

# Lecture V: From Stable to Weakly Bound Nuclei

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# Outline

- 1 Introduction
  - Overall motivation and aims
- 2 Many-Body Methods
- 3 Reminder of Coupled Cluster Theory
  - Why Coupled-Cluster theory
  - Formalism
- 4 Effective Interactions for Weakly Bound Systems
  - Complex Effective Interactions
  - Complex Scaling for Realistic Interactions
- 5 Summary

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# Aims and Motivation

- ① RIKEN/FAIR/Eurisol/RIA(?) can offer unprecendeted data on weakly bound systems. Increased experimental intensities.
- ② Crucial for NP next 10 years : understand how shells evolve
- ③ Identify and investigate methods that will extend to unstable systems
- ④ Combine effective interactions for unstable systems and the shell model
- ⑤ Single-particle level density increasing (more active particles)
- ⑥ Want an 'ab initio' and reductionist approach starting with both NN and NNN interactions
- ⑦ Complement the shell model for heavier systems

# Nuclear Many-Body Methods

## Widely used Methods

- 1 Variational and Diffusion Monte Carlo/GFMC  
(Benchmark-test  $A \leq 12$ )
- 2 Shell-model, Monte Carlo shell model and No-core shell-model
- 3 Coupled cluster theory
- 4 Perturbative many-body methods and shell-model
- 5 Shell-model with phenomenological interactions
- 6 Extension to weakly bound systems : Complex scaling and complex shell model, Gamow shell model.
- 7 Parquet diagrams, Green's function method, FHNC, UMOA...

# Progress in our QCD understanding of the NN force

- CEBAF 12 GeV upgrade: Explore the limits of our understanding of the atomic nuclei based on nucleonic and mesonic degrees of freedom
  - ① Experimental plans aim at identifying and exploring the transition from the nucleon/meson description of nuclei to the underlying quark and gluon description.
  - ② Test the short-range behavior of the NN interaction via deep inelastic scattering
- Effective field theory has made progress in constructing NN and NNN forces from the underlying symmetries of QCD
- Three-body forces emerge naturally and have explicit expressions at every order in the chiral expansion.
- Recent progress in Lattice QCD may hold great promise for the construction of the nucleon-nucleon interaction.

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# Selected Problems, $^{48}\text{Ca}$

There are 90  $T = 1$  twobody matrix elements. Except a few matrix elements there is an amazing agreement with empirical ones and

| $2j_a$ | $2j_b$ | $2j_c$ | $2j_d$ | $2T$ | $2J$ | A       | B      | C      | Emp    |
|--------|--------|--------|--------|------|------|---------|--------|--------|--------|
| 7      | 3      | 7      | 3      | 2    | 4    | -1.0055 | -.9716 | -.9546 | -.9036 |
| 7      | 3      | 7      | 3      | 2    | 6    | -.0411  | -.0506 | -.0612 | .2396  |
| 7      | 3      | 7      | 3      | 2    | 8    | -.0421  | -.0596 | -.0727 | .1891  |
| 7      | 3      | 7      | 3      | 2    | 10   | .1900   | .1748  | .1533  | .5781  |

No way to make the theoretical matrix elements more repulsive with two-body interactions only. These matrix elements yield a spectroscopic catastrophe in  $^{47}\text{Ca}$ ,  $^{48}\text{Ca}$  and  $^{48}\text{Ca}$ .

# Selected Problems, $^{48}\text{Ca}$

The energy (in MeV) difference  $0_1^+ - 2_1^+$  in  $^{48}\text{Ca}$ :

| Expt | Empirical | Theory |
|------|-----------|--------|
| 3.83 | 3.90      | 1.26   |

If we change the  $J = 5$  matrix element, only one of 90  $T = 1$  matrix elements, and set it equal the empirical value I get 3.95 MeV! And good spectroscopy for all Ca isotopes. No sound theoretical understanding why two-body effective interactions are unable to reproduce shell closures. Great challenge for nuclear structure.

Similarly, in the  $sd$ -shell we obtain even  $^{28}\text{O}$  as a stable and bound nucleus without fitting the matrix elements. **How much is due to three-body forces and other missing degrees of freedom such as proper treatment of the continuum?** We would like to have a many-body formalism with which we can answer such questions.

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# Why Coupled-Cluster theory?

## Advantages

- Fully microscopic. Only linked diagrams enter, size extensive
- Can be improved upon systematically, e.g., by inclusion of three-body interactions and more complicated correlations.
- Allows for description of both closed-shell systems and valence systems
- Derivation of effective two and three-body interactions for the shell model
- Amenable to parallel computing
- Huge development in Quantum Chemistry. Exploit this for the nuclear many-body problem.

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# More on Coupled Cluster

## More advantages

- Can be used to generate excited spectra for nuclei like  $^{16}\text{O}$  or  $^{40}\text{Ca}$  with many shells. Hard for the shell model to go beyond one major shell. Huge dimensionalities in shell-model calcs

| System          | 4 shells | 7 shells |
|-----------------|----------|----------|
| $^4\text{He}$   | 4E4      | 9E6      |
| $^8\text{B}$    | 4E8      | 5E13     |
| $^{12}\text{C}$ | 6E11     | 4E19     |
| $^{16}\text{O}$ | 3E14     | 9E24     |

Standard shell-model codes can today reach dimensionalities of  $d \sim 10^{10}$  basis states. Monte Carlo shell model codes can reach  $d \sim 10^{15}$ .

- Can include complex effective interactions, today's topic.

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# Coupled Cluster, Basics

Formally, the coupled cluster method begins by postulating that the correlated many-body wave function is given by

$$|\Psi\rangle = \exp(T) |\Phi_0\rangle,$$

where we define the reference Slater determinant as  $|\Phi_0\rangle$  and the correlation operator as

$$T = T_1 + T_2 + T_3 + \cdots + T_A.$$

The terms of the correlation operator are defined in terms of  $n$ -particle  $n$ -hole ( $np$ - $nh$ ) excitation amplitudes as

$$T_1 = \sum_{i < \varepsilon_f, a > \varepsilon_f} t_i^a a_a^+ a_i$$

for single excitations (S)

$$T_2 = \sum_{i,j < \varepsilon_f; ab > \varepsilon_f} t_{ij}^{ab} a_a^+ a_b^+ a_j a_i$$

for double excitations (D).

# Coupled Cluster, the Energy

We compute the expectation of the energy from

$$E = \langle \Psi_0 | \exp(-T) H \exp(T) | \Psi_0 \rangle .$$

The energy is quite easy to calculate and is given by

$$E_{\text{CCSD}} - E_0 = \sum_{ia} f_{ia} t_i^a + \frac{1}{4} \sum_{aibj} \langle ij || ab \rangle t_{ij}^{ab} + \frac{1}{2} \sum_{aibj} \langle ij || ab \rangle t_i^a t_j^b ,$$

where  $E_0 = \langle \Psi_0 | H_{\text{int}} | \Psi_0 \rangle$ . For two-body Hamiltonians, this equation is general and is not restricted to the CCSD approximation (singles and doubles) since higher-order cluster operators such as  $T_3$  and  $T_4$  cannot produce fully contracted terms with the Hamiltonian and therefore contribute zero to the energy.

# Coupled Cluster, the $t_i$ Equations

The equations for the amplitudes are found by left projection of excited Slater determinants so that

$$0 = \langle \Psi_i^a | \exp(-T) H(T) | \Psi_0 \rangle ,$$

$$0 = \langle \Psi_{ij}^{ab} | \exp(-T) H(T) | \Psi_0 \rangle .$$

The Baker-Campbell-Hausdorf relation

$$\begin{aligned} \exp(-T) H(T) &= H + [H, T_1] + [H, T_2] \\ &+ \frac{1}{2} [[H, T_1], T_1] + \frac{1}{2} [[H, T_2], T_2] \\ &+ [[H, T_1], T_2] + \dots \end{aligned}$$

can be used to terminate exactly at quadruply nested commutators when the Hamiltonian contains at most two-body terms. We stress that this termination is exact, thus allowing for a derivation of exact expressions for the  $T_1$  and  $T_2$  amplitudes. To derive these equations is straight-forward but tedious work.

# Coupled Cluster Equations, $t_1$ Equation

The  $t_1$  amplitude equations are given by

$$\begin{aligned}
 0 = & f_{ai} + \sum_c f_{ac} t_i^c - \sum_k f_{ki} t_k^a + \sum_{kc} \langle ka || ci \rangle t_k^c + \sum_{kc} f_{kc} t_{ik}^{ac} \\
 & + \frac{1}{2} \sum_{kcd} \langle ka || cd \rangle t_{ki}^{cd} - \frac{1}{2} \sum_{klc} \langle kl || ci \rangle t_{kl}^{ca} \\
 & - \sum_{kc} f_{kc} t_i^c t_k^a - \sum_{klc} \langle kl || ci \rangle t_k^c t_j^a \\
 & + \sum_{kcd} \langle ka || cd \rangle t_k^c t_i^d \\
 & - \sum_{klcd} \langle kl || cd \rangle t_k^c t_i^d t_j^a + \sum_{klcd} \langle kl || cd \rangle t_k^c t_{li}^{da} \\
 & - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{ki}^{cd} t_l^a - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{kl}^{ca} t_i^d
 \end{aligned}$$

# Coupled Cluster Equations, $t_2$ Equation

The  $t_2$  amplitude equations are given by

$$\begin{aligned}
 0 = & \langle ab || ij \rangle + \sum_c \left( f_{bc} t_{ij}^{ac} - f_{ac} t_{ij}^{bc} \right) - \sum_k \left( f_{kj} t_{ik}^{ab} - f_{ki} t_{jk}^{ab} \right) \\
 & + \frac{1}{2} \sum_{kl} \langle kl || ij \rangle t_{kl}^{ab} + \frac{1}{2} \sum_{cd} \langle ab || cd \rangle t_{cd}^{ij} + P(ij)P(ab) \sum_{kc} \langle kb || cj \rangle t_{ac}^{ik} \\
 & + P(ij) \sum_c \langle ab || cj \rangle t_i^c - P(ab) \sum_k \langle kb || ij \rangle t_k^a \\
 & + \frac{1}{2} P(ij)P(ab) \sum_{klcd} \langle kl || cd \rangle t_{ik}^{ac} t_{lj}^{db} + \frac{1}{4} \sum_{klcd} \langle kl || cd \rangle t_{ij}^{cd} t_{kl}^{ab} - \frac{1}{2} P(ab) \sum_{klcd} \langle kl || cd \rangle t_{ij}^{ac} t_{kl}^{bd} \\
 & + \frac{1}{2} P(ab) \sum_{kl} \langle kl || ij \rangle t_k^a t_l^b + \frac{1}{2} P(ij) \sum_{cd} \langle ab || cd \rangle t_i^c t_j^d - P(ij)P(ab) \sum_{kc} \langle kb || ic \rangle t_k^a t_j^c \\
 & + P(ab) \sum_{kc} f_{kc} t_k^a t_{ij}^{ab} + P(ij) \sum_{kc} f_{kc} t_i^c t_{jk}^{ab}
 \end{aligned}$$

# Coupled Cluster Equations, $t_2$ Equation, contrn.

$t_2$  continued

$$\begin{aligned}
 & - P(ij) \sum_{klc} \langle kl || ci \rangle t_k^c t_{lj}^{ab} + P(ab) \sum_{kcd} \langle ka || cd \rangle t_k^c t_{ij}^{db} + P(ij)P(ab) \sum_{kcd} \langle ak || dc \rangle t_i^d t_{jk}^{bc} \\
 & + P(ij)P(ab) \sum_{klc} \langle kl || ic \rangle t_l^a t_{jk}^{bc} + \frac{1}{2} P(ij) \sum_{klc} \langle kl || ck \rangle t_i^c t_{kl}^{ab} - \frac{1}{2} P(ab) \sum_{kcd} \langle kb || cd \rangle t_k^a t_{ij}^{cd} \\
 & - \frac{1}{2} P(ij)P(ab) \sum_{kcd} \langle kb || cd \rangle t_i^c t_k^a t_j^d + \frac{1}{2} P(ij)P(ab) \sum_{klc} \langle kl || cj \rangle t_i^c t_k^a t_l^b \\
 & - P(ij) \sum_{klcd} \langle kl || cd \rangle t_k^c t_i^d t_{lj}^{ab} - P(ab) \sum_{klcd} \langle kl || cd \rangle t_k^c t_l^a t_{ij}^{db} + \frac{1}{4} P(ij) \sum_{klcd} \langle kl || cd \rangle t_i^c t_j^d t_{kl}^{ab} \\
 & + \frac{1}{4} P(ab) \sum_{klcd} \langle kl || cd \rangle t_k^a t_l^b t_{ij}^{cd} + P(ij)P(ab) \sum_{klcd} \langle kl || cd \rangle t_i^c t_l^b t_{kj}^{ad} \\
 & + \frac{1}{4} P(ij)P(ab) \sum_{klcd} \langle kl || cd \rangle t_i^c t_k^a t_j^d t_l^b .
 \end{aligned}$$

with  $P = P(ij)f(ij) = f(ij) - f(ji)$ .

# Coupled Cluster, Selected Results with $N^3\text{LO}$

| Nucleus              | $N = 5$            | $N = 6$            | $N = 7$            | $N = 8$            | Expt               |
|----------------------|--------------------|--------------------|--------------------|--------------------|--------------------|
| $^{15}\text{O}$      | 113.904<br>(7.594) | 101.150<br>(6.743) | 99.869<br>(6.658)  | 99.646<br>(6.643)  | 111.955<br>(7.464) |
| $^{15}\text{N}$      | 116.983<br>(7.799) | 103.810<br>(6.921) | 102.341<br>(6.823) | 102.360<br>(6.824) | 115.492<br>(7.699) |
| $^{16}\text{O}$      | 131.800<br>(8.787) | 120.720<br>(7.545) | 119.101<br>(7.444) | 118.491<br>(7.406) | 127.619<br>(7.976) |
| $^{17}\text{O}$      | 132.075<br>(8.805) | 122.910<br>(7.230) | 121.980<br>(7.175) | 121.547<br>(7.150) | 131.762<br>(7.751) |
| $^{17}\text{F}$      | 128.954<br>(8.597) | 120.250<br>(7.074) | 119.430<br>(7.026) | 118.780<br>(6.987) | 128.220<br>(7.542) |
| $\hbar\Omega$        | 13                 | 11                 | 10                 | 11                 |                    |
| $\beta_{\text{CoM}}$ | 1.50               | 0.15               | 0.05               | 0.0                |                    |

# Coupled Cluster, Results with $N^3\text{LO}$

| Excited state             | $N = 5$ | $N = 6$ | $N = 7$ | $N = 8$ | Expt  |
|---------------------------|---------|---------|---------|---------|-------|
| $^{15}\text{O} (3/2)_1^-$ | 6.515   | 6.602   | 6.166   | 6.264   | 6.176 |
| $^{15}\text{N} (3/2)_1^-$ | 6.354   | 6.680   | 6.256   | 6.318   | 6.323 |
| $^{17}\text{O} (3/2)_1^+$ | 6.298   | 6.031   | 5.489   | 5.675   | 5.084 |
| $^{17}\text{O} (1/2)_1^+$ | 0.328   | 0.130   | -0.349  | -0.025  | 0.870 |
| $^{17}\text{F} (3/2)_1^+$ | 6.460   | 6.207   | 5.686   | 5.891   | 5.000 |
| $^{17}\text{F} (1/2)_1^+$ | 0.748   | 0.544   | 0.088   | 0.428   | 0.495 |

# Coupled Cluster and Shell Model

**Preliminary** comparison of SM and CC results for  ${}^4\text{He}$ , Av8 interaction, No-core similarity transformation, no energy dependence of effective two-body interaction. (No CoM correction).

| $\hbar\omega$ [MeV] | 10      | 15      | 20      | 25      | 30      |
|---------------------|---------|---------|---------|---------|---------|
| 4 SM                | -24.894 | -28.207 | -28.164 | -27.17  | -25.869 |
| CCSD                | -24.606 | -28.027 | -28.033 | -26.917 | -25.308 |
| CR(T)L              | -24.822 | -28.156 | -28.118 | -27.101 | -25.766 |
| 5 SM                | -26.484 | -28.336 | -27.228 | -25.9   | -24.702 |
| CCSD                | -26.156 | -28.101 | -27.015 | -25.439 | -23.738 |
| CR(T)L              | -26.365 | -28.272 | -27.175 | -25.817 | -24.602 |
| 6 SM                | -26.604 | -27.526 | -26.189 | -25.053 | -24.147 |
| CCSD                | -25.86  | -27.195 | -25.903 | -24.38  | -22.755 |
| CR(T)L              | -26.396 | -27.46  | -26.134 | -24.967 | -24.077 |
| 7 SM                |         |         | -25.18  |         |         |
| CCSD                | -25.834 | -26.256 | -24.802 | -23.385 | -21.857 |
| CR(T)L              | -26.447 | -26.574 | -25.147 | -24.261 | -23.762 |
| 8 SM                | -26.4   | -25.8   | -24.44  | -23.7   | -23.25  |

# Coupled Cluster Summary

## Challenges

- CCSD in 8 major shells in  $^{16}\text{O}$  seems to yield stable results for the binding energy. Quick calculations compared to no-core shell-model.
- Can now do valence systems: first test for  $^{15,17}\text{O}$ .
- Can now do all closed core nuclei up to  $^{100}\text{Sn}$ , 10 major shells.
- Three-body forces implemented, Hagen *et al*
- Problem: harmonic oscillator basis. Even if we can do many shells, wave function not correct for many states. Now complex coupled cluster, Hagen *et al* nucl-th/0610072.
- How do we construct effective interactions which reflect the fact that we have a weakly bound system? And can we use the coupled-cluster machinery to study such systems?

# Exotic Systems

## Challenges

Exotic phenomena emerge in weakly bound and resonant many-body quantum systems. These phenomena include ground states that are embedded in the continuum, melting and reorganizing of shell structures, extreme matter clusterizations and halo densities. These unusual features occur in many branches of physics; as examples, in quantum, ultracold atom gases, auto-ionizing or molecules and exotic nuclei. In nuclear physics we find such exotic systems moving away from the valley of nuclear stability towards the drip lines, where the outermost nucleons literally start to drip from the nuclei.

The theoretical description of weakly bound and unbound quantum many-body systems is a challenging undertaking. The proximity of the scattering continuum in these systems implies that they should be treated as open quantum systems where coupling with the scattering continuum can take place. Recent work with Gamow states employed in Hamiltonian diagonalization have shown that these basis states correctly depict properties associated with open quantum systems.

Can we construct effective interactions for such systems?

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# Complex Scaling, Definitions

In nuclear physics, like in atomic physics, the expansion of many-body wavefunctions on single particle bases, generated by a suitable potential has been common practice. For a given potential the single particle eigenstates form a complete set of states,

$$\mathbf{1} = \sum_b |\psi_{nl}\rangle \langle \psi_{nl}| + \frac{1}{2} \int_{-\infty}^{\infty} dk k^2 |\psi_I(k)\rangle \langle \psi_I(k)|,$$

This completeness relation is known as the *resolution of unity*. The relation also applies to the binary interaction of say two nucleons and their relative motion. The sum is over the bound states in the system, while the integral is over the positive energy continuum states. The infinite space spanned by this basis is given by all square integrable functions on the real energy axis, known as the  $L^2$  space, which forms a Hilbert space. In the case of a confining harmonic oscillator potential there is an infinite number of bound states and no continuum integral.

# Complex Scaling, Definitions

The momentum space Schrödinger equation, for relative motion in partial wave  $l$  in a central potential, reads

$$\frac{\hbar^2}{2\mu} k^2 \psi_{nl}(k) + \frac{2}{\pi} \int_0^\infty dq q^2 V_l(k, q) \psi_{nl}(q) = E_{nl} \psi_{nl}(k).$$

With real momenta the momentum space Schrödinger equation corresponds to a hermitian Hamiltonian. The energy eigenvalues will in this case always be real, corresponding to discrete bound states ( $E_{nl} < 0$ ) and a continuum of scattering states ( $E_{nl} > 0$ ). Resonant and antibound states can never be obtained by directly solving this equation as it stands. In a sense, one can say that the spectrum of a hermitian Hamiltonian does not display all information about the physical system.

# Complex Scaling

Generalizing  $k$  to the complex  $k$ -plane, i.e.  $k = \text{Re}[k] + i\text{Im}[k]$ , an integral equation for the bound state wavefunctions may be written as

$$\psi_{nl}(k) = \frac{1}{E_{nl} - k^2/2\mu} \frac{2}{\pi} \int_0^\infty dq q^2 V_l(k, q) \psi_{nl}(q).$$

$\psi(k)$  is analytic in the upper half complex  $k$ -plane corresponding to the physical energy sheet, except for simple poles at the bound state energies (positive imaginary  $k$ ) and a cut in the complex  $E$ -plane along the real energy axis. The interaction between the particles,  $V_l(k, q)$ , is assumed to be spherically symmetric without tensor components. Our discussion does not involve the particle spins explicitly.

# Complex Scaling

The Fourier-Bessel transform of a non-local potential  $V_I(r, r')$  in coordinate space is given by

$$V_I(k, k') = \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 j_l(kr) j_l(k'r') V_I(r, r').$$

In the case of a local potential,

$$V_I(r, r') = \frac{\delta(r - r')}{r^2} V_I(r),$$

yielding

$$V_I(k, k') = \int_0^\infty dr r^2 j_l(kr) j_l(k'r) V_I(r).$$

The interaction in momentum space is given in units of  $\text{MeVfm}^3$ .

# Complex Scaling

Antibound states are not to be interpreted as physical states, i.e. a quantal system cannot be put in such a state. Nevertheless, antibound states close to the scattering threshold may have impact on observables such as phase shifts. For a system with antibound states close to the scattering threshold, a large enhancement of the scattering cross section will take place. This enhancement can be understood in terms of the antibound states.

From a mathematical point of view an antibound state is defined as a pole of the scattering matrix located on the negative imaginary  $k$ -axis.

# Complex Scaling

Resonant states can be divided into two subclasses; decay and capture states. Decay states are associated with poles of the scattering matrix located in the fourth quadrant of the complex  $k$ -plane. They have outgoing boundary conditions at infinity. Capture states are on the other hand associated with poles in the third quadrant of the complex  $k$ -plane, and have incoming waves at infinity. Naturally only capture states can be given physical meaning. Capture states may be interpreted as quasi-stationary states formed inside a potential barrier in the positive energy regime.

# Complex Scaling

Resonant states will have a definite lifetime before they decay through the barrier. This lifetime varies inversely with the probability of tunneling through the barrier, and the probability of tunneling is given by the width  $\Gamma$  of the resonant states. The width is in turn given by the absolute value of the imaginary part of the resonance energy squared. The closer the resonance energy is to the real energy axis, the smaller the width becomes and the lifetime of the quasi-stationary states increases. This indicates that resonant states with energy close to the real energy axis may have larger impact on observable quantities, e.g. phase shifts and scattering cross sections. Physical decay states are those with positive real energy. Gamow states are to be understood as physical resonant decay states close to the real energy axis, i.e. resonant states with narrow widths.

# Complex Scaling

Antibound and resonant states are located on the second (non-physical) energy Riemann sheet. The momentum is a multivalued function of energy;  $k(E) = \sqrt{2\mu E}$ . Multivalued functions may be represented by Riemann surfaces of branch cuts. The upper half complex  $k$ -plane and the lower half complex  $k$ -plane maps into the same complex energy plane. This problem is resolved by defining a Riemann surface with two sheets. The physical energy sheet (first sheet) is a mapping of the upper half complex  $k$ -plane while the so called *non-physical* energy sheet (second sheet) is a mapping of the lower half complex  $k$ -plane.

To reach into the non-physical energy sheet where antibound and resonant states are to be found one has to analytically continue the scattering equations through the cut along the real energy axis and into the lower half complex energy plane. We study here the analytic continuation of the Schrödinger equation into the non-physical sheet by the contour deformation method.

# Complex Scaling

In the 1960's Berggren discussed the use of resonant states in eigenfunction expansions of scattering and reaction amplitudes.

The resonant states form an incomplete set of states, for completeness the non-resonant continuum states has to be taken into account. Berggren found that the regularized resonant states along with a set of non-resonant continuum states defined on deformed contours in the complex momentum plane, form a bi-orthogonal set of states. This bi-orthogonal set can in turn be used as expansion basis for various physical quantities, where the resonant character of the system is displayed explicitly.

# Complex Scaling

The method Berggren studied is based on analytic continuation of the completeness relation to the complex  $k$ -plane by deforming the integration contour.

The sum over bound states are then the residues calculated at the poles of the scattering matrix along the positive imaginary  $k$  - axis. The integration along the real axis may then be distorted into some *inversion symmetric* contour, meaning that if  $k$  is on  $C$ , then  $-k$  is also on  $C$ . By redefining the completeness relation on distorted contours in the complex  $k$  plane, one can show by using Cauchy's residue theorem that the summation over discrete states will in general include bound, antibound and resonant states. By this procedure the norm integral of the resonant states is regularized along the distorted contours.

The eigenfunctions defined along distorted contours form a *biorthogonal* set, and the normalization follows the generalized c-product

$$\langle\langle \psi_{nI} | \psi_{n'I} \rangle\rangle \equiv \langle \psi_{nI}^* | \psi_{n'I} \rangle = \delta_{n,n'}.$$

# General Completeness Relation

The most general completeness relation on an arbitrary *inversion symmetric* contour  $C = C^+ + C^-$  can then be written as

$$\mathbf{1} = \sum_{n \in \mathbf{C}} |\psi_n\rangle \langle \psi_n^*| + \int_{C^+} dz |\psi_I(z)\rangle \langle \psi_I^*(z)|,$$

where  $C^+$  is the distortion of the positive real  $k$ -axis, and  $C^-$  is the distortion of the negative real  $k$ -axis.

$$\int_{C^-} dz |\psi_I(z)\rangle \langle \psi_I^*(z)| = \int_{C^+} dz |\psi_I(z)\rangle \langle \psi_I^*(z)|.$$

The summation is over all discrete states (bound, virtual and resonant states) located in the domain  $\mathbf{C}$ , defined as the area above the contour  $C$ , and the integral is over the non-resonant complex continuum defined on  $C^+$ .

# Complex Scaling

Here the symmetry of the integrand has been taken into account, that is

$$\int_{C^-} dk k^2 |\psi_I(k)\rangle \langle \psi_I^*(k)| = \int_{C^+} dk k^2 |\psi_I(k)\rangle \langle \psi_I^*(k)|.$$

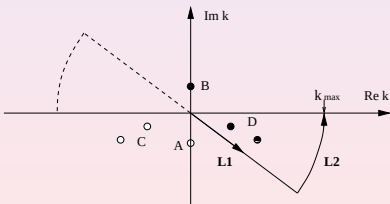
The summation is over all discrete states (bound, antibound and resonant states) located in the domain  $\mathbf{C}$ , defined as the area above the contour  $C$ , and the integral is over the non-resonant complex continuum defined on  $C^+$ . The space spanned by the basis includes all square integrable functions defined in the domain  $\mathbf{C}$ , defining a generalized Hilbert space.

In analytic continuation of integral equations we state the general rule

*Continuing an integral in the complex plane, the moving singularities of the integrand must not intercept the integration contour.*

The contour  $C_1^+$

- $$\begin{aligned} & \left( \exp(-2i\theta) \frac{k^2}{2\mu} - E_{nl} \right) \psi_{nl}(z) \\ & + \exp(-3i\theta) \frac{2}{\pi} \times \\ & \int_0^\infty dq q^2 V_l(z, z') \psi_{nl}(z') = 0. \end{aligned}$$



# Problems with contour $C_1^+$

Yukawa type interaction model (Malfliet-Tjon model)

$$V(r) = V_A \frac{\exp(-\mu_A r)}{r}$$

This interaction can be made to support bound and virtual states for several partial waves. In momentum space it reads for e.g.,  $s$ -waves

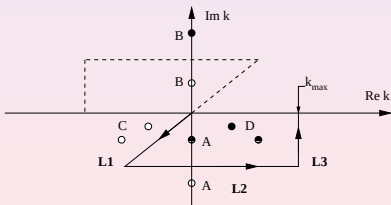
$$V(k, k') = V_A \frac{1}{4kk'} \ln \left( \frac{(k + k')^2 + \mu_A^2}{(k - k')^2 + \mu_A^2} \right).$$

By analytic continuation of the interaction to the complex  $k$ -plane, there will be singularities in the interaction for

$$(z - z')^2 + \mu_A^2 = 0 \quad (z + z')^2 + \mu_A^2 = 0.$$

For certain values of  $k, k'$  the contour  $C_1^+$  will pass through the singularity of the interaction and Cauchy's integral theorem cannot be applied.

# A modified contour



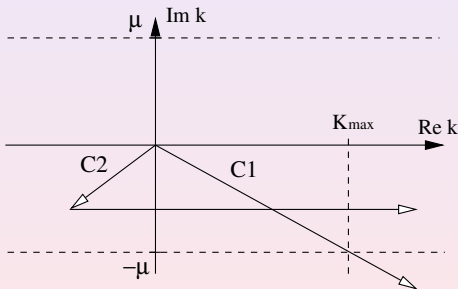
## The contour $C_2^+$

- The line segment  $L_1$  is given by a rotation  

$$z_1 = k_1 \exp(-i\theta)$$
- $k_1 \in [0, b]$ ,  $L_2$  is given by a translation  

$$z_2 = k_2 - ib \sin(\theta)$$
 where  
 $k_2 \in [b \cos(\theta), k_{\max}]$  and
- $b$  determines the translation into the lower-half  $k$ -plane and  $L_3$  by  $z_3 = k_{\max} - ic$  where  $c \in [b \sin(\theta) 0]$ .

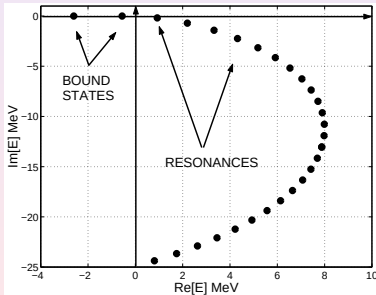
# Sketch of both contours



## Interaction Singularity

For  $k, k' > \mu_A / \tan(\theta) = k_{\max}$  the contour  $C_1^+$  will pass through the singularity of the interaction and Cauchy's integral theorem cannot be applied.

# Complex Scaling



How the bound state of the system approaches the scattering threshold and develop into decay resonant states for decreasing interaction strength  $\nu_A$ . The interaction strength  $\nu_A$  is varied from  $-5.6$  to  $-4.1$  in steps of  $0.1$  MeV. For  $\nu_A = -5.6$  and  $\nu_A = -5.5$  we have a bound state.

# Complex interaction, the $t$ -matrix

We can then obtain a complex  $t$ -matrix defined in operator form by

$$t(\omega) = V + VG(\omega)V,$$

with

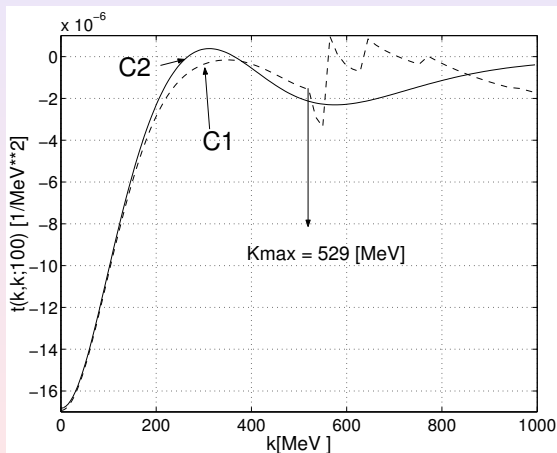
$$G(\omega) = \sum_b \frac{|\psi_b\rangle\langle\psi_b|}{\omega - E_b} + \int_0^\infty dE_c \frac{|\psi_c\rangle\langle\psi_c|}{\omega - E_c},$$

or in full glory (real  $k, k'$ )

$$t_I(k, k', \omega) = V_I(k, k') + \frac{4}{\pi^2} \sum_\alpha \int_C \int_{C'} dz dz' z^2 z'^2 V_I(k, z) \frac{\psi_\alpha(z) \psi_\alpha(z')}{\omega - E_\alpha} V_I(z', k'),$$

Here  $C$  is either  $C_1^+$  or  $C_2^+$ . This applies to  $C'$  as well. The last equation can be solved via matrix inversion or as an eigenvalue problem.

# $t$ -Matrix for Malfliet-Tjon like potential



# Applications to Nuclei: ${}^5, {}^6, {}^7\text{He}$

Here phenomenological NN model, separable Gaussian

$$V_{ij}(\mathbf{r}_i, \mathbf{r}_j) = V_0 \exp(-\alpha^2(r_i^2 + r_j^2)) \sum_{\lambda} (Y_{\lambda}(i) \cdot Y_{\lambda}(j)).$$

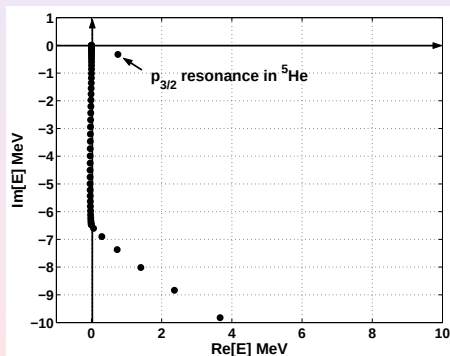
and sp potential

$$V_{ij}(k, k') = V_{ij}^c(k, k') + (\vec{\sigma} \cdot \vec{l}) V_{ij}^{\sigma l}(k, k'),$$

fitted to reproduce the resonances in  ${}^5\text{He}$ .

- Define the model space to consist of  $p_{3/2}$  and  $p_{1/2}$  and choose a number of mesh points along contours  $C_R$  and  $C_T$ .
- Setup complex scaled NN interaction and Hamiltonian and diagonalize.
- Dimensionalities can be huge. Reduce this through similarity transformation.
- Next step (see later) is to use a realistic NN force.

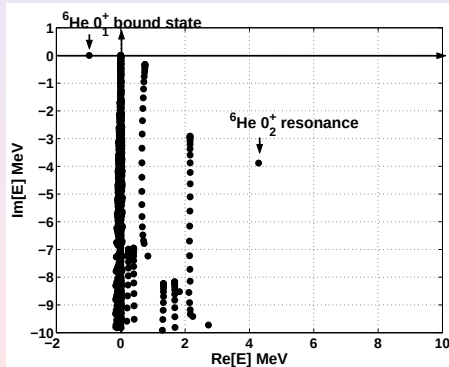
# Complex Scaling and $^5\text{He}$ results



## $J = 3/2^-$ Resonance

| $N_R$ | $N_T$ | Re[E]  | Im[E]   |
|-------|-------|--------|---------|
| 10    | 10    | 0.7523 | -0.3298 |
| 12    | 12    | 0.7525 | -0.3280 |
| 20    | 20    | 0.7525 | -0.3280 |
| 40    | 40    | 0.7525 | -0.3280 |

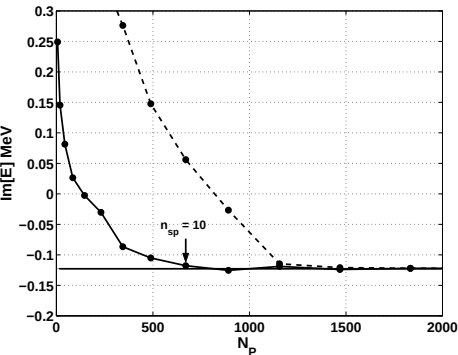
# Complex Scaling and ${}^6\text{He}$ results



## $0^+_1$ Ground State

| $N_{2p}$ | $\text{Re}[E]$ | $\text{Im}[E]$ |
|----------|----------------|----------------|
| 300      | -0.980067      | -0.000759      |
| 820      | -0.979508      | 0.000000       |
| 1275     | -0.979509      | 0.000000       |

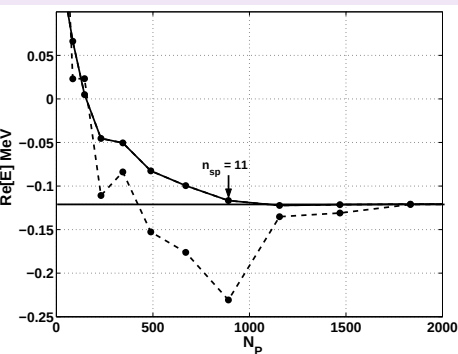
# Complex Scaling and Imaginary $^7\text{He}$ results



## $J = 3/2^-$ Resonance

- $N_P$  total dimensionality
- $n_{sp}$  number of single particle momenta for  $p_{3/2}$ .
- Similarity transformation done for three-body problem

# Complex Scaling and Real $^7\text{He}$ results



## $J = 3/2^-$ Resonance

- Dimension becomes too big
- Use similarity transformed equation for smaller space, where model space consists of selected states.
- Dim reduced to 4 – 8% of total

# Outline

- 1 Introduction
  - Overall motivation and aims
- 2 Many-Body Methods
- 3 **Reminder of Coupled Cluster Theory**
  - Why Coupled-Cluster theory
  - **Formalism**
- 4 Effective Interactions for Weakly Bound Systems
  - Complex Effective Interactions
  - Complex Scaling for Realistic Interactions
- 5 Summary

# Hamiltonian and Basis

The  $A$ -body Hamiltonian  $H$  is defined as

$$H = \frac{1}{2m} \sum_{i=1}^A \mathbf{k}_i^2 + \sum_{i<j}^A V_{\text{low-k}}(i,j). \quad (2)$$

The spurious center of mass energy is removed by writing the internal kinetic energy as

$$T_{\text{in}} = T - T_{\text{c.m.}} = \left(1 - \frac{1}{A}\right) \sum_{i=1}^A \frac{\mathbf{k}_i^2}{2m} - \sum_{i<j}^A \frac{\mathbf{k}_i \cdot \mathbf{k}_j}{mA}. \quad (3)$$

The introduction of an additional two-body term yields a modified two-body interaction

$$H_{\text{I}} = V_{\text{low-k}} + V_{\text{c.m.}} = \sum_{i<j}^A \left( V_{\text{low-k}}(i,j) - \frac{\mathbf{k}_i \cdot \mathbf{k}_j}{mA} \right), \quad (4)$$

resulting in a total Hamiltonian given by

$$H = \left(1 - \frac{1}{A}\right) \sum_{i=1}^A \frac{\mathbf{k}_i^2}{2m} + H_{\text{I}}. \quad (5)$$

# Hamiltonian and Basis

Two-particle state in the laboratory system is given via transformation from the relative and center of mass system.

$$\begin{aligned}
 |(k_a l_a j_a t_{z_a})(k_b l_b j_b t_{z_b})JT_z\rangle = & \sum_{IL\lambda S\mathcal{J}} \int k^2 dk \int K^2 dK \left\{ \begin{array}{ccc} l_a & l_b & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_a & j_b & J \end{array} \right\} \\
 & \times (-1)^{\lambda+\mathcal{J}-L-S} F_{\hat{\mathcal{J}}\hat{\lambda}^2\hat{j}_a\hat{j}_b\hat{S}} \left\{ \begin{array}{ccc} L & l & \lambda \\ S & j & \mathcal{J} \end{array} \right\} \\
 & \times \langle kIKL|k_a l_a k_b l_b \lambda \rangle |kIKL(\mathcal{J})SJT_z\rangle,
 \end{aligned}$$

# Hartree-Fock Diagram

The HF contribution

$$\mathcal{V}_{HF}(k_a k_c l_a j_a t_{z_a}) = \frac{1}{\hat{x}^2} \sum_{j_a} \sum_{J \quad n_h l_h j_h t_{z_h}} \hat{j}^2 \langle (k_a l_a j_a t_{z_a})(n_h l_h j_h t_{z_h}) J T_z | H_1 | (k_c l_a j_a t_{z_a})(n_h l_h j_h t_{z_h}) J T_z \rangle ,$$

where  $\hat{x} = \sqrt{2x+1}$  and  $n_h l_h j_h t_{z_h}$  are the quantum numbers of the nucleon hole states. The variables  $l_a, j_a, t_{z_a}$  are the orbital angular momentum, total angular momentum and isospin projection ( $t_{z_a} = \pm 1/2$ ) of the incoming/outgoing nucleon, and  $k_a (k_c)$  the outgoing (incoming) particle momenta.

# Self-Energy

We limit ourselves to the computation of the HF contribution, the expression for the self-energy reads

$$\Sigma(j_a l_a k_a k_c) = \mathcal{V}_{HF}(j_a l_a k_a k_c).$$

This equation is only valid along the real-energy axis. However,  $\Sigma(j_a l_a k_a k_c)$  has to be analytically continued from the real  $k$ -axis to the complex  $k$ -plane in order to obtain a genuine Gamow shell-model single-particle basis.

# Recipe I

- The first step is to calculate  $\mathcal{V}_{HF}$  self-consistently on a grid on the real momentum axis using the interaction  $H_I$
- When a self-consistent solution has been obtained,  $\mathcal{V}_{HF}$  is calculated in position space via a double Fourier-Bessel transform.

$$\mathcal{V}_{HF}(jlrr') = \frac{2}{\pi} \int_0^\infty dk k^2 \int_0^\infty dk k^2 j_l(kr) j_l(k'r') \mathcal{V}_{HF}(jlkk'). \quad (6)$$

- Having obtained  $\mathcal{V}_{HF}$  in the  $r$ -plane we may go back to the complex  $k$ -plane using one more Fourier-Bessel transformation. On an inversion symmetric contour  $L^+$  in the complex  $k$ -plane, the HF potential becomes

$$\mathcal{V}_{HF}(jlkk') = \int_0^\infty dr r^2 \int_0^\infty dr' r'^2 j_l(kr) j_l(k'r') \mathcal{V}_{HF}(jlrr'), \quad (7)$$

where  $k$  and  $k'$  belong to the contour  $L^+$  and are therefore complex.

# Recipe II

The analytically continued single-particle Schrödinger equation on a general inversion symmetric contour then takes the form

$$\frac{\hbar^2}{m_{\text{eff}}} k^2 \psi_{nlj}(k) + \int_{L^+} dk' k'^2 \mathcal{V}_{HF}(jlk k') \psi_{nl}(k') = E_{nl} \psi_{nl}(k),$$

with  $m_{\text{eff}} = 2m(1 - 1/A)^{-1}$ . Here both  $k$  and  $k'$  are defined on an inversion symmetric contour  $L^+$  in the lower half complex  $k$ -plane, resulting in a closed integral equation. In order to solve this equation, the integral has to be discretized, and we finally end up with a complex symmetric matrix diagonalization problem. This procedure results in a self-consistent Gamow Hartree-Fock basis, which is complete within the discretization space, and includes bound, resonant and a finite set of non-resonant continuum states.

Results for  $^{16}\text{O}$  with  $\text{N}^3\text{LO}$ 

| $lj$      | $\Lambda = 1.9 \text{ fm}^{-1}$ |        | $\Lambda = 2 \text{ fm}^{-1}$ |        | $\Lambda = 2.1 \text{ fm}^{-1}$ |        | Expt.   |        |
|-----------|---------------------------------|--------|-------------------------------|--------|---------------------------------|--------|---------|--------|
|           | Re[E]                           | Im[E]  | Re[E]                         | Im[E]  | Re[E]                           | Im[E]  | Re[E]   | Im[E]  |
| $s_{1/2}$ | -73.977                         | 0.000  | -68.496                       | 0.000  | -63.078                         | 0.000  | -44.000 | 0.000  |
| $p_{3/2}$ | -37.082                         | 0.000  | -33.824                       | 0.000  | -30.650                         | 0.000  | -21.840 | 0.000  |
| $p_{1/2}$ | -23.981                         | 0.000  | -21.749                       | 0.000  | -19.680                         | 0.000  | -15.664 | 0.000  |
| $d_{5/2}$ | -5.060                          | 0.000  | -3.810                        | 0.000  | -2.541                          | 0.000  | -4.143  | 0.000  |
| $s_{1/2}$ | -3.531                          | 0.000  | -2.556                        | 0.000  | -1.781                          | 0.000  | -3.273  | 0.000  |
| $d_{3/2}$ | 5.189                           | -1.669 | 5.353                         | -1.928 | 5.419                           | -2.155 | 0.937   | -0.048 |

The number of nodes for each  $lj$  combination is 25.

Results for  ${}^4\text{He}$  with  $\text{N}^3\text{LO}$ 

|           | $\Lambda = 1.8\text{fm}^{-1}$ |        | $\Lambda = 1.9\text{fm}^{-1}$ |        | $\Lambda = 2.0\text{fm}^{-1}$ |        | Expt.   |        |
|-----------|-------------------------------|--------|-------------------------------|--------|-------------------------------|--------|---------|--------|
| $lj$      | Re[E]                         | Im[E]  | Re[E]                         | Im[E]  | Re[E]                         | Im[E]  | Re[E]   | Im[E]  |
| $s_{1/2}$ | -25.731                       | 0.000  | -24.541                       | 0.000  | -23.079                       | 0.000  | -20.578 | 0.000  |
| $p_{3/2}$ | 0.819                         | -0.325 | 1.041                         | -0.479 | 1.287                         | -0.667 | 0.890   | -0.324 |
| $p_{1/2}$ | 2.497                         | -3.697 | 2.514                         | -3.777 | 2.648                         | -4.029 | 2.160   | -2.785 |

# Two-body Matrix Elements I

The renormalized nucleon-nucleon interaction in an arbitrary two-particle basis in the laboratory frame is given by

$$\langle ab | V_{\text{low-k}} | cd \rangle = \langle (n_a l_a j_a t_{z_a}) (n_b l_b j_b t_{z_b}) J T_z | V_{\text{low-k}} | (n_c l_c j_c t_{z_c}) (n_d l_d j_d t_{z_d}) J T_z \rangle. \quad (8)$$

The two-body state  $|ab\rangle$  is implicitly coupled to good angular momentum  $J$ . The labels  $n_{a\dots d}$  number all bound, resonant and discretized scattering states with orbital and angular momenta  $(l_{a\dots d}, j_{a\dots d})$ .

In order to efficiently calculate the matrix elements of Eq. (8), we introduce a two-particle harmonic oscillator basis completeness relation

$$\sum_{\alpha \leq \beta} |\alpha\beta\rangle \langle \alpha\beta| = \mathbf{1}, \quad (9)$$

where the sum is not restricted in the neutron-proton case. We introduce the greek single particle labels  $\alpha, \beta$  for the single-particle harmonic oscillator states in order to distinguish them from the latin single-particle labels  $a, b$  referring to Gamow states.

## Two-body Matrix Elements II

The interaction can then be expressed in the complete basis of Eq. (9)

$$V_{\text{osc}} = \sum_{\alpha \leq \beta} \sum_{\gamma \leq \delta} |\alpha\beta\rangle \langle\alpha\beta| V_{\text{low-k}} |\gamma\delta\rangle \langle\gamma\delta|, \quad (10)$$

where the sums over two-particle harmonic oscillator states are infinite. The expansion coefficients

$$\langle\alpha\beta| V_{\text{low-k}} |\gamma\delta\rangle = \left\langle (n_\alpha l_\alpha j_\alpha t_{z\alpha}) (n_\beta l_\beta j_\beta t_{z\beta}) J T_z \right| V_{\text{low-k}} \left| (n_\gamma l_\gamma j_\gamma t_{z\gamma}) (n_\delta l_\delta j_\delta t_{z\delta}) J T_z \right\rangle,$$

represent the nucleon-nucleon interaction in an antisymmetrized two-particle harmonic oscillator basis, and may easily be calculated using the well known Moshinsky transformation coefficients.

# Two-body Matrix Elements III

Matrix elements of Eq. (8) are calculated numerically in an arbitrary two-particle Gamow basis by truncating the completeness expansion of Eq. (10) up to  $N$  harmonic oscillator two-body states

$$\langle ab|V_{\text{osc}}|cd\rangle \approx \sum_{\alpha \leq \beta}^N \sum_{\gamma \leq \delta}^N \langle ab|\alpha\beta\rangle \langle \alpha\beta|V_{\text{low-k}}|\gamma\delta\rangle \langle \gamma\delta|cd\rangle. \quad (11)$$

The two-particle overlap integrals  $\langle ab|\alpha\beta\rangle$  read

$$\langle ab|\alpha\beta\rangle = \frac{\langle a|\alpha\rangle\langle b|\beta\rangle - (-1)^{J-j_\alpha-j_\beta}\langle a|\beta\rangle\langle b|\alpha\rangle}{\sqrt{(1+\delta_{ab})(1+\delta_{\alpha\beta})}} \quad (12)$$

for identical particles (proton-proton or neutron-neutron states) and

$$\langle ab|\alpha\beta\rangle = \langle a|\alpha\rangle\langle b|\beta\rangle \quad (13)$$

for the proton-neutron case.

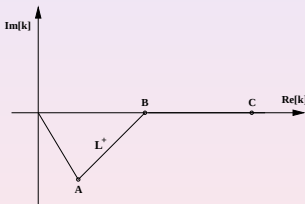
## Two-body Matrix Elements IV

The one-body overlaps  $\langle a|\alpha\rangle$  are given by,

$$\langle a|\alpha\rangle = \int d\tau \tau^2 \varphi_a(\tau) R_\alpha(\tau) \delta_{l_a l_\alpha} \delta_{j_a j_\alpha} \delta_{t_a t_\alpha}, \quad (14)$$

where  $\varphi_a$  is a Gamow single-particle state and  $R_\alpha$  is a harmonic oscillator wave function. The radial integral is either evaluated in momentum or position space, indicated by the integration variable  $\tau$ . The important point to notice is that the only numerical calculations involving Gamow states are the overlaps of Eq. (14). Hence, this expansion provides a simple analytical continuation of the nuclear interaction in the complex  $k$ -plane. More precisely, the expansion coefficients of Eq. (11) can always be calculated with real harmonic oscillator wave functions, and in the case of Gamow functions spanning a complex contour  $L^+$  (as in the momentum space representation), it is only the overlap integrals of Eq. (14) which are analytically continued in the complex plane. These one-body overlap integrals converge in all regions of the complex plane which are of physical importance, due to the gaussian fall off of the harmonic oscillator wave functions.

# Contour and Number of States



## The contour $L^+$

- $s_{1/2}$ ,  $p_{3/2}$ ,  $p_{1/2}$ ,  $d_{5/2}$  and  $d_{3/2}$  single-particle states
- Each combination of the quantum numbers  $lj$  consists of 25 single-particle orbitals, totalling 115 orbitals.
- These states are used to build two-particle states

# Results

The same integration contour  $L^+$  in the complex  $k$ -plane is used for all single-particle states. In our  ${}^6\text{He}$  calculations the contour is defined with  $A = 0.28 - 0.12i$   $\text{fm}^{-1}$ ,  $B = 0.5$   $\text{fm}^{-1}$  and  $C = 4$   $\text{fm}^{-1}$ , and in our  ${}^{18}\text{O}$  calculations it is defined with  $A = 0.52 - 0.12i$   $\text{fm}^{-1}$ ,  $B = 0.64$   $\text{fm}^{-1}$  and  $C = 4$   $\text{fm}^{-1}$ . Using Gauss-Legendre quadrature, the discretization of  $L^+$  has been carried out with 5 points in the interval  $(0, A)$ , 7 points in the interval  $(A, B)$  and 13 points in the interval  $(B, C)$ . Our discretization of  $L^+$  yields a precision of the energy calculation better than 0.1 keV for all states considered.

# Results

Convergence of the  $0_1^+$  and the  $2_1^+$  energies in  ${}^6\text{He}$  as functions of the number of harmonic oscillator nodes in the expansion of the realistic low-momentum  $\text{N}^3\text{LO}$  nucleon-nucleon interaction. The model space is given by  $\Lambda = 1.9 \text{ fm}^{-1}$ . The harmonic oscillator length is chosen at  $b = 2 \text{ fm}$ .

|                  | $J^\pi = 0_1^+$ |        | $J^\pi = 2_1^+$ |         |
|------------------|-----------------|--------|-----------------|---------|
| $n_{\text{max}}$ | Re[E]           | Im[E]  | Re[E]           | Im[E]   |
| 4                | -0.4760         | 0.0000 | 0.9504          | -0.0467 |
| 6                | -0.4714         | 0.0000 | 0.9546          | -0.0461 |
| 8                | -0.4719         | 0.0000 | 0.9597          | -0.0453 |
| 10               | -0.4721         | 0.0000 | 0.9602          | -0.0452 |
| 12               | -0.4721         | 0.0000 | 0.9600          | -0.0452 |
| 14               | -0.4721         | 0.0000 | 0.9601          | -0.0452 |
| 16               | -0.4721         | 0.0000 | 0.9601          | -0.0453 |
| 18               | -0.4721         | 0.0000 | 0.9601          | -0.0453 |
| 20               | -0.4721         | 0.0000 | 0.9601          | -0.0453 |

# Results

Convergence of the  $0_1^+$ ,  $0_2^+$ ,  $4_1^+$  and the  $4_2^+$  energies in  $^{18}\text{O}$  as functions of the number of harmonic oscillator nodes in the harmonic oscillator expansion. A model space defined by  $\Lambda = 1.9\text{fm}^{-1}$  was used. The harmonic oscillator length is fixed at  $b = 2\text{ fm}$ . Energies are in units of MeV.

|                  | $J^\pi = 0_1^+$ |       | $J^\pi = 0_2^+$ |       | $J^\pi = 4_1^+$ |        | $J^\pi = 4_2^+$ |         |
|------------------|-----------------|-------|-----------------|-------|-----------------|--------|-----------------|---------|
| $n_{\text{max}}$ | Re[E]           | Im[E] | Re[E]           | Im[E] | Re[E]           | Im[E]  | Re[E]           | Im[E]   |
| 4                | -12.225         | 0.000 | -8.438          | 0.000 | -11.0641        | 0.0000 | -1.4373         | -0.8275 |
| 6                | -12.226         | 0.000 | -8.498          | 0.000 | -11.0907        | 0.0000 | -1.4292         | -0.7600 |
| 8                | -12.228         | 0.000 | -8.499          | 0.000 | -11.0922        | 0.0000 | -1.4380         | -0.7405 |
| 10               | -12.229         | 0.000 | -8.499          | 0.000 | -11.0921        | 0.0000 | -1.4400         | -0.7390 |
| 12               | -12.228         | 0.000 | -8.499          | 0.000 | -11.0923        | 0.0000 | -1.4393         | -0.7401 |
| 14               | -12.228         | 0.000 | -8.499          | 0.000 | -11.0923        | 0.0000 | -1.4394         | -0.7401 |
| 16               | -12.228         | 0.000 | -8.499          | 0.000 | -11.0923        | 0.0000 | -1.4394         | -0.7401 |
| 18               | -12.228         | 0.000 | -8.499          | 0.000 | -11.0923        | 0.0000 | -1.4394         | -0.7401 |
| 20               | -12.228         | 0.000 | -8.499          | 0.000 | -11.0923        | 0.0000 | -1.4394         | -0.7401 |

Convergence of the  $2_1^+$ ,  $2_2^+$ ,  $2_3^+$  and the  $2_4^+$  energies in  $^{18}\text{O}$  as functions of the number of harmonic oscillator nodes in the harmonic oscillator expansion. A model space defined by  $\Lambda = 1.9\text{fm}^{-1}$  was used. The harmonic oscillator length is fixed at  $b = 2\text{ fm}$ .

|            | $J^\pi = 2_1^+$ |        | $J^\pi = 2_2^+$ |        | $J^\pi = 2_3^+$ |         | $J^\pi = 2_4^+$ |         |
|------------|-----------------|--------|-----------------|--------|-----------------|---------|-----------------|---------|
| $n_{\max}$ | Re[E]           | Im[E]  | Re[E]           | Im[E]  | Re[E]           | Im[E]   | Re[E]           | Im[E]   |
| 4          | -12.1398        | 0.0000 | -10.0488        | 0.0000 | -0.0772         | -1.4465 | 1.1632          | -1.4478 |
| 6          | -12.1465        | 0.0000 | -10.0830        | 0.0000 | -0.1321         | -1.3038 | 1.1628          | -1.5059 |
| 8          | -12.1452        | 0.0000 | -10.0853        | 0.0000 | -0.1539         | -1.2929 | 1.1836          | -1.5346 |
| 10         | -12.1450        | 0.0000 | -10.0857        | 0.0000 | -0.1595         | -1.2922 | 1.1807          | -1.5331 |
| 12         | -12.1453        | 0.0000 | -10.0858        | 0.0000 | -0.1570         | -1.2938 | 1.1820          | -1.5343 |
| 14         | -12.1453        | 0.0000 | -10.0858        | 0.0000 | -0.1571         | -1.2938 | 1.1821          | -1.5342 |
| 16         | -12.1453        | 0.0000 | -10.0858        | 0.0000 | -0.1573         | -1.2936 | 1.1822          | -1.5342 |
| 18         | -12.1453        | 0.0000 | -10.0858        | 0.0000 | -0.1573         | -1.2936 | 1.1822          | -1.5342 |
| 20         | -12.1453        | 0.0000 | -10.0858        | 0.0000 | -0.1573         | -1.2936 | 1.1822          | -1.5342 |

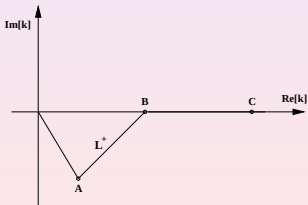
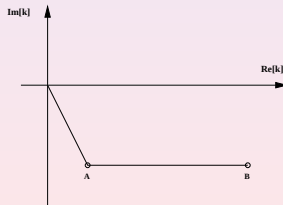
# Complex Scaling

To make calculations numerically feasible at present we therefore initialize our Hartree-Fock calculations with a mixed basis consisting of a finite set of Complex Woods-Saxon bound, resonant and non-resonant continuum states and a finite set of Harmonic Oscillator basis states for chosen partial waves. For protons we strictly define the space by a finite set of harmonic oscillator wave functions, while for the neutron space we use a complex Woods-Saxon basis for the  $s - p$  partial waves and harmonic oscillator wave functions for the higher partial waves  $d - g$ . This choice of mixed basis may be justified since we are dealing with the ground states of the  $^3\text{-}^5\text{He}$  isotopes. For these nuclei the proton separation energy is typically at the order of 20 – 30 MeV and they are mainly occupying deeply bound  $s$ -orbits. On the other hand it is well known that the  $^5\text{He}$  ground state is a resonance with width  $\sim 0.65\text{MeV}$  and with spin and parity  $J^\pi = 3/2^-$ , implying that the outermost neutron in  $^5\text{He}$  is mainly in the  $p_{3/2}$  shell.

# Complex Scaling

In order to check the validity and convergence of our results, we construct our single-particle Berggren basis on two very different contours in the complex  $k$ -plane. We sketch a contour  $L_1^+$  and that is of triangular shape and defined by three line segments joined by the points  $A$  and  $B$  in the complex  $k$ -plane. The contour  $L_2^+$  consists of a rotated and a translated line segment joined at the point  $A$  in the complex  $k$ -plane. Utilizing a contour of the type  $L_2^+$  both resonant and anti-bound states converge quickly with respect to the number of integration points. Further, the contour  $L_2^+$ , yields stable solutions of all physical scattering amplitudes, such as the  $t$ -matrix, which may be obtained by a spectral representation of the Green's function. We discretize the contours  $L_1^+$  and  $L_2^+$  by Gauss-Legendre quadrature.

# Countours $L_1$ and $L_2$



# Complex Scaling

Convergence of the  $s_{1/2}$  hole and the  $p_{3/2}$  particle states in  $^4\text{He}$  with increasing number of discretization points along the triangular contour  $L_1^+$ . The initial proton space was given by  $5s5p$  oscillator states.

|     |       |       |       | Neutrons  |       |           |        | Protons   |       |           |       |
|-----|-------|-------|-------|-----------|-------|-----------|--------|-----------|-------|-----------|-------|
|     |       |       |       | $s_{1/2}$ |       | $p_{3/2}$ |        | $s_{1/2}$ |       | $p_{3/2}$ |       |
| $n$ | $n_1$ | $n_2$ | $n_3$ | Re[E]     | Im[E] | Re[E]     | Im[E]  | Re[E]     | Im[E] | Re[E]     | Im[E] |
| 15  | 3     | 3     | 9     | -24.323   | 0.000 | 1.027     | -0.536 | -23.350   | 0.000 | 2.933     | 0.000 |
| 20  | 5     | 4     | 11    | -24.323   | 0.000 | 1.000     | -0.546 | -23.350   | 0.000 | 2.930     | 0.000 |
| 25  | 7     | 5     | 13    | -24.323   | 0.000 | 1.002     | -0.548 | -23.350   | 0.000 | 2.930     | 0.000 |
| 30  | 8     | 6     | 16    | -24.323   | 0.000 | 1.002     | -0.548 | -23.350   | 0.000 | 2.930     | 0.000 |

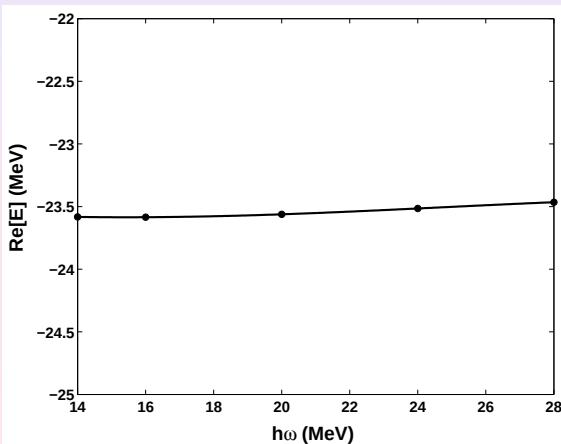
# Complex Scaling

Convergence of the  $s_{1/2}$  hole and the  $p_{3/2}$  particle states in  ${}^4\text{He}$  with increasing number of discretization

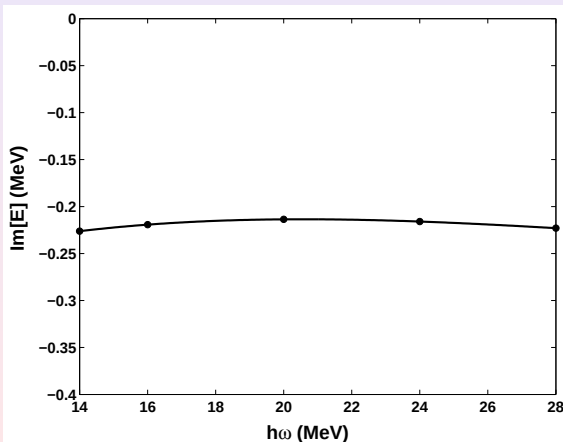
points along the contour  $L_2^+$ . The initial proton space was given by  $5s5p$  oscillator states.

| Neutrons |       |       |           |        |           | Protons |           |       |           |       |
|----------|-------|-------|-----------|--------|-----------|---------|-----------|-------|-----------|-------|
|          |       |       | $s_{1/2}$ |        | $p_{3/2}$ |         | $s_{1/2}$ |       | $p_{3/2}$ |       |
| $n$      | $n_1$ | $n_2$ | Re[E]     | Im[E]  | Re[E]     | Im[E]   | Re[E]     | Im[E] | Re[E]     | Im[E] |
| 15       | 3     | 12    | -24.324   | -0.001 | 1.003     | -0.547  | -23.352   | 0.001 | 2.926     | 0.001 |
| 20       | 4     | 16    | -24.323   | 0.000  | 1.002     | -0.547  | -23.350   | 0.000 | 2.930     | 0.000 |
| 25       | 7     | 18    | -24.323   | 0.000  | 1.002     | -0.548  | -23.350   | 0.000 | 2.930     | 0.000 |
| 30       | 8     | 16    | -24.323   | 0.000  | 1.002     | -0.548  | -23.350   | 0.000 | 2.930     | 0.000 |

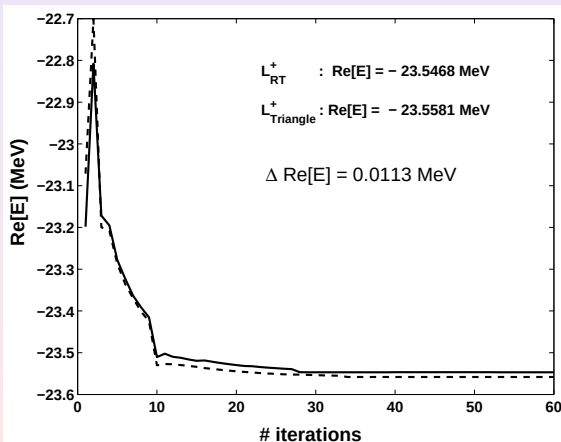
# $\hbar\omega$ dependence of the real part of the $^5\text{He}$ ground state energy



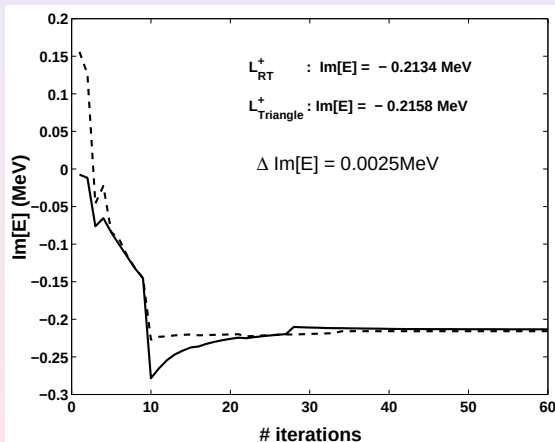
# $\hbar\omega$ dependence of the imaginary part of the $^5\text{He}$ ground state energy



# Convergence of the real part of the $^5\text{He}$ ground state energy



# Convergence of the imag part of the $^5\text{He}$ ground state energy



# Coupled Cluster and He Isotopes

Comparison of CCSD results and triples-corrected CCSD(T) results with exact calculations for the ground states of helium isotopes. The energies  $E$  are given in MeV, and the results are displayed for different basis sets.

| Method           | $^3\text{He}$ | $^4\text{He}$ | $^5\text{He}$ | $^6\text{He}$ |
|------------------|---------------|---------------|---------------|---------------|
| CCSD (OSC)       | -6.21         | -26.19        | -21.53        | -20.96        |
| CCSD (RHF)       | -6.10         | -26.06        | -21.55        | -20.99        |
| CCSD (SC-RHF)    | -6.11         | -26.06        | -21.55        | -21.04        |
| CCSD(T) (OSC)    | -6.40         | -26.30        | -21.91        | -22.83        |
| CCSD(T) (RHF)    | -6.35         | -26.24        | -21.90        | -22.56        |
| CCSD(T) (SC-RHF) | -6.34         | -26.24        | -21.91        | -22.62        |
| Exact            | -6.45         | -26.3         | -22.1         | -22.7         |

# Coupled Cluster and He Isotopes

|         | $^3\text{He}$ |       | $^4\text{He}$ |       | $^5\text{He}$ |       | $^6\text{He}$ |       | $^7\text{He}$ |       |
|---------|---------------|-------|---------------|-------|---------------|-------|---------------|-------|---------------|-------|
| $lj$    | Re[E]         | Im[E] | Re[E]         | Im[E] | Re[E]         | Im[E] | Re[E]         | Im[E] | Re[E]         | Im[E] |
| $s - p$ | -4.94         | 0.00  | -24.97        | 0.00  | -20.08        | -0.54 | -19.03        | -0.18 | -17.02        | -0.00 |
| $s - d$ | -6.42         | 0.00  | -26.58        | 0.00  | -23.56        | -0.22 | -23.26        | -0.09 | -22.19        | -0.00 |
| $s - f$ | -6.81         | 0.00  | -27.27        | 0.00  | -24.56        | -0.17 | -24.69        | -0.07 | -24.13        | -0.00 |
| $s - g$ | -6.91         | 0.00  | -27.35        | 0.00  | -24.87        | -0.16 | -25.16        | -0.06 | -24.83        | -0.00 |
| Expt.   | -7.72         | 0.00  | -28.30        | 0.00  | -27.41        | -0.33 | -29.27        | 0.00  | -28.82        | -0.00 |

CCSD calculation of the  $^3\text{--}^{10}\text{He}$  ground states with the low-momentum  $\text{N}^3\text{LO}$

nucleon-nucleon interaction for increasing number partial waves. The energies  $E$  are given in MeV for both real and imaginary parts.

# Summary: much Work in Progress

- Inclusion of continuum effects, complex coupled-cluster code and complex effective interactions
- Complicated algorithm for self-energy in  $k$ -space not needed. Can use any basis and just a complex  $G$ -matrix in an oscillator basis as starting point for Hartree-Fock and/or improved self-consistency.
- Need to introduce a complex  $G$ -matrix
- Derive better effective interactions for heavy nuclei and the shell model via similarity transformations to smaller spaces
- Helium and Oxygen isotopes, especially from  $^{20}\text{O}$  till  $^{28}\text{O}$ . several experiments at for example NSCL-MSU,  $^{23}\text{O}$ ,  $^{24}\text{O}$  and  $^{25}\text{O}$ .
- How much due to three-body forces and how much due to coupling to continuum with only two-body?
- Can we understand how shells evolve?

## For Further Reading

-  Kowalski, Dean, Hjorth-Jensen, Piecuch and Papenbrock, Phys. Rev. Lett. **92**, 132501 (2004).
-  Hagen, Vaagen, and Hjorth-Jensen J. Phys. **A 37**; Math. Gen., 8991-9021 (2004).
-  Hagen, Hjorth-Jensen, and Michel, Phys. Rev. C **73**, 064307 (2006).
-  Hagen, Dean, Hjorth-Jensen, and Papenbrock, nucl-th/0610072
-  Hagen, Papenbrock and Dean, Three-Body interactions and coupled cluster calculations.