Towards Optical Potentials from Coupled Cluster Calculations

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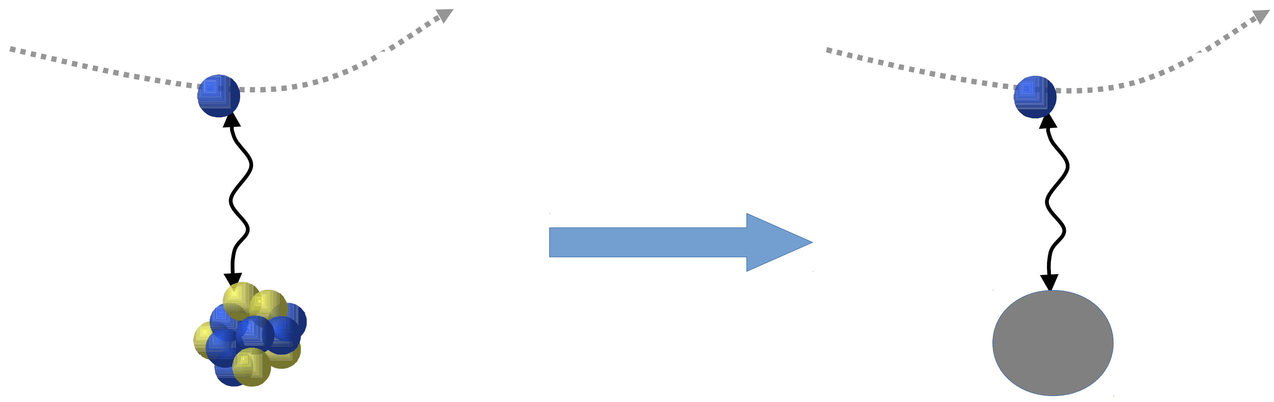
Goals

* microscopic construction of optical potentials : nucleons as degrees of freedom, modern realistic n-n, 3n forces...



$$H|\Psi(1,\ldots,A)\rangle = E|\Psi(1,\ldots,A)\rangle \qquad H^{eff}|\Psi'(\vec{r})\rangle = E|\Psi'(\vec{r})\rangle$$

Goals

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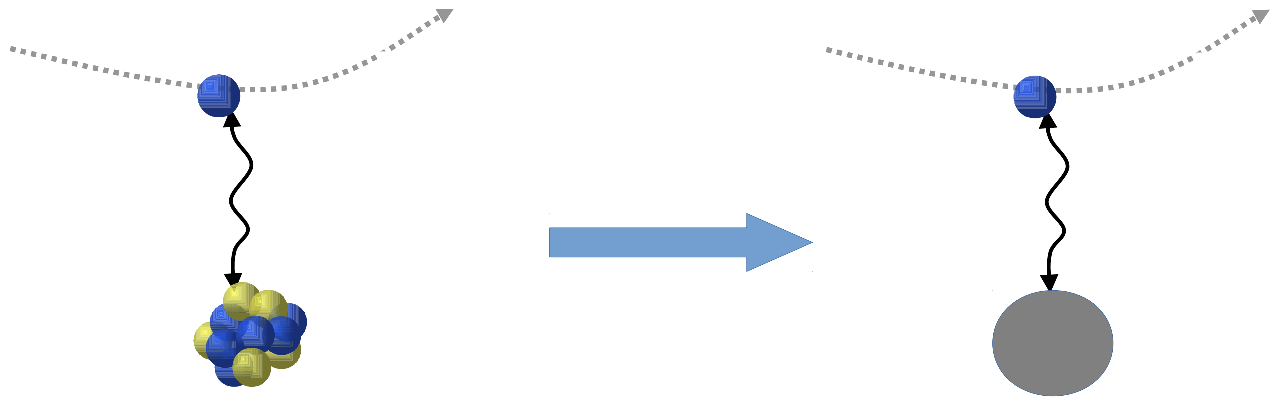
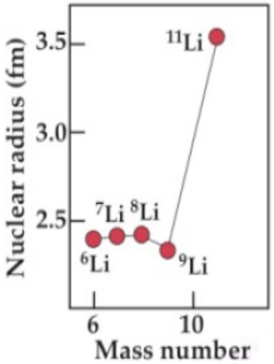


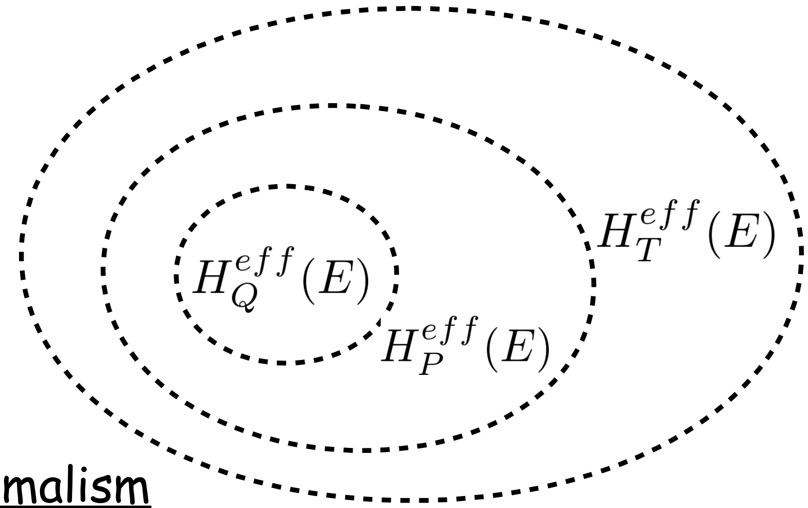
$$H|\Psi(1,\ldots,A)\rangle = E|\Psi(1,\ldots,A)\rangle \qquad H^{eff}|\Psi'(\vec{r})\rangle = E|\Psi'(\vec{r})\rangle$$

* predictive theory for nuclear reactions

* reliable/accurate extrapolations for systems far from stability.



Microscopic approaches for a unified description of structure and reactions



Continuum (real-energy) Shell Model

H.W.Bartz et al, NPA (1977) ; R.J. Philpott, NPA (1977) ;
K. Bennaceur et al, NPA(1999) ;J. Okołowicz et al PR (2003)
J. R et al, PRL (2005).

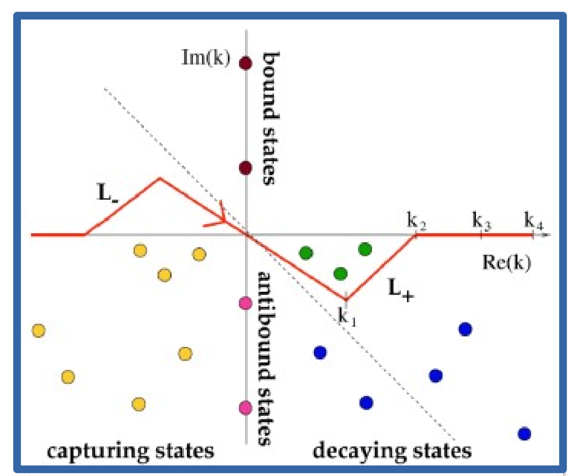
$$\boxed{\begin{aligned} \mathcal{Q} &= A \\ \mathcal{P} &= [A-1] \otimes 1 \\ \mathcal{T} &= [A-2] \otimes 2 \end{aligned}}$$

Feshbach projection formalism

Gamow (complex-energy) Shell Model

N. Michel et al, PRL (2002) ; N. Michel et al, JPG (2009) ; G. Hagen et al PRC (2005) ;
G. Papadimitriou et al, PRC (2014); Y. Jaganathen et al JP (2012) ; K. Fossez et al PRA (2015).

Berggren basis



No-Core Shell Model with continuum

S. Quaglioni et al PRC (2009),P Navratil et al (PRC) (2011), G. Hupin PRL (2015)

+ R-matrix, Complex scaling, Cluster-orbital Shell Model....

Single-particle Green's function

$$\boxed{G(\alpha,\beta,t,t') = -\frac{i}{\hbar}\langle\Psi_0^A|\mathcal{T}[a_\alpha(t)a_\beta^\dagger(t')]|\Psi_0^A\rangle}$$

Time ordering operator :

$$\mathcal{T}[a_\alpha(t)a_\beta^\dagger(t')] = \theta(t-t')a_\alpha(t)a_\beta^\dagger(t') - \theta(t'-t)a_\beta^\dagger(t')a_\alpha(t)$$

After a Fourier transformation:

$$\boxed{\begin{aligned} G(\alpha,\beta,E) = \langle\Psi_0^A|a_\alpha \frac{1}{E-(H-E_0^A)+i\eta}a_\beta^\dagger|\Psi_0^A\rangle \\ +\langle\Psi_0^A|a_\beta^\dagger \frac{1}{E+(E_0^A-H)-i\eta}a_\alpha|\Psi_0^A\rangle \end{aligned}}$$

$$\boxed{\eta \to 0}$$

Single-particle Green's function

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Hamiltonian for the A+1 system

$$\boxed{\begin{aligned} G(\alpha,\beta,E) = {} & \langle\Psi_0^A|a_\alpha\frac{1}{E-(H-E_0^A)+i\eta}a_\beta^\dagger|\Psi_0^A\rangle \\ & +\langle\Psi_0^A|a_\beta^\dagger\frac{1}{E+(E_0^A-H)-i\eta}a_\alpha|\Psi_0^A\rangle \end{aligned}}$$

$$\boxed{\eta \to 0}$$

Hamiltonian for the A-1 system

Lehman representation

$$\boxed{G(\alpha,\beta;E) = \sum_n \frac{\langle\Psi_0^A|a_\alpha|\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}|a_\beta^\dagger|\Psi_0^A\rangle}{E-[E_n^{A+1}-E_0^A]+i\eta} + \sum_m \frac{\langle\Psi_0^A|a_\beta^\dagger|\Psi_m^{A-1}\rangle\langle\Psi_m^{A-1}|a_\alpha|\Psi_0^A\rangle}{E-[E_0^A-E_m^{A-1}]-i\eta}}$$

<u>Connection to experimental data:</u>

i) poles: energy of the A+1 and A-1 nuclei with respect to the g.s. of the A-nucleon system

ii) spectral functions :

$$\boxed{E \le \epsilon_F^- = E_0^A - E_0^{A-1}}$$

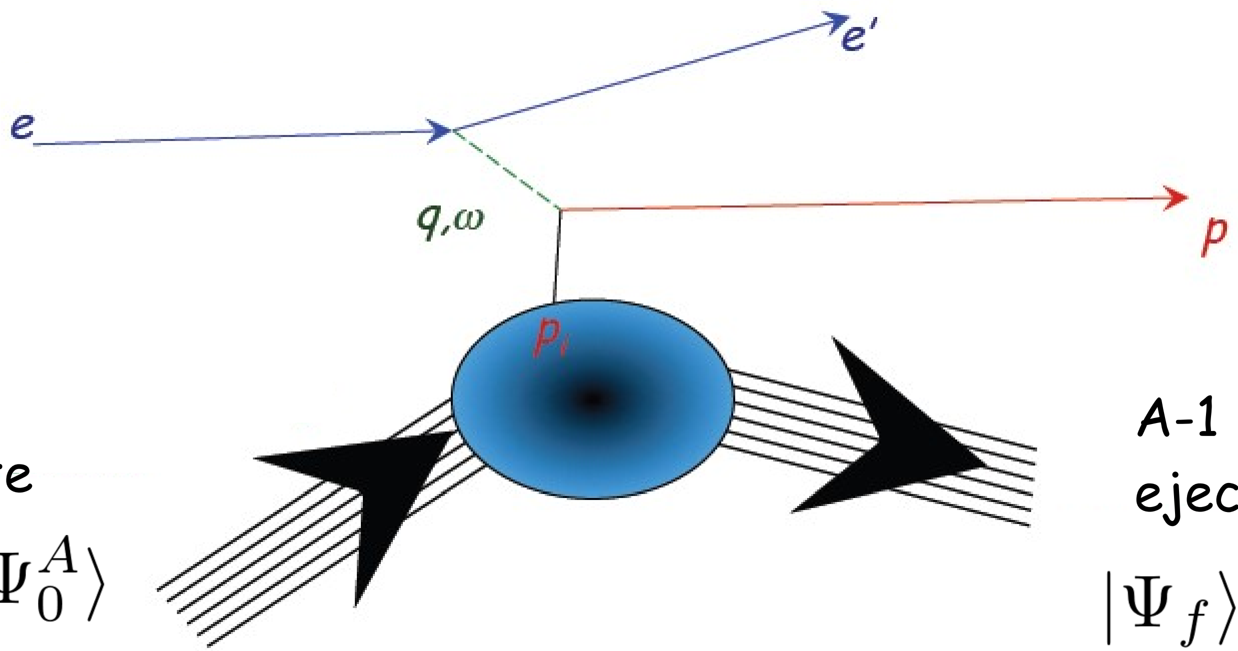
$$S_h(\alpha;E) = \frac{1}{\pi}\mathrm{Im}\ G(\alpha,\alpha;E) = \sum_m |\langle\Psi_m^{A-1}|a_\alpha|\Psi_0^A\rangle|^2\delta(E-(E_0^A-E_m^{A-1}))$$

$$S_p(\alpha;E) = -\frac{1}{\pi}\mathrm{Im}\ G(\alpha,\alpha;E) = \sum_n |\langle\Psi_n^{A+1}|a_\alpha^\dagger|\Psi_0^A\rangle|^2\delta(E-(E_n^{A+1}-E_0^A))$$

$$\boxed{E \ge \epsilon_F^+ = E_0^{A+1} - E_0^A}$$

"measure" of the correlations in nuclei as their behaviors deviate from an independent particle model

Spectroscopy with knockout reactions



intial state

$$|\Psi_i\rangle = |\Psi_0^A\rangle$$

A-1 body system+
ejected particle

$$|\Psi_f\rangle = a^\dagger_{\mathbf{p}}|\Psi_n^{A-1}\rangle$$

(ejectile with <u>**large**</u> momentum **p**)

$$\begin{aligned} d\sigma &\sim \sum_n \delta(E_n^{A-1} + \frac{\mathbf{p}^2}{2m} - E_0^A - \hbar\omega)\langle\Psi_n^{A-1}|a_{\mathbf{p}-\hbar\mathbf{q}}|\Psi_0^A\rangle \\ &= S_h(\mathbf{p}-\hbar\mathbf{q}; \frac{\mathbf{p}^2}{2m} - \hbar\omega) \end{aligned}$$

Dyson equation

$$G(\alpha,\beta;E) = G^{(0)}(\alpha,\beta;E) + \sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\Sigma(\gamma,\delta;E)G(\delta,\beta;E)$$

self-energy = optical potential

Dyson equation

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self-energy = optical potential

$$\left\{ \begin{array}{l} z_n^{A-1}(r) = \langle \Psi_n^{A-1} | a_r | \Psi_0^A \rangle \\ \\ \xi_{E+}^c(r) = \langle \Psi_0^A | a_r | \Psi_{E+}^c \rangle \end{array} \right\}$$

solutions of a one-body Schrödinger-like equation with the self-energy .

wave function for the elastic scattering from the g.s of the A-nucleon system

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wave function for the elastic scattering from the g.s of the A-nucleon system

Applications in Nuclear Physics :

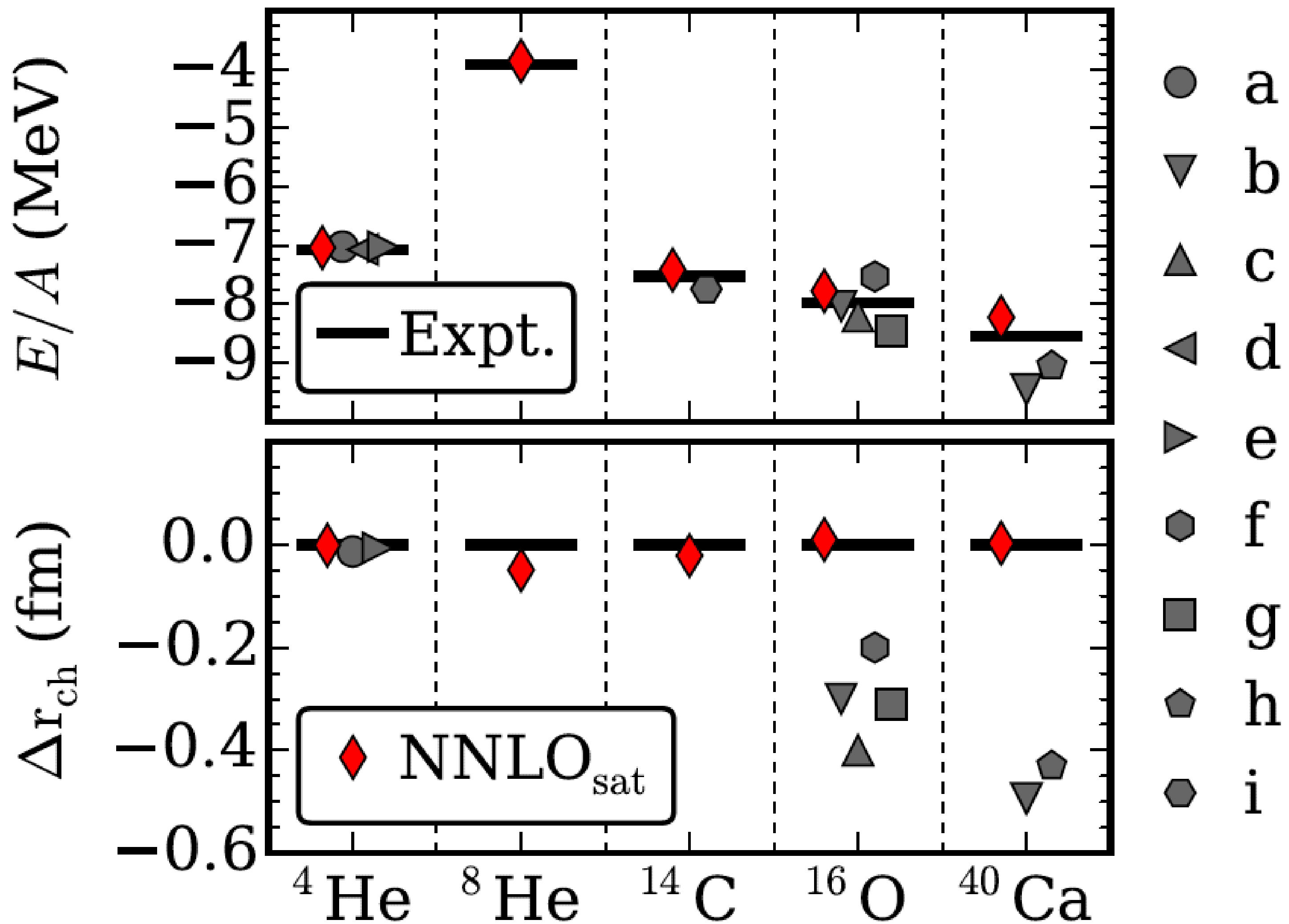
Self consistent Green's function : W. H. Dickhoff et al (2004), C. Barbieri et al (2009)....

See talk by C. Barbieri during week 4 of the workshop.

Coupled Cluster Green's function

CC talks by G. Hagen and T. Papenbrock during the week 4 of the workshop.

Coupled Cluster calculations of g.s. energies and charge radii



A. Ekström et al, PRC (R) 91 (2015)

Coupled cluster (i)

Exponential ansatz for the many-body wave function :

$$\boxed{|\Psi\rangle = e^{T}|\Phi\rangle}$$

G. Hagen, T. Papenbrock, M. Hjorth-Jensen, D. J. Dean, Rep. Prog. Phys.(2014)

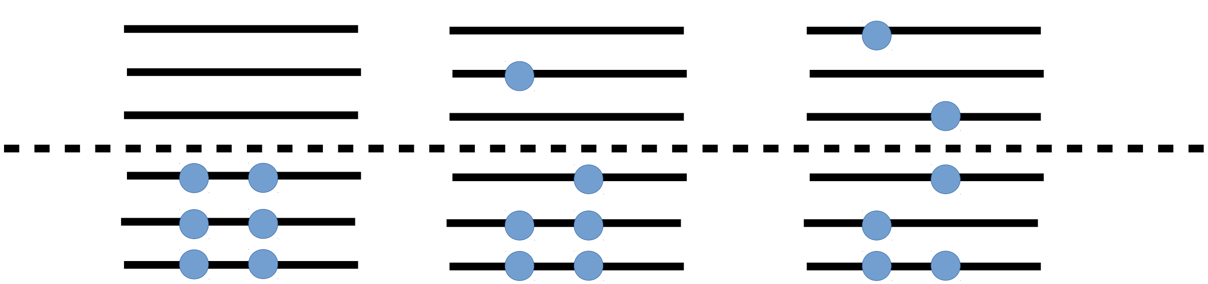
Similarity-transformed Hamiltonian

$$\boxed{\bar{H} \quad = \quad e^{-T} H e^{T}}$$

1p-1h operator

$$T = T_1 + T_2 + \ldots$$

2p-2h operator



$|\Phi\rangle$ 1p-1h 2p-2h

Coupled-cluster equations

$$\boxed{\begin{aligned} E &= \langle \Phi | \bar{H} | \Phi \rangle \\ 0 &= \langle \Phi_i^a | \bar{H} | \Phi \rangle \\ 0 &= \langle \Phi_{ij}^{ab} | \bar{H} | \Phi \rangle \\ & \ldots \end{aligned}}$$

Coupled Cluster Green's function

$$
\begin{aligned}
G(\alpha,\beta;E) &= \langle\Phi_L|\bar{a}_\alpha \frac{1}{E-[\bar{H}-E_0^A]+i\eta}\bar{a}_\beta^\dagger|\Phi\rangle \\
&+ \langle\Phi_L|\bar{a}_\beta^\dagger \frac{1}{E-[E_0^A-\bar{H}]-i\eta}\bar{a}_\alpha|\Phi\rangle
\end{aligned}
$$

solution of the Coupled Cluster equations

→The first step is the resolution of CC equations to get the cluster operator $T=T_1+T_2+\ldots$.

→Similarity-transformed operators

$$
\boxed{
\begin{aligned}
\bar{a}^\dagger{}_\alpha &= e^{-T}a_\alpha^\dagger e^{T} \\
\bar{a}_\alpha &= e^{-T}a_\alpha e^{T}
\end{aligned}
}
$$

→Inversion of the (similarity-transformed) Hamiltonian is avoided by using the Lanczos method....

Particle spectral function

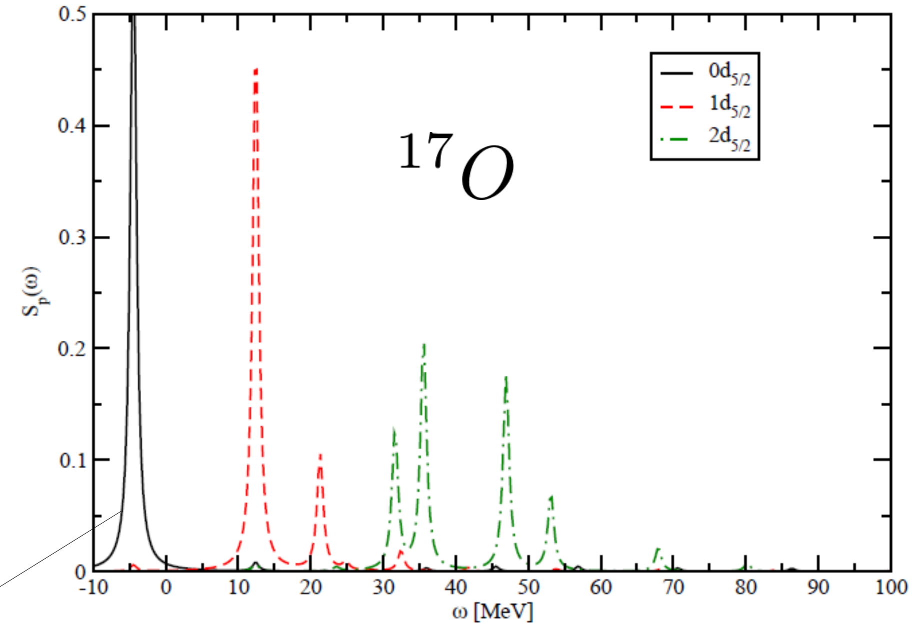
$$S_p(\alpha; E) = -\frac{1}{\pi}\mathrm{Im}\ G(\alpha, \alpha; E)$$

CC Single-Double:

-> Harmonic Oscillator basis:
N_{max} =10, hw=22 MeV.

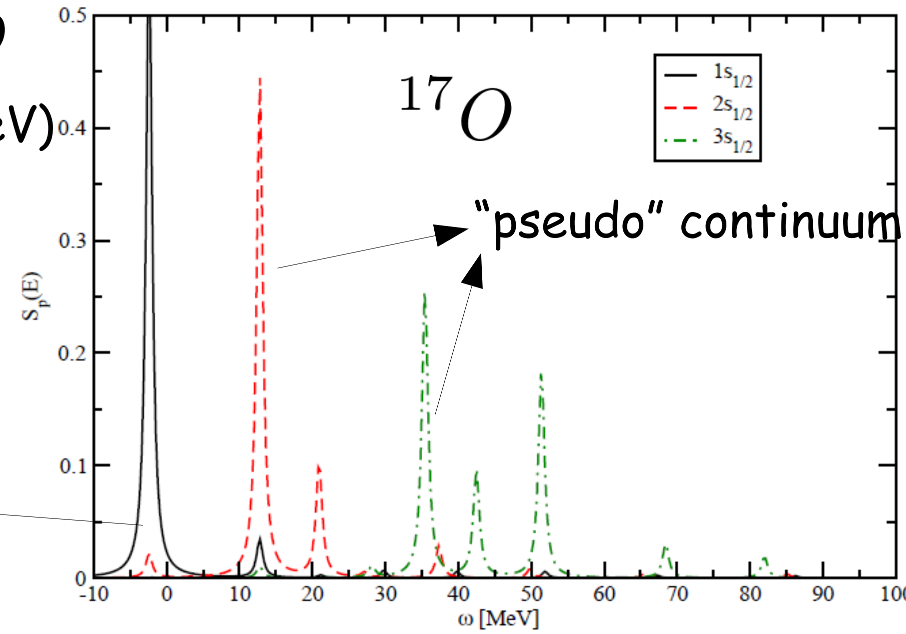
→ Interaction : N^2LO_{opt}

(A. Ekström et al [2013])



g.s. in ^{17}O

(E_{ccsd}=-4.459 MeV)



1st excited state in ^{17}O

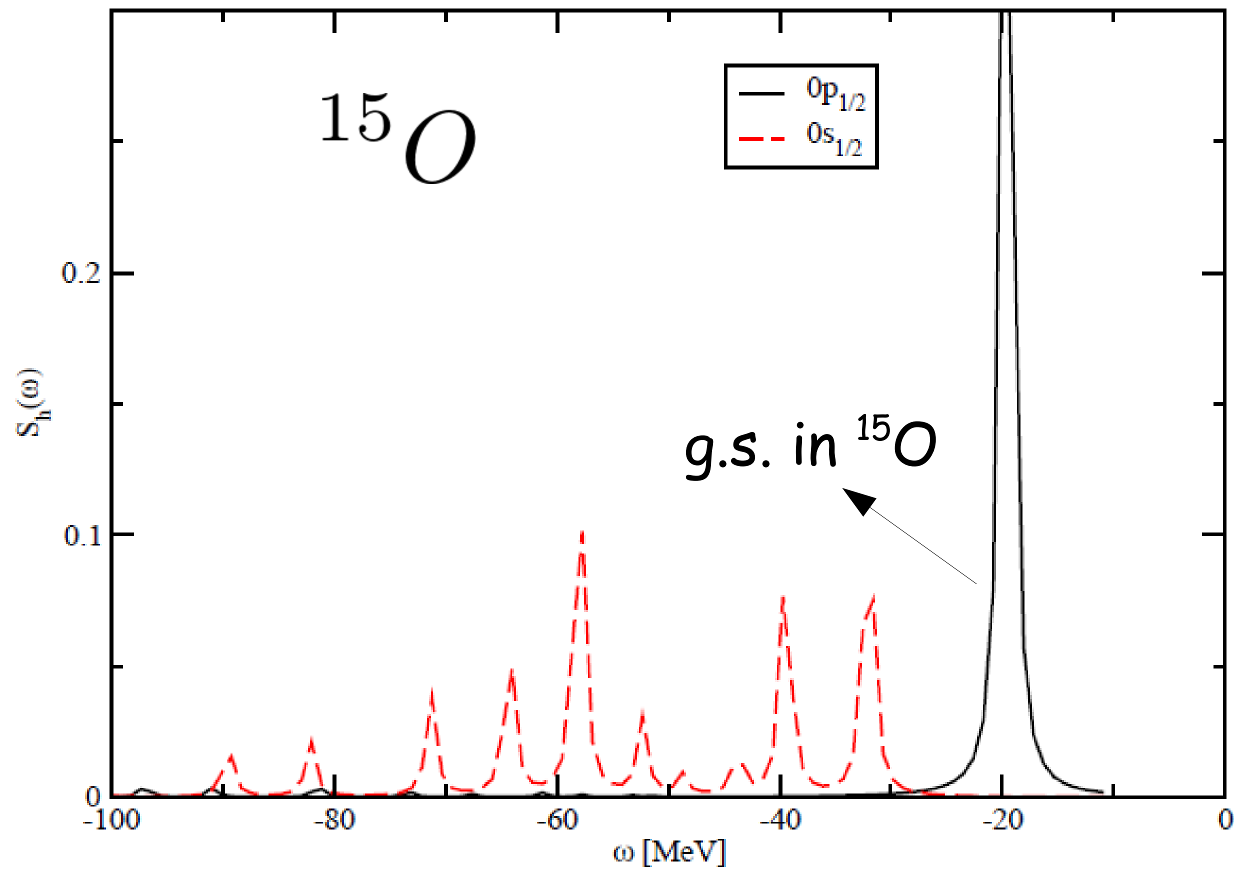
(E_{ccsd}=-2.387 MeV)

Hole spectral function

CC Single-Double:

-> Harmonic Oscillator basis: N_{max} =10, hw=22 MeV.

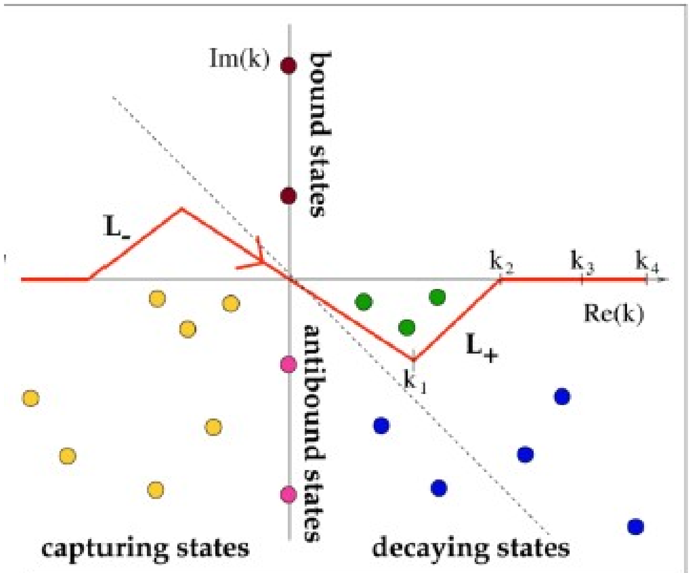
→ Interaction : N^2LO_{opt} (A. Ekström et al [2013])

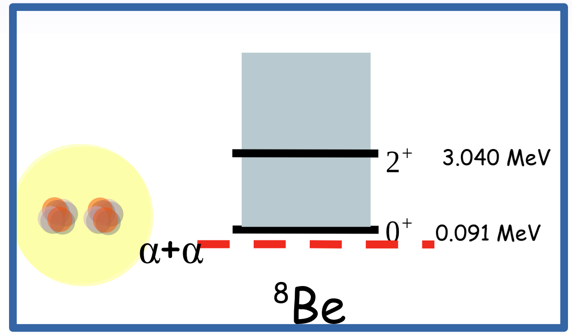


$$\boxed{S_h(\alpha;E) = \sum_m |\langle \Psi_m^{A-1}|a_\alpha|\Psi_0^A\rangle|^2 \delta\left(E-(E_0^A - E_m^{A-1})\right)}$$

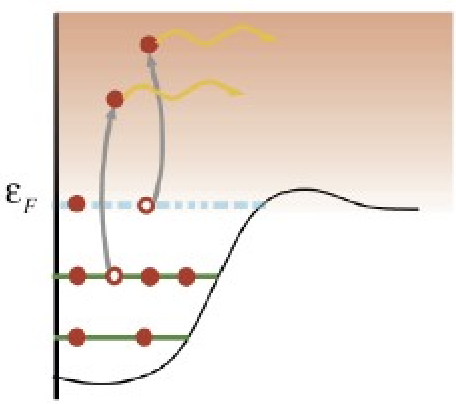
Coupled cluster with the Berggren basis

Physics of nuclei at the edges of stability

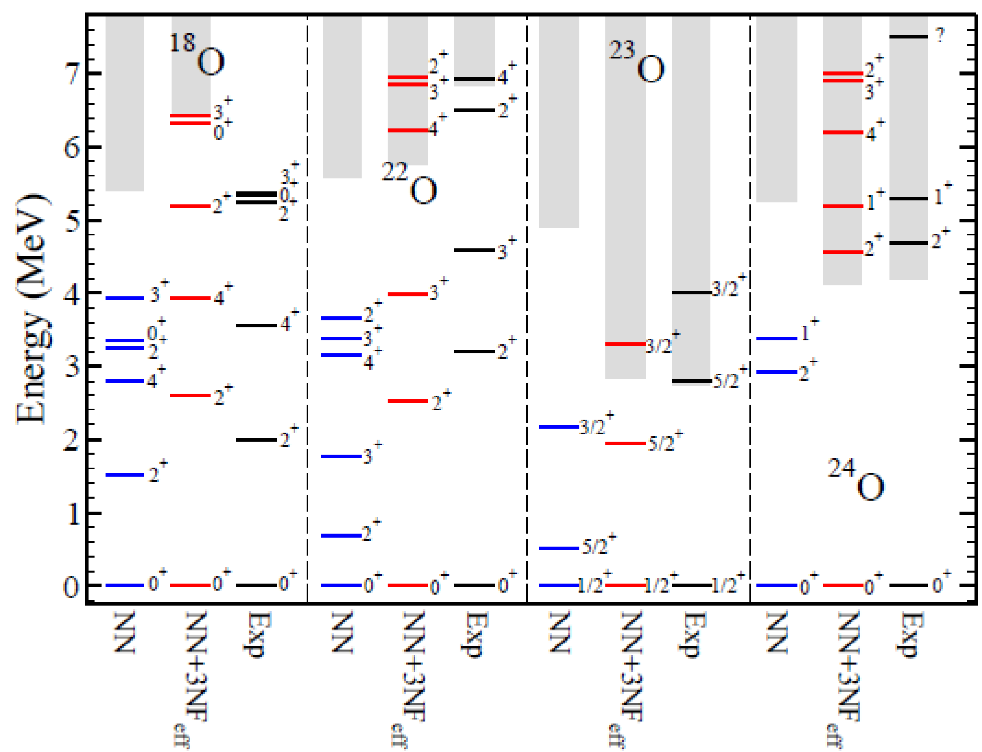




*coupling to the continuum is an essential feature of systems far from stability.
*taken into account by using the Berggren basis which includes bound, resonant and scattering states.



Hagen et al (2012)

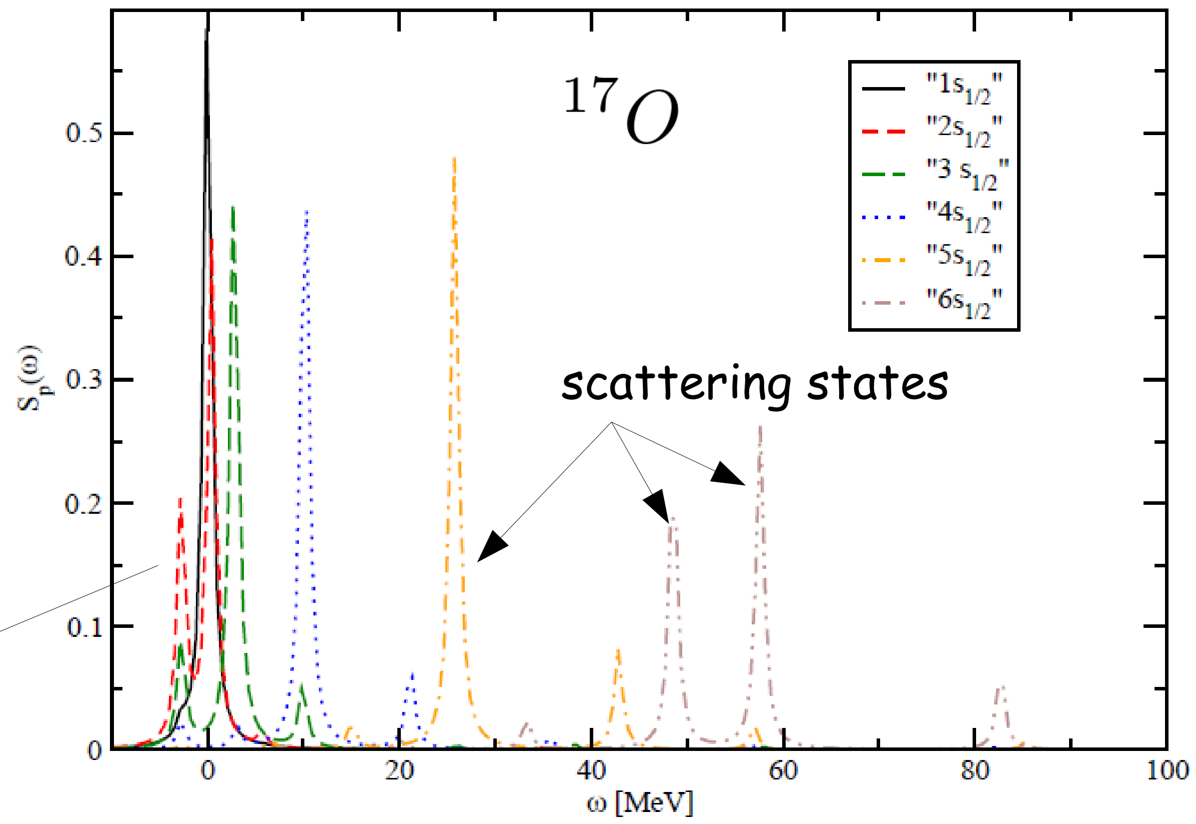


See also talks by M. Ploszajczak, Y. Jaganathen, K. Fossez, G. Papadimitriou.

Particle spectral function with the Berggren basis

CC Single-Double:

Harmonic Oscillator shells
+ s-wave real (discretized)
neutron continuum



first excited
state in ^{17}O
(E_{ccsd}=-2.731 MeV)

Towards Optical Potentials from Coupled Cluster Calculations

Combining the Many-body Green's function
and the Coupled-Cluster method.

Ab-initio approach with n-n,
3n forces and coupling to the
continuum

Microscopic construction of optical potentials