

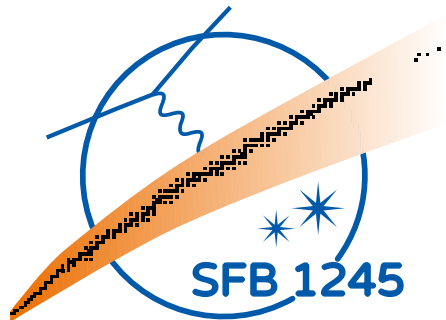
Continuum extension of the NCSM: HORSE and ACCC



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Stefan Alexa, Thomas Hüther, Robert Roth

TRIUMF Workshop 2019



DFG



Hessisches Kompetenzzentrum
für Hochleistungsrechnen

- Describe possible resonance of the four neutron system from ab initio bound state calculations

Kisamori et al. PRL **116**, 052501 (2016)

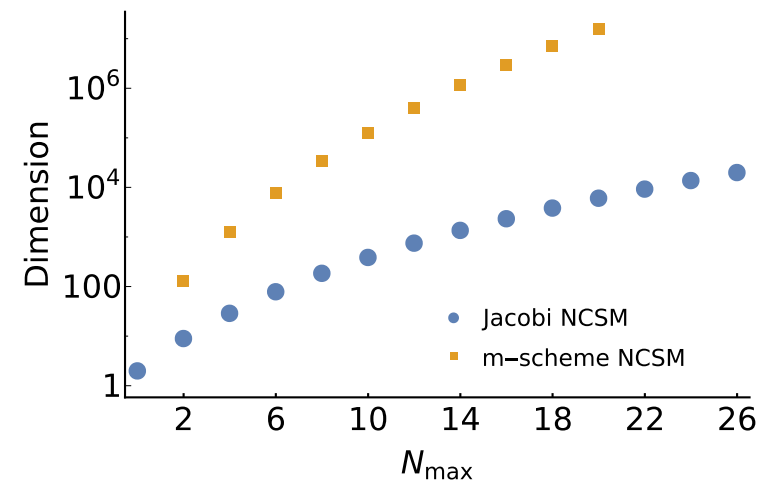
- Use existing Jacobi-NCSM framework with favourable model space scaling behaviour

- Single state HORSE calculations of $4n$ with large model spaces and different chiral interactions

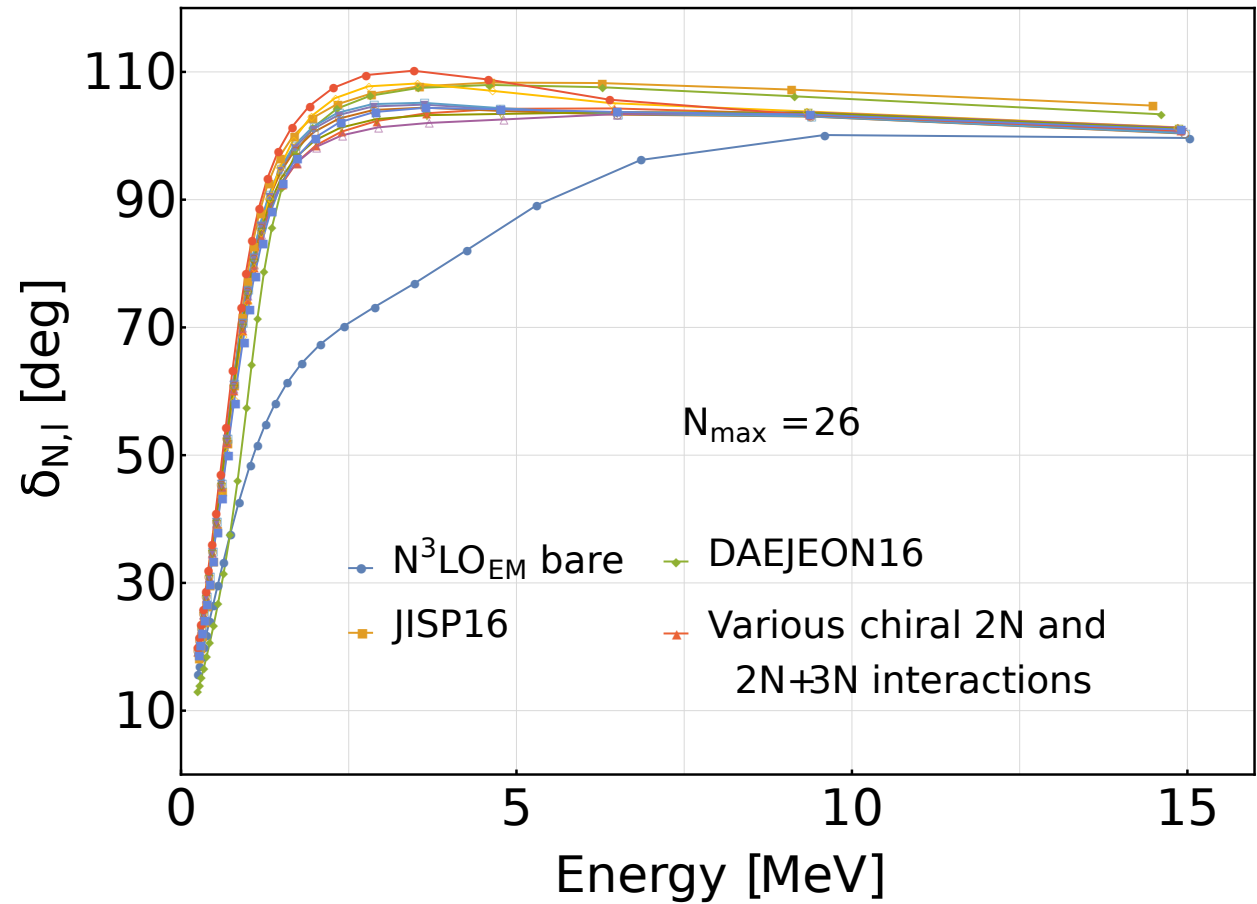
Shirokov et al. PRL **117**, 182502 (2016)

- Combine Jacobi-NCSM with analytic continuation in the coupling constant

Kukulin et al. Theory of Resonances, Springer (1989)



- **H**armonic
Oscillator
Representation of
Scattering
Equation
- Single-state
version
- Large model
spaces
- Interactions
consistent



- Obtain resonance from unbound system by artificially binding system, e.g.

$$H(\lambda) = H + \lambda V_{\text{ext}} \quad \text{or} \quad H(\lambda) = T + \lambda V_{\text{init}}$$

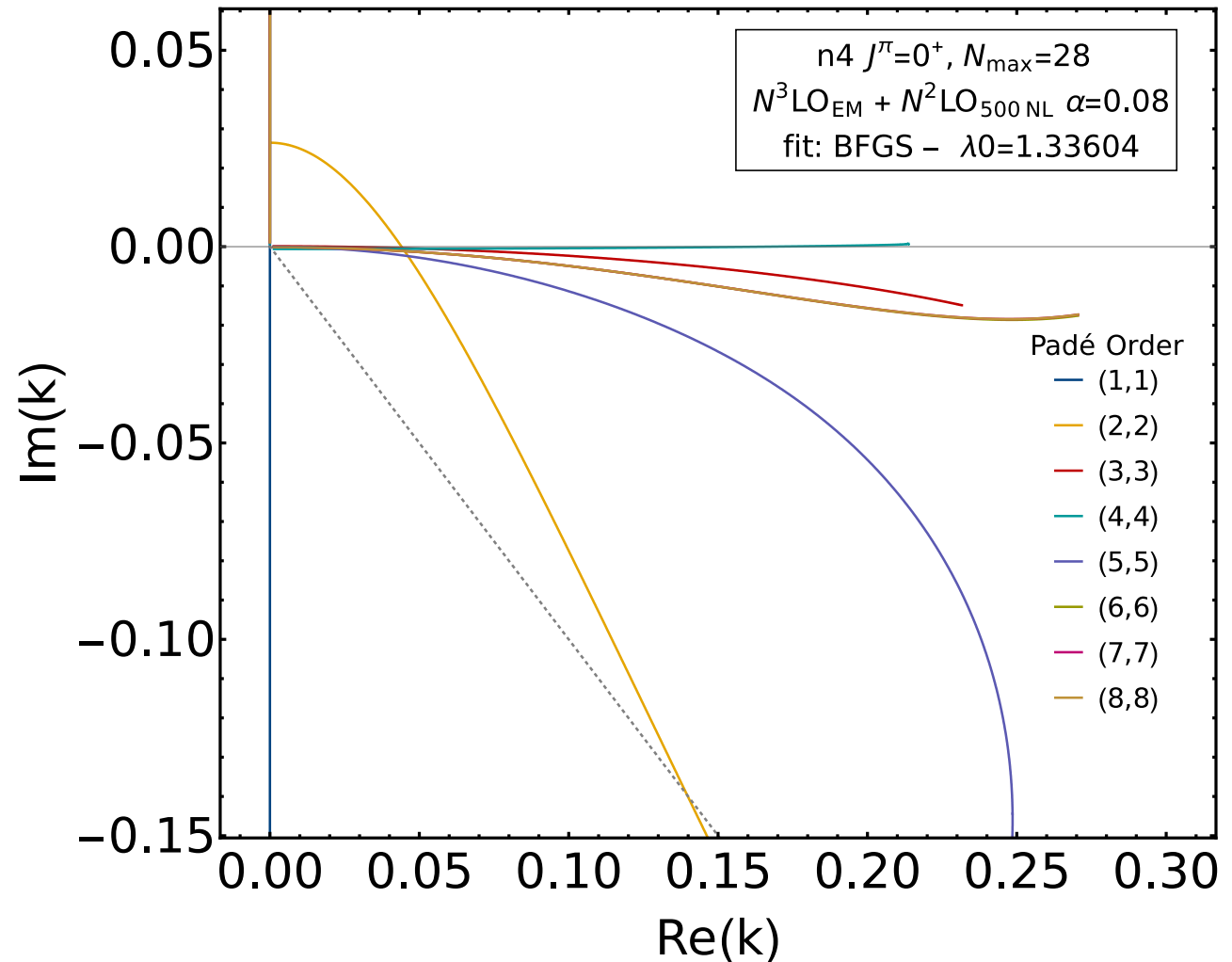
- Generate set of binding energies $\{E_i, \lambda_i\}$
- Padé fit of wavenumber for analytic continuation

$$k^{[N,M]}(x) = i \frac{c_0 + c_1 x + \dots + c_N x^N}{1 + d_1 x + \dots + d_M x^M} \quad x = \sqrt{\lambda - \lambda_0}$$

- Resonance energy and width

$$E_R = \frac{\hbar^2 (k_{\text{Re}}^2 - k_{\text{Im}}^2)}{2m} \quad \Gamma = \frac{2\hbar^2}{m} k_{\text{Re}} k_{\text{Im}}$$

- Modification: $H(\lambda) = T + \lambda V_{2N} + V_{3N}$
- Di-neutron not accounted for
- Padé extrapolation unstable
- Effect of modification?



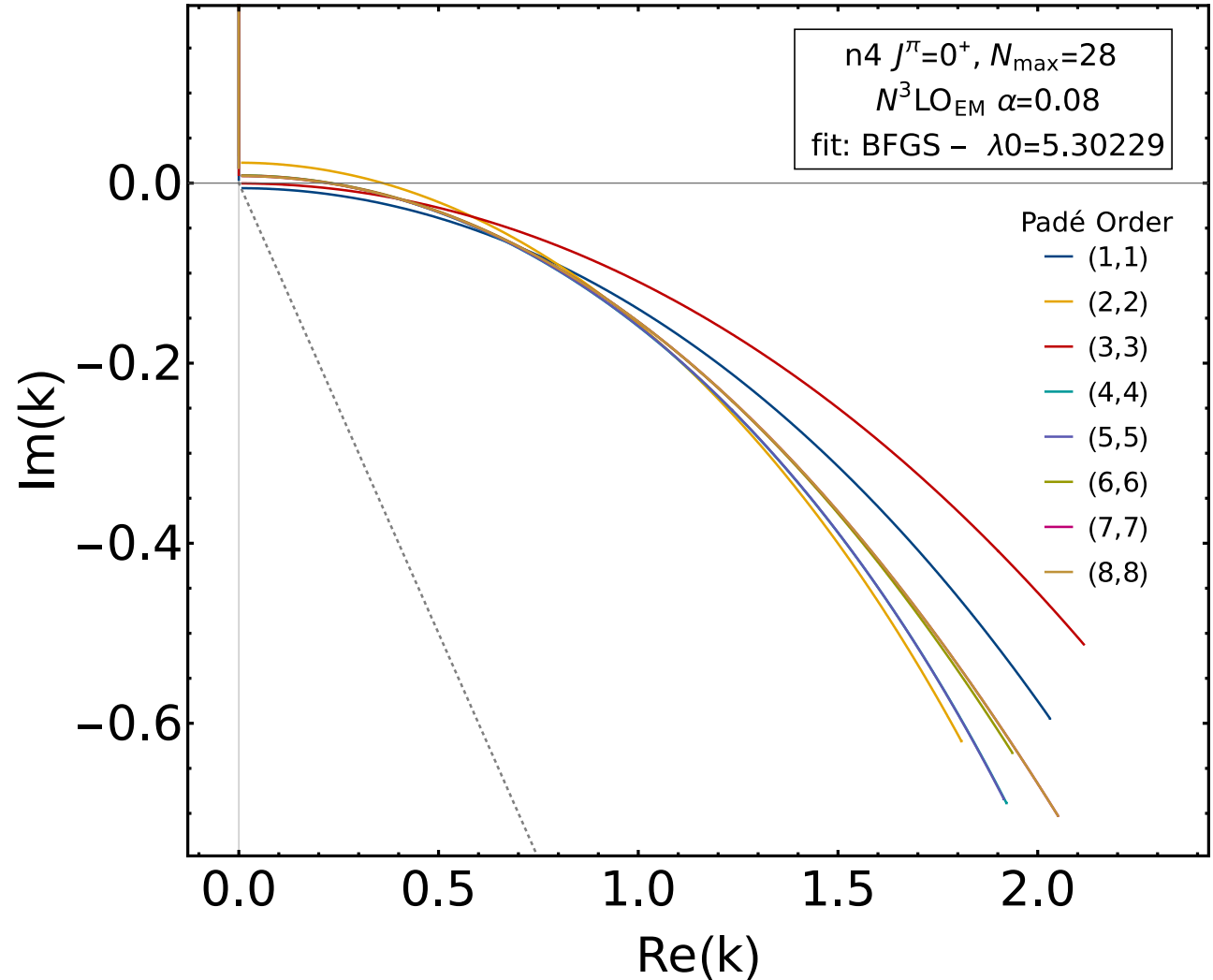
▪ Modification: $H(\lambda) = T + V_{2N}({}^1S_0) + \lambda V_{2N}$

▪ Di-neutron unbound

▪ Padé orders “better behaved”

▪ Far extrapolation due to large λ_0

▪ Modification too strong?



ACCC - 4n - Statistical ACCC

▪ Modification: $H(\lambda) = T + V_{2N}(^1S_0) + \lambda V_{2N}$

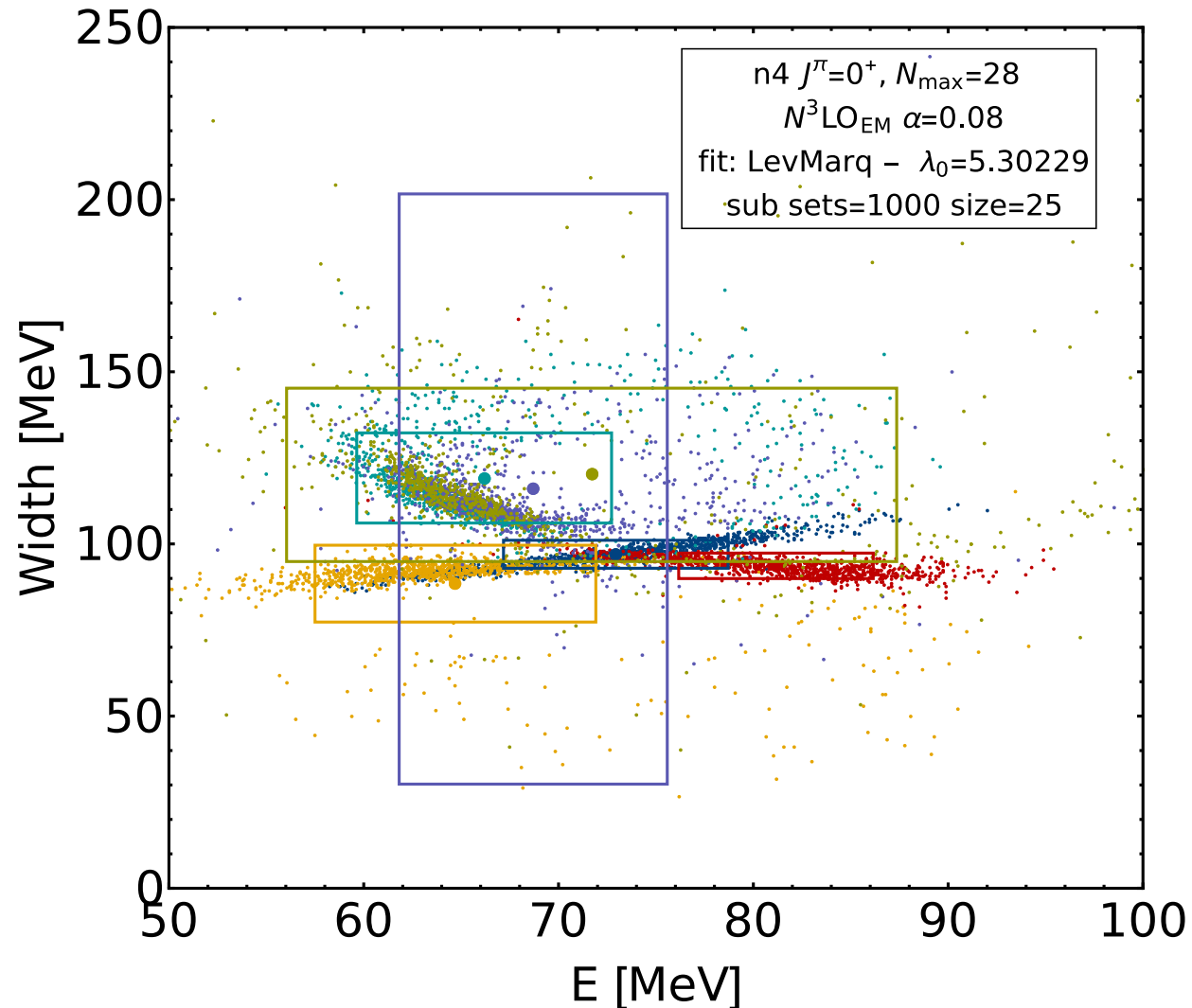
▪ Statistical approach

Papp et al. Chem.Phys
418 (2013)

▪ Number of data points impact fit

▪ Modification generates unphysical state?

▪ External potential necessary?



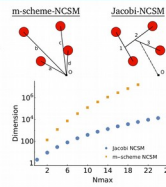
Continuum extension of the NCSM: HORSE and ACCC



Stefan Alexa, Thomas Hütter, Robert Roth

Motivation

- Describe possible resonance of the four neutron system [1] from ab initio nuclear structure bound state calculations:
 - Use existing Jacobi-NCSM framework with favourable model space scaling behaviour
 - Supply single state HORSE calculations of $4n$ [2] with
 - Large model spaces
 - Different chiral interactions
- Combine Jacobi-NCSM with analytic continuation in the coupling constant [3]
- ACCC actively developed in conjunction with CI codes in quantum chemistry.

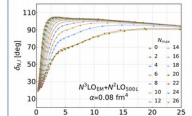
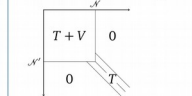


HORSE: Harmonic Oscillator Representation of Scattering Equations

- The HORSE formalism [2, 5] allows to extract scattering phase shifts from bound-state methods, like the NCSM
- Variation of the HO frequency $\hbar\Omega$ and the model space size N_{max}
- Democratic Decay Approximation and hyper-spherical expansion
- Expand solution to radial Schrödinger equation in (hyper)spherical HO functions

$$u_l(k, r) = \sum_{n=0}^{\infty} a_{nl}(k) R_{nl}(r)$$

- Truncate model space at $\mathcal{A}' = \frac{N_{\text{max}} \hbar\Omega \tau}{\hbar^2}$



- Phase shift behaviour with increasing N_{max} for the $N^16O_{\text{int}} + N^16O_{\text{out}}$ interaction
- Phase shifts quickly rise well above 90° , indicating a resonance
- Convergence w.r.t. N_{max} reached at higher energies
- Convergence at lower energies not reached

- Matching the inner and outer region
- $$\sum_{n=0}^{\infty} (H'_{nl} - \delta_{nl} E) a_{nl}(k) = -\delta_{nl} T_{l, \mathcal{A}' + 1} \times a_{n, \mathcal{A}' + 1}(k)$$

- Solve via Green's function of truncated model space

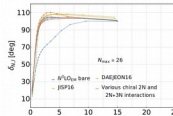
$$G_{\mathcal{A}' + 1} = \sum_{n=0}^{\infty} \frac{Y_{nl} Y_{n, \mathcal{A}' + 1}^*}{E - E_{n, \mathcal{A}' + 1}}$$

- Obtain partial wave phase shifts

$$\tan(\delta_l(E)) = \frac{S_{l, \mathcal{A}'}(E) - G_{l, \mathcal{A}' + 1}^* S_{l, \mathcal{A}' + 1}(E)}{C_{l, \mathcal{A}'}(E) - G_{l, \mathcal{A}' + 1}^* C_{l, \mathcal{A}' + 1}(E)}$$

- Single-State HORSE for $E \rightarrow E_r$ of truncated Hamiltonian

$$\tan(\delta_l(E_r)) = \frac{S_{l, \mathcal{A}' + 1}(E_r)}{C_{l, \mathcal{A}' + 1}(E_r)}$$



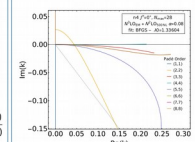
- Comparison of a selection of interactions at $N_{\text{max}} = 26$ [6-10]
- All interactions show resonance
- Chiral 3N force contributions small
- Bare interaction not converged. Significant improvement with SRG

ACCC: Analytic Continuation in the Coupling Constant

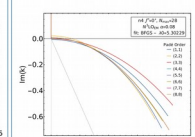
- Resonances can emerge from bound eigenstates when the interaction strength is decreased [3]
- Binding the Hamiltonian can be achieved by adding an external potential or multiplying the whole or parts of the initial interaction with a 'coupling constant':
 - $H(\lambda) = H + \lambda V_{\text{ext}}$
 - $H(\lambda) = T + \lambda V_{\text{int}}$
 - $H(\lambda) = T + (V - V^*) + \lambda V^*$
- The position at which $H(\lambda)$ becomes bound is denoted by λ_0
- Generate set of binding energies $\{E_i, \lambda_i\}$
- Switching to wavenumber $k = \sqrt{2mE/\hbar^2}$ and introducing the variable $x = \sqrt{\lambda - \lambda_0}$ one can write Padé expansion for k :

$$k^{N, M}(x) = \frac{P_N(x)}{Q_M(x)} = \frac{c_0 + c_1 x + \dots + c_N x^N}{1 + d_1 x + \dots + d_M x^M}$$

- Parameters c_i and d_i are real and fitted to positive and real $k = -ik$ for $\lambda > \lambda_0$



- $H(\lambda) = T + \lambda \sum_{i,j} V_{ij} + \sum_{i,j,k} V_{ijk}$
- Ignores possible subsystems
- Trajectories change with Padé order



- $H(\lambda) = T + V_l(S_0) + \lambda \sum V_l^{\text{pert}}$
- Trajectories well behaved, spreading owed to far extrapolation
- Ignoring dominant two-body channel leads to extreme increase in λ_0

Conclusion: Choice of modification critical. Obtaining reliable data possible with the Jacobi-NCSM, but will require some form of suitable many-body binding potential

- Extrapolation of $k^{N, M}(x)$ to desired interaction strength λ
- Resonance parameters are obtained via

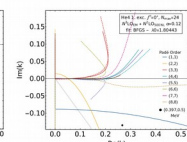
$$E_R = \frac{\hbar^2(k_R^2 - k_0^2)}{2m} \text{ and } \Gamma = \frac{2\hbar^2}{m} k_0 k_R$$

- Accommodate substructures:

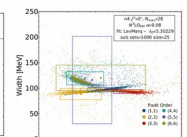
$$k(\lambda) \propto \sqrt{E_i(\lambda) - E_{\text{int}}(\lambda)} = \frac{P_i(\lambda)}{Q_{\text{int}}(\lambda)}$$

- Changes in data impact fit and thus the extrapolation
- Statistical ACCC approach [4]:
 - Select random subsets of full data set
 - Perform ACCC with subsets
 - Changes in extrapolated results indicate of fit stability

- Challenges:**
 - Choice of binding potential influences fit
 - Generating binding potential suitable for the use with Jacobi-NCSM non-trivial



- "He ex. 0" state trajectories unstable
- Simultaneous fit of λ_0 (dashed lines) does not improve result



- Statistical ACCC for the case to the left
- Squares mark $E_R \pm \sigma$ and $\Gamma \pm \sigma$
- Large values owed to choice of binding

Technische Universität Darmstadt, Germany

References:

[1] K. Saito, S. Shimizu, and H. Miyata, *Physical Review Letters* **110**, 112301 (2013).
 [2] A. Blomberg, C. Pascazio, A. Maza, S. Maza, and S. Maza, *Physical Review Letters* **117**, 172301 (2016).
 [3] V. T. Stetsko, M. M. Romo-Exposito, and J. Hübner, *Theory of Resonance Optics* (Springer, 2019).
 [4] D. B. Steunin, and B. Machleidt, *Physical Review Letters* **111**, 112301 (2013).
 [5] P. Papoušek, and J. Hübner, *Chemical Physics* **484**, 1 (2016).
 [6] A. B. Blomberg, A. Maza, J. A. Maza, and J. Hübner, *Physical Review Letters* **117**, 172301 (2016).
 [7] D. B. Steunin, G. E. Johnson, K. A. Wood, G. Rupen, T. Papoušek, B. D. Carlsson, C. Pascazio, M. Hjorth-Jensen, P. Navrátil, and M. Hjorth-Jensen, *Physical Review Letters* **111**, 112301 (2013).
 [8] A. Blomberg, J. Vogt, A. Maza, and S. Maza, *Physical Review Letters* **116**, 162301 (2016).
 [9] A. B. Blomberg, G. E. Johnson, K. A. Wood, G. Rupen, T. Papoušek, B. D. Carlsson,



Thank you for your attention!

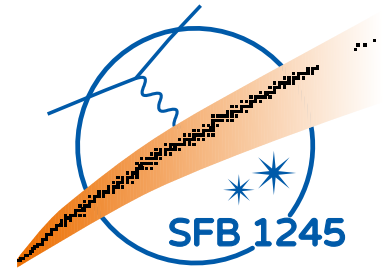


TECHNISCHE
UNIVERSITÄT
DARMSTADT

▪ Thanks to my group and collaborators

M. Deuker, T. Hüther, P. Käse, M. Knöll, L. Mertes,
T. Mongelli, J. Müller, R. Roth, K. Vobig, C. Walde,
T. Wolfgruber

Institut für Kernphysik, TU Darmstadt



▪ Special thanks

R. Wirth

Michigan State University



Hessisches Kompetenzzentrum
für Hochleistungsrechnen