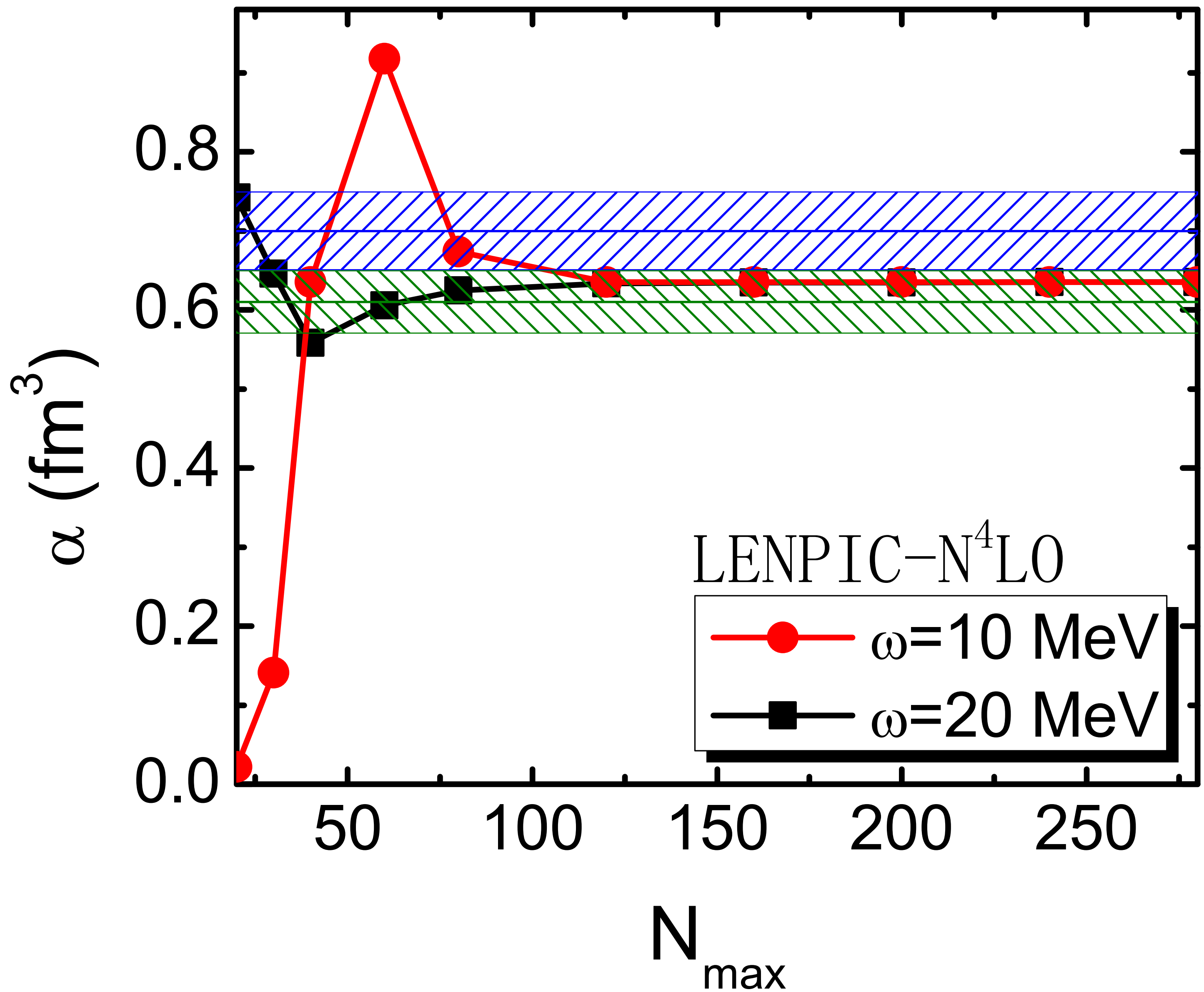


- Scattering states of *np* system: LENPIC N4LO in 3DHO basis with large N_{max}
- Rutherford + polarization potential trajectory of CM
- Scattering basis space: coherent superposition of hundreds of states
- E1 transition included; M1 transitions found to be very weak in comparison

➢ Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, arXiv:1910. 10586.

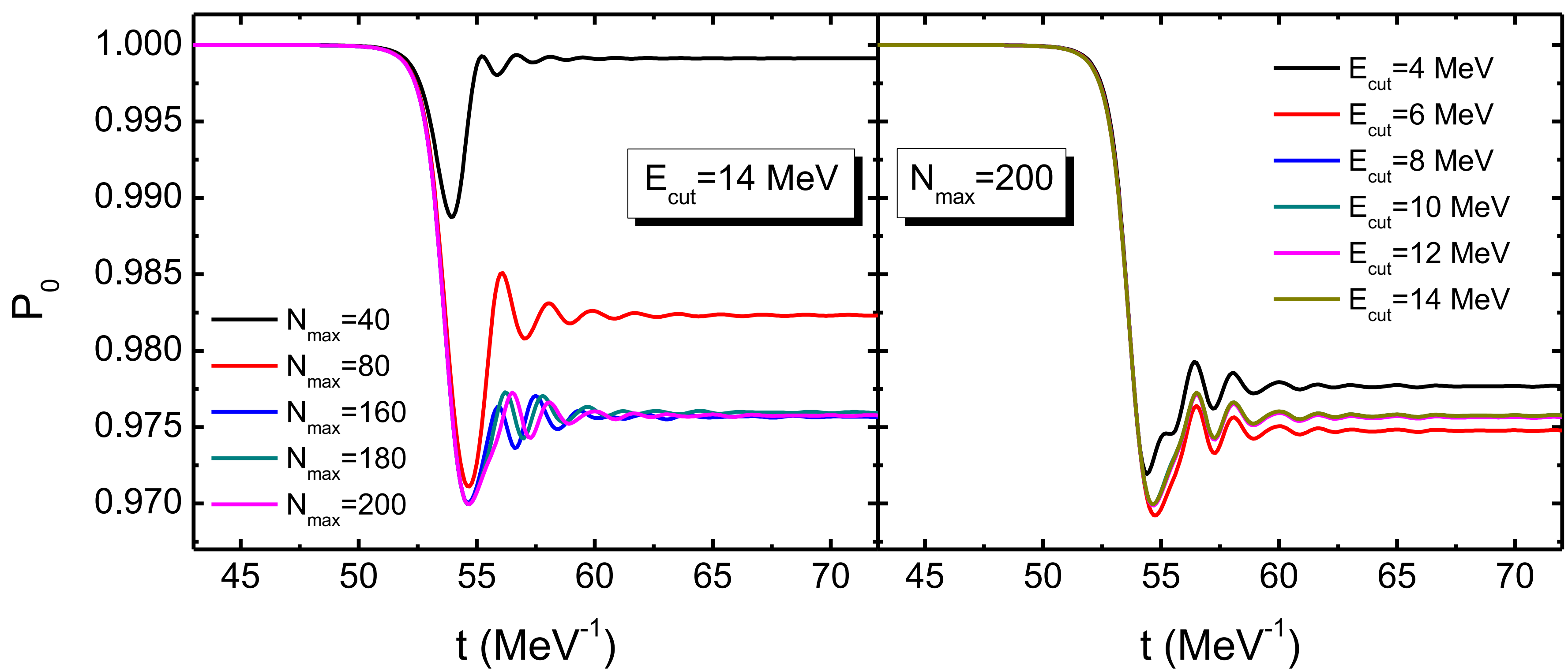
$$\alpha = \frac{8\pi}{9}\sum_{n\neq 0}\frac{B(E1;0\to n)}{(E_n - E_0)}$$

Implies: $$V_{\rm pol} = -\frac{1}{2}\alpha\frac{Z^2e^2}{[r^2(t)+r_0^2]^2}$$



Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, arXiv:1910.10586

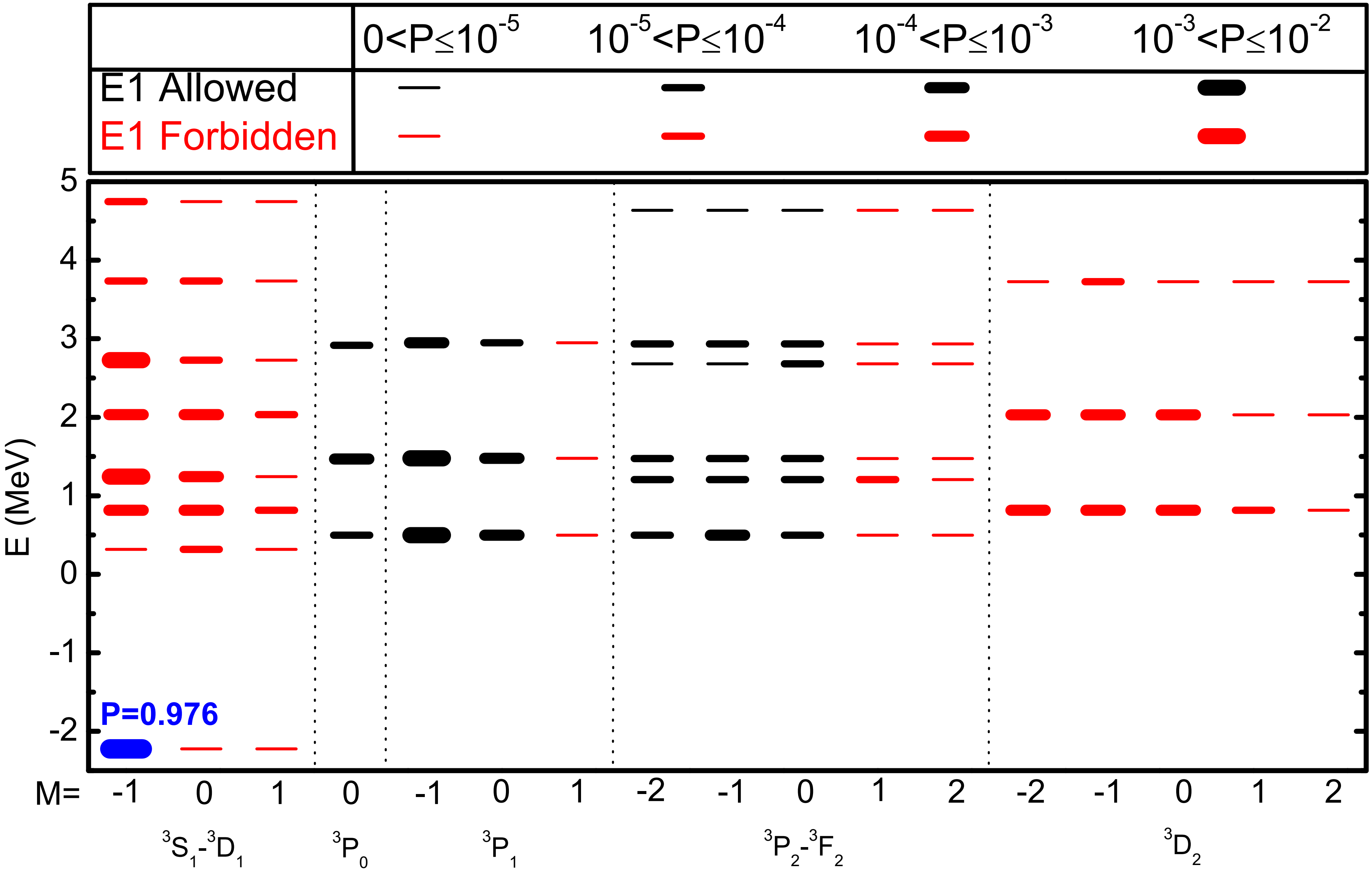
d+^{208}Pb scattering at E_d=7 MeV and θ=150°
Convergence with respect to N_{max} and E_{cut}



- Initial state: deuteron ground state with M=-1;
- P_0 is the probability of the initial state;
- The asymptotic value is well converged with respect to N_{max} and E_{cut}.

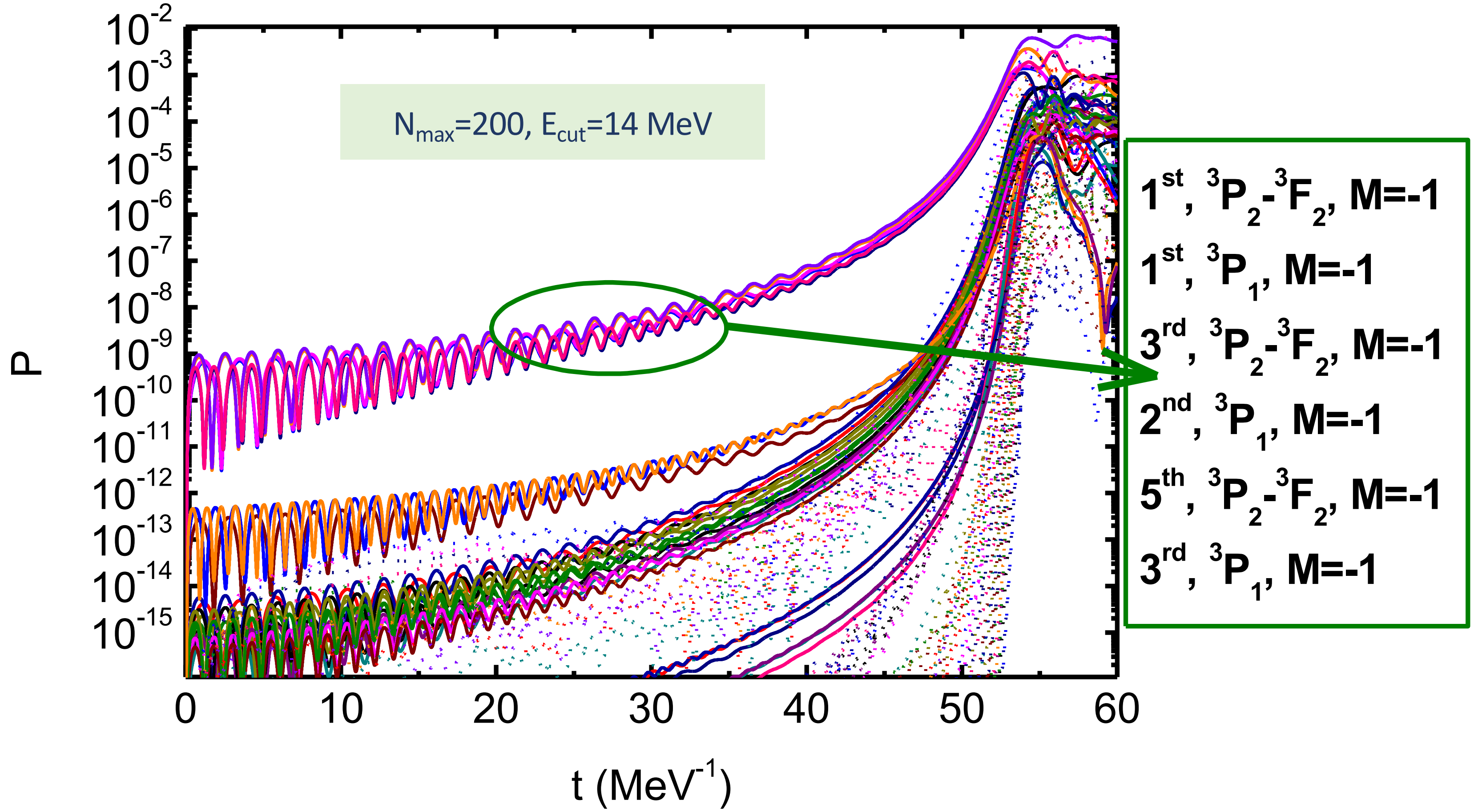
Peng Yin, et al., in preparation

Occupation probabilities of np states after d+208Pb scattering
E_d=7 MeV; LENPIC NN (N4LO) interaction



Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, arXiv:1910.10586

d+^{208}Pb scattering at E_d=7 MeV and θ=150°
Sequence of population

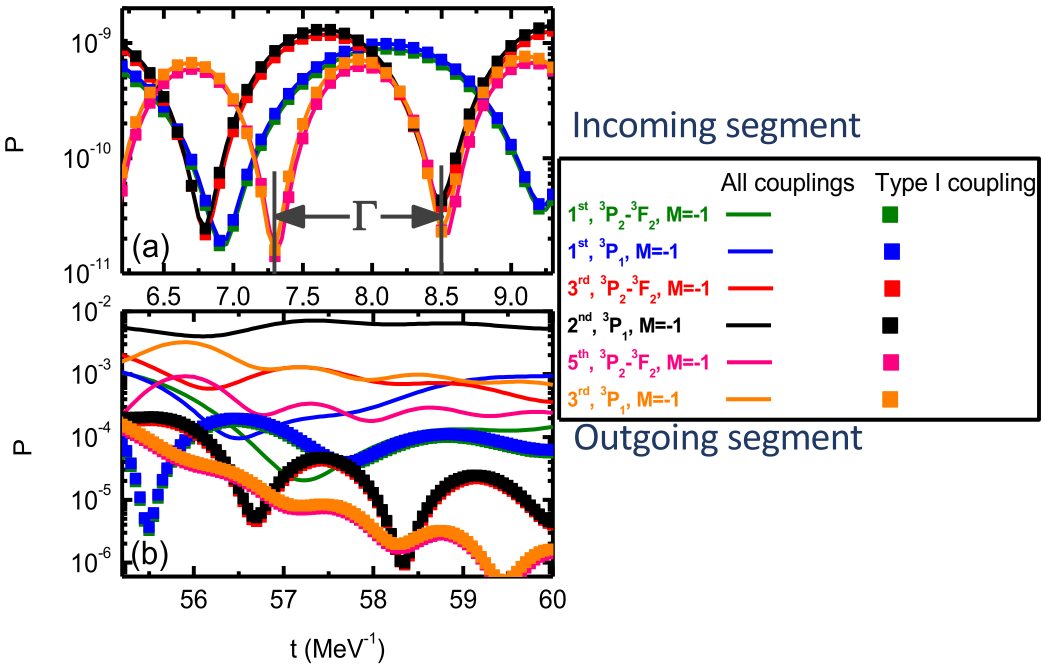


- Initial state: deuteron ground state with M=-1;
- P is the probability of states other than the initial state;
- Allowed states (solid lines) populate first. Forbidden states (dotted lines) populate afterwards.
- 6 allowed states populate dominantly in the early stage of the time evolution.

Peng Yin, et al., in preparation

d+^{208}Pb scattering at E_d=7 MeV and θ =150°

Phase coherence and decoherence



Peng Yin, et al., in preparation

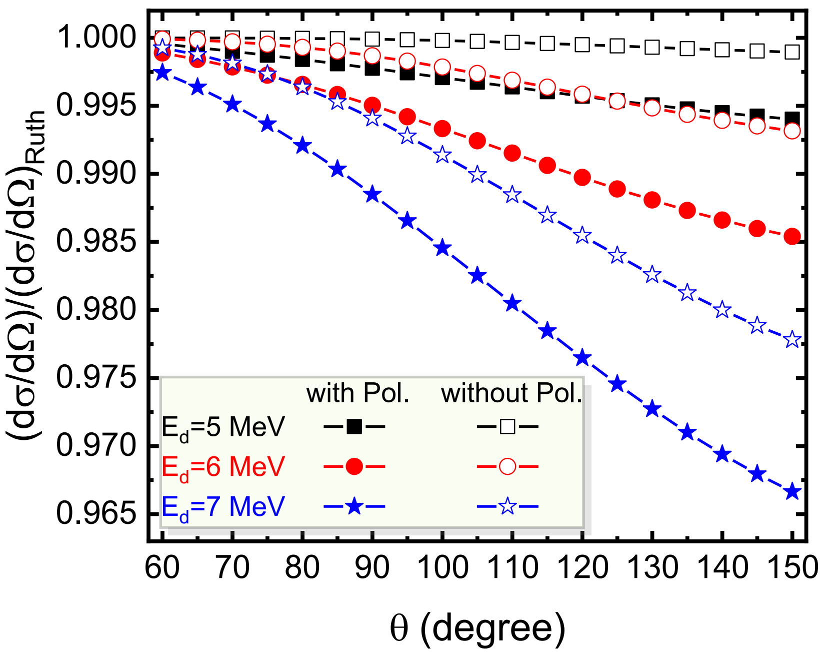
Transitions to forbidden states generate phase decoherence.

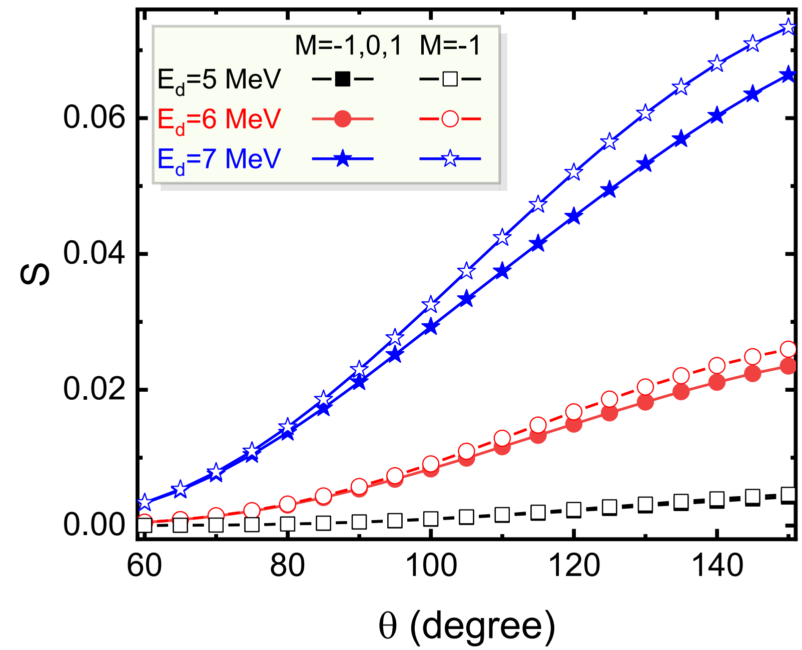
~2π ~2π No~2π

	E_{exc} (MeV)	Γ (MeV^{-1}) (Incoming segment)		Γ (MeV^{-1}) (Outgoing segment)		E_{exc}*Γ (Incoming segment)		E_{exc}*Γ (Outgoing segment)	
		Type I coupling	All couplings	Type I coupling	All couplings	Type I coupling	All couplings	Type I coupling	All couplings
2nd, $^3P_1$, M=-1	3.70	1.70	1.70	1.65	2.13	6.29	6.29	6.11	7.88
3rd, $^3P_2$-$^3F_2$, M=-1	3.69	1.70	1.70	1.65	2.13	6.27	6.27	6.09	7.86
1st, $^3P_1$, M=-1	2.72	2.35	2.35	2.21	2.09	6.39	6.39	6.01	5.68
1st, $^3P_2$-$^3F_2$, M=-1	2.72	2.35	2.35	2.21	2.34	6.39	6.39	6.01	6.36
3rd, $^3P_1$, M=-1	5.17	1.20	1.20	1.18	1.86	6.20	6.20	6.10	9.62
5th, $^3P_2$-$^3F_2$, M=-1	5.15	1.23	1.23	1.18	1.32	6.33	6.33	6.08	6.80

d+^{208}Pb scattering

Observables: cross section and Von-Neumann entropy





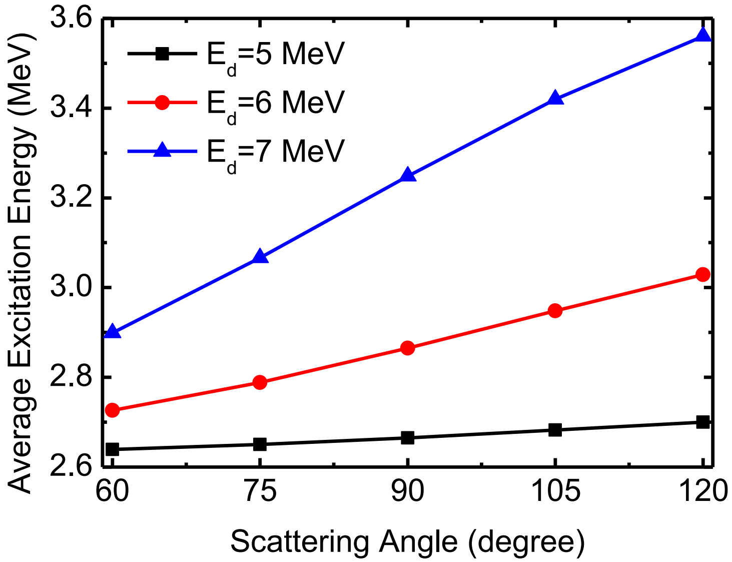
Unpolarized initial state:
equal probability ($\frac{1}{3}$) for M=-1,0,1 at t=0.

$$S_{M=-1} = -\sum_i P_i log P_i$$
$$S_{M=-1,0,1} = -\sum_i P_i log P_i + 3\times\frac{1}{3}\log\frac{1}{3}$$

Peng Yin, et al., in preparation

d+^{208}Pb scattering

Average excitation energy and inelastic probability distribution

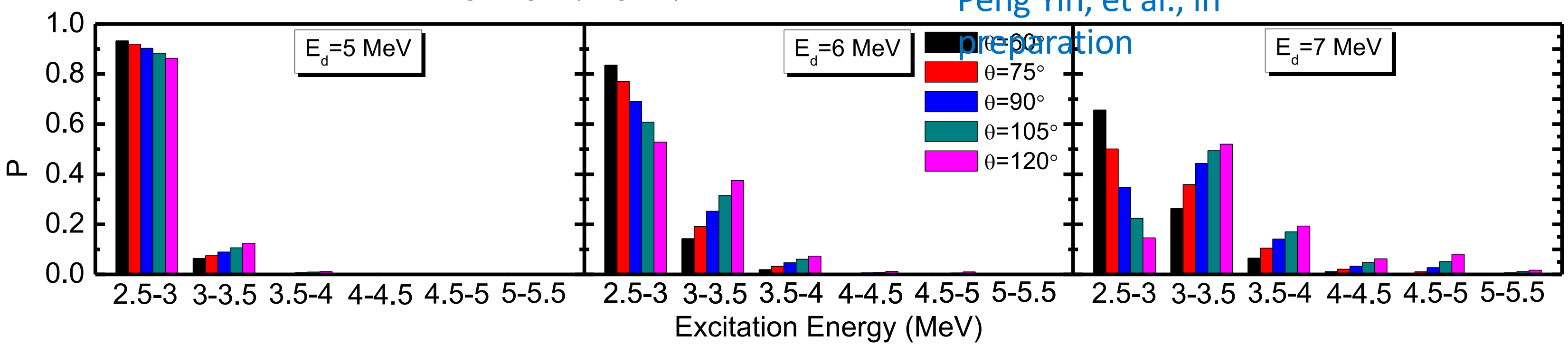


$$\bar{E} = \sum_{i \neq g.s.} E_i P_i^{res}$$

$$P_i^{res} = \frac{P_i}{\sum_{i \neq g.s.} P_i}$$

Unpolarized initial state

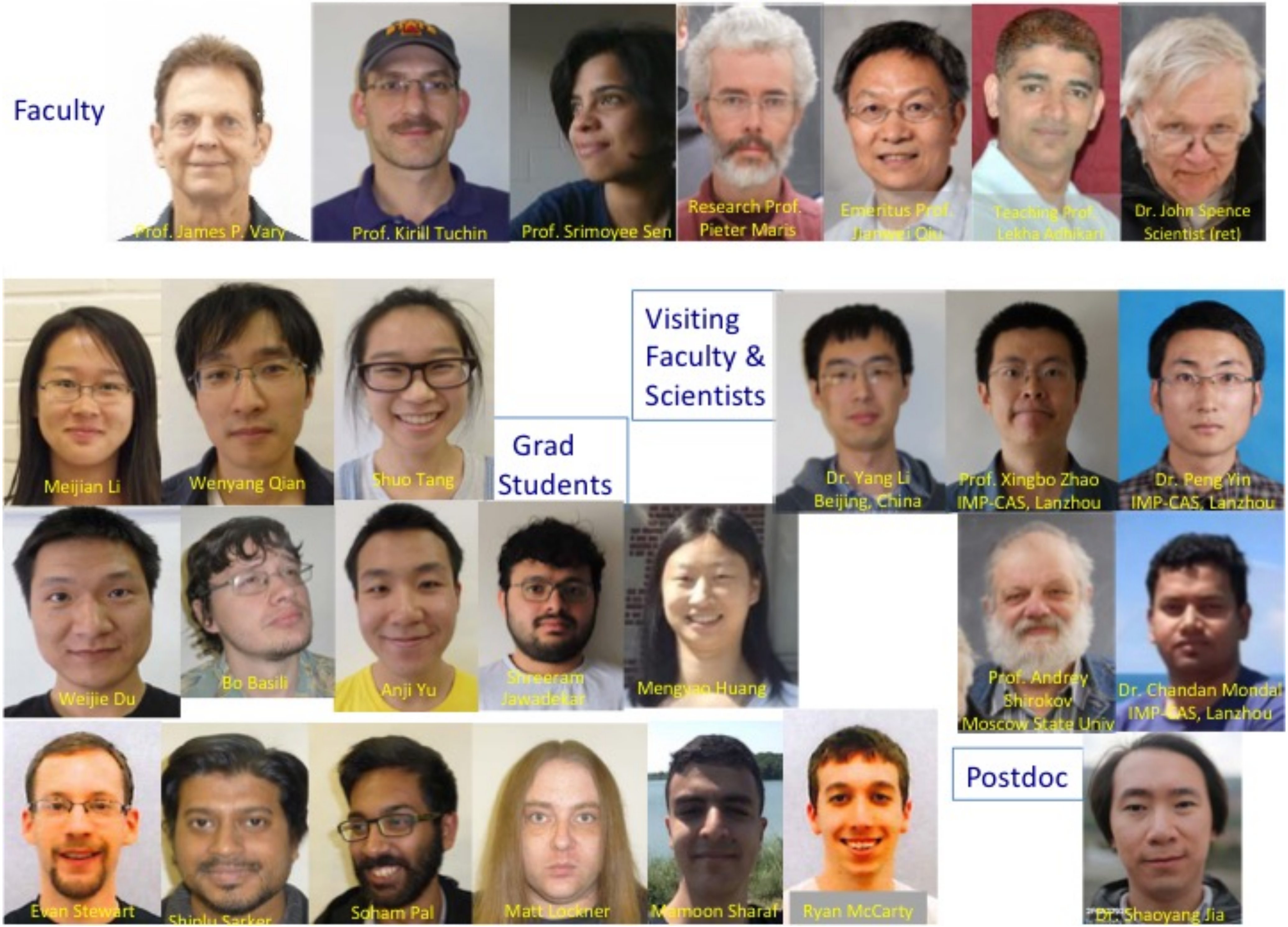
Peng Yin, et al., in preparation



Conclusions/Perspectives

- ✧ New scattering application opportunities with the SS-HORSE formalism
- ✧ ^{7}He and Tetraneutron examples illustrate the recent progress and challenges
- ✧ Extensions to proton-nucleus resonances such as p + ^{4}He have been reported
- ✧ tBF offers access to dynamics that complements stationary state approaches
- ✧ tBF provides opportunities to test strong and electromagnetic interactions from chiral EFT in precision reaction studies
- ✧ Higher energy diffractive dissociation of rare isotope beams under investigation

Iowa State University Nuclear Theory Group Fall 2019



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