Microscopic Optical Potentials from Coupled Cluster Calculations

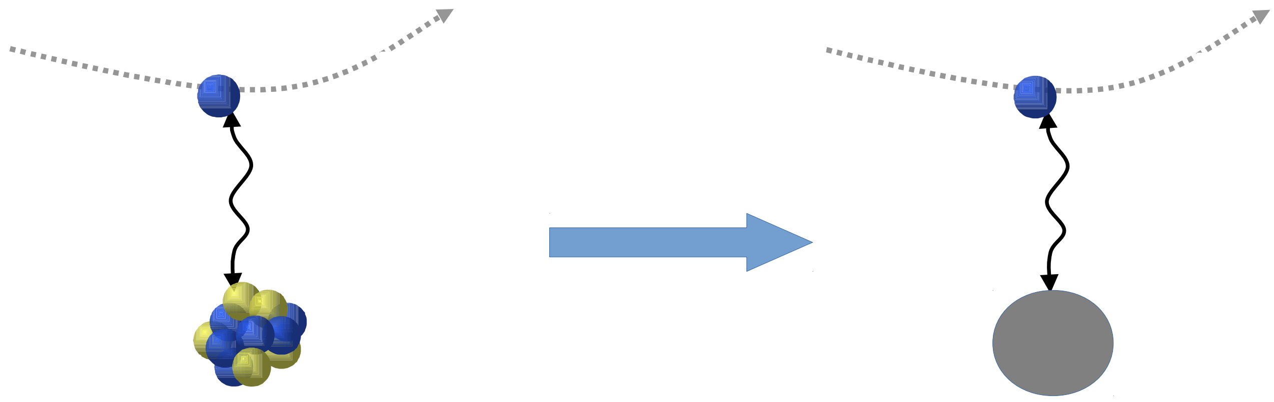
J. Rotureau

In collaboration with:
P. Danielewicz
G. Hagen
F. Nunes
T. Papenbrock

"Future directions for nuclear structure and reaction theories: *Ab initio* approaches for 2020", Fustipen meeting, March 14-18 2016.

Goals

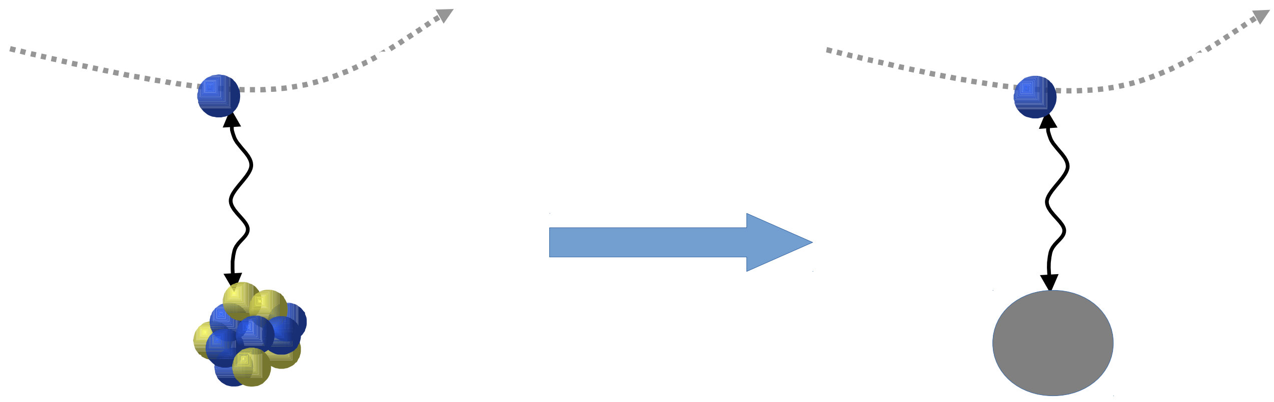
* microscopic construction of optical potentials : nucleons as degrees of freedom, modern realistic n-n, 3n forces...



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

Goals

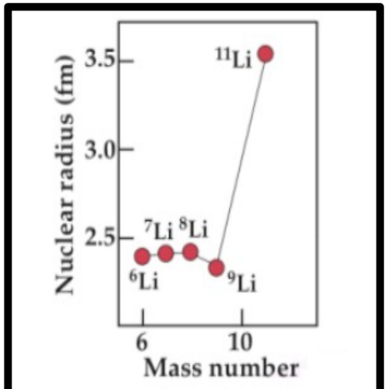
* microscopic construction of optical potentials : nucleons as degrees of freedom, modern realistic n-n, 3n forces...



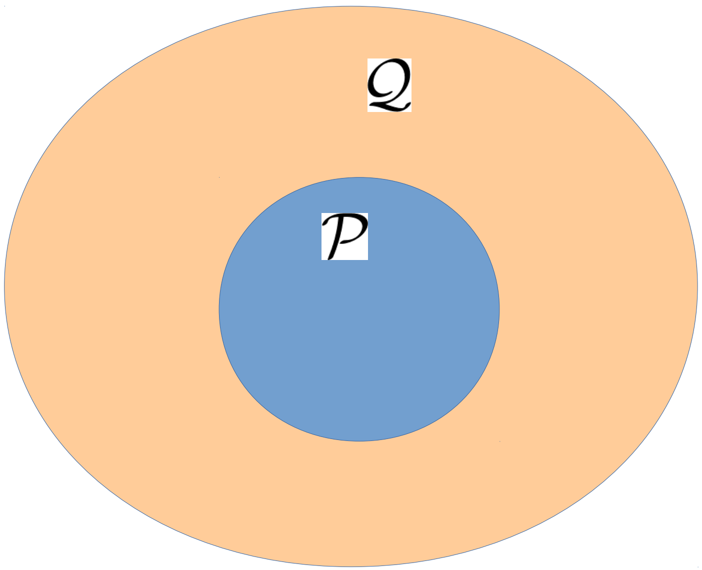
$$H|\Psi(1,\ldots,A)\rangle = E|\Psi(1,\ldots,A)\rangle \qquad H^{eff}|\Psi'(\vec{r})\rangle = E|\Psi'(\vec{r})\rangle$$

* predictive theory for nuclear reactions

* reliable/accurate extrapolations for systems far from stability.



Feshbach projection technique



$$\begin{cases} |\Psi\rangle = |\Psi_P\rangle + |\Psi_Q\rangle \\ H = H_{PP} + H_{PQ} + H_{QP} + H_{QQ} \end{cases}$$

$$(E - H_{PP})|\Psi_P\rangle = H_{PQ}|\Psi_Q\rangle$$

$$(E - H_{QQ})|\Psi_Q\rangle = H_{QP}|\Psi_P\rangle$$

$$\left[E - H_{PP} - H_{PQ}\frac{1}{E - H_{QQ}}H_{QP}\right]|\Psi_P\rangle = 0$$

Effective (optical) potential:
→ energy-dependent, non local
→ complex (open quantum system)

ContinuumShell Model/Shell Model Embedded in the continuum:

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

Phenomenological Optical Potential

$$\mathcal{U}(r,E) = -\mathcal{V}_V(r,E) - i\mathcal{W}_V(r,E) - i\mathcal{W}_D(r,E) + \mathcal{V}_{SO}(r,E).\mathbf{l}.\sigma + i\mathcal{W}_{SO}(r,E).\mathbf{l}.\sigma + \mathcal{V}_C(r),$$

$$\left\{\begin{aligned}
\mathcal{V}_V(r,E) &= V_V(E)f(r,R_V,a_V),\\
\mathcal{W}_V(r,E) &= W_V(E)f(r,R_V,a_V),\\
\mathcal{W}_D(r,E) &= -4a_D W_D(E)\frac{d}{dr}f(r,R_D,a_D),\\
\mathcal{V}_{SO}(r,E) &= V_{SO}(E)\left(\frac{\hbar}{m_\pi c}\right)^2\frac{1}{r}\frac{d}{dr}f(r,R_{SO},a_{SO}),\\
\mathcal{W}_{SO}(r,E) &= W_{SO}(E)\left(\frac{\hbar}{m_\pi c}\right)^2\frac{1}{r}\frac{d}{dr}f(r,R_{SO},a_{SO}).
\end{aligned}\right\}$$

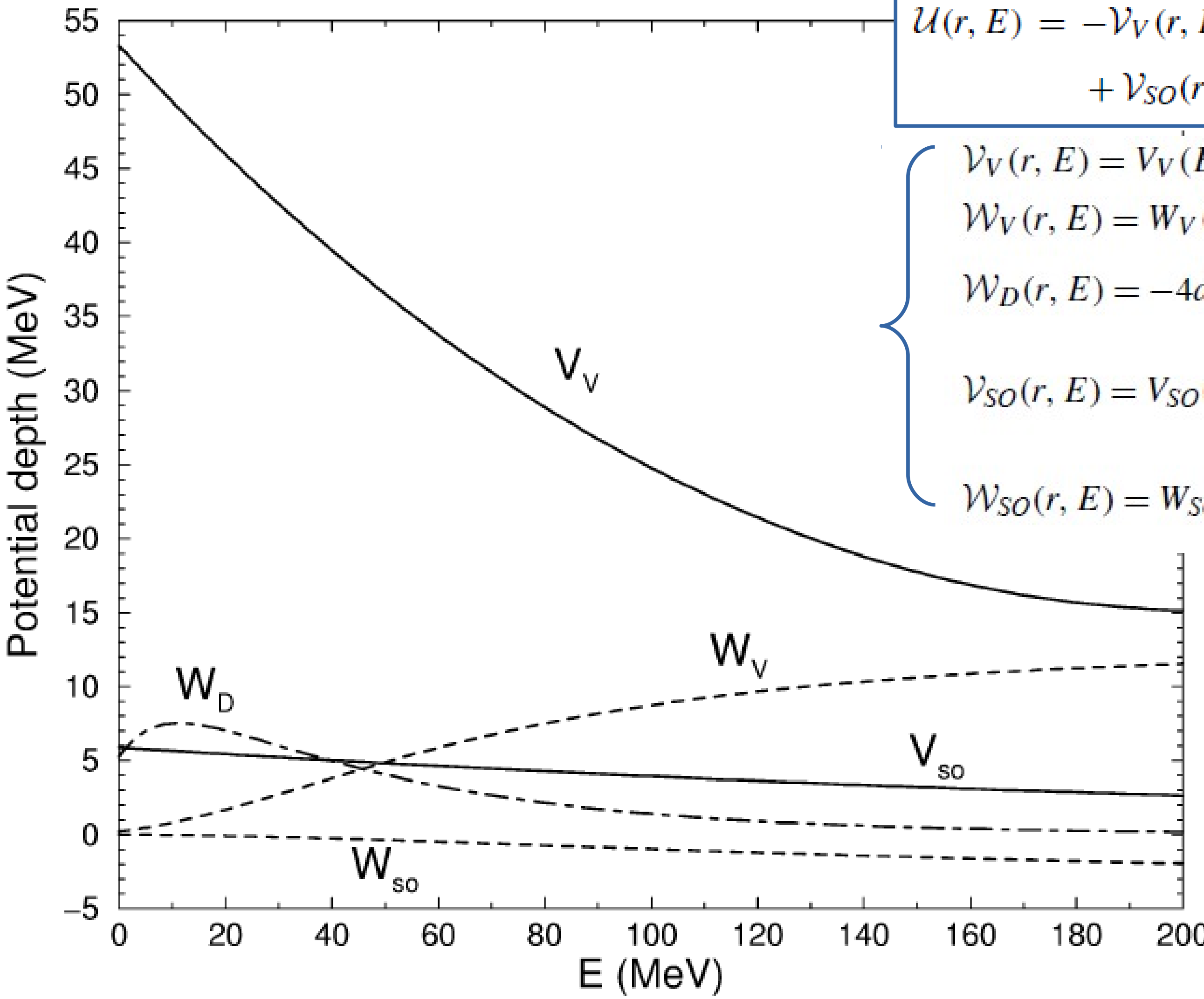


Fig. 1. The various potential well depths as a function of incident (laboratory) energy, see Eq. (7). As an example, the values for neutrons incident on ^{56}Fe are plotted.

A.J Koning, J. P. Delaroche, NPA 713 (2003)

Single-particle Green's function

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

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:

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

$$\eta \to 0$$

Lehman representation

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

Connection to experimental data:

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 :

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

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

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

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

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

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

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

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

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

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

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

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

Applications in Nuclear Physics:

W. H. Dickhoff, C. Barbieri; Prog.Part.Nucl.Phys. 52 (2004) 377-496

.....

H. Dussan, M. H. Mahzoon, R. J. Charity, W. H. Dickhoff, A. Polls, Phys. Rev. C90, 061603(R) (2014).

Our approach: calculation of the Green's function with the Coupled Cluster method.

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

Previous applications in Quantum Chemistry:

M. Nooijen, J. G. Snijders; J. Quantum Chem. 44 (1992) 55,...,
Kowalski K, K Bhaskaran-Nair, and WA Shelton; J. Chem. Phys. 141 (2014) 094102.

Coupled cluster

Exponential ansatz for the many-body wave function :

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

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

1p-1h operator

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

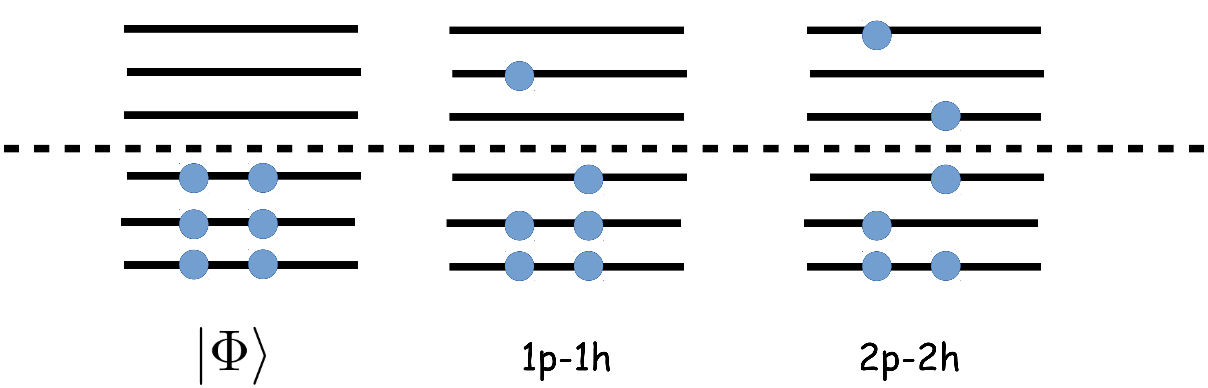
2p-2h operator

Similarity-transformed Hamiltonian

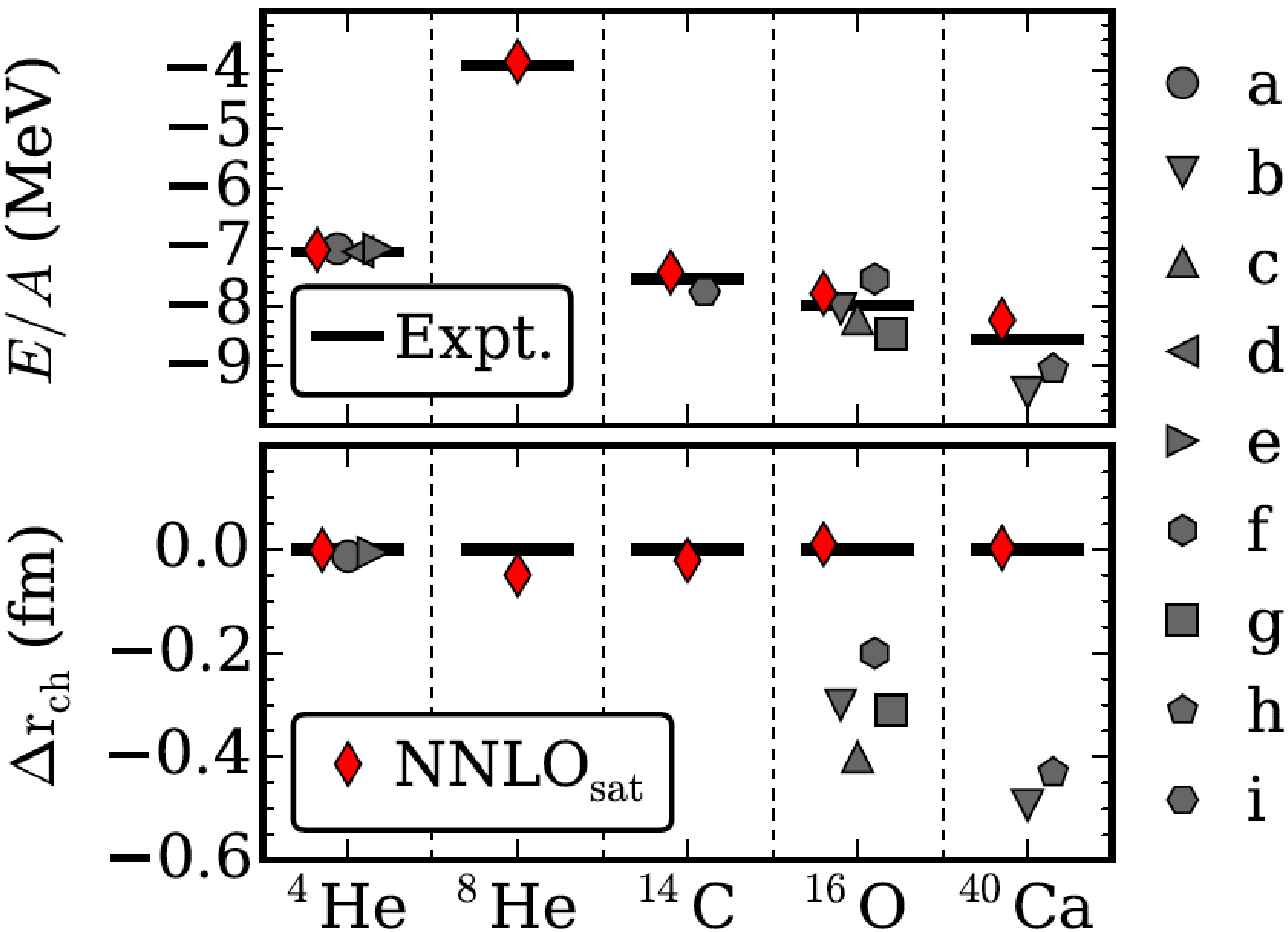
$$\bar{H} \quad = \quad e^{-T} H e^{T}$$

Coupled-cluster equations

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



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



A. Ekström et al, PRC (R) 91 (2015)

Coupled Cluster Green's function

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

→ similarity-transformed operators :

$$\overline{a^\dagger}_\alpha = e^{-T}a_\alpha^\dagger e^T$$
$$\bar{a}_\alpha = e^{-T}a_\alpha e^T$$

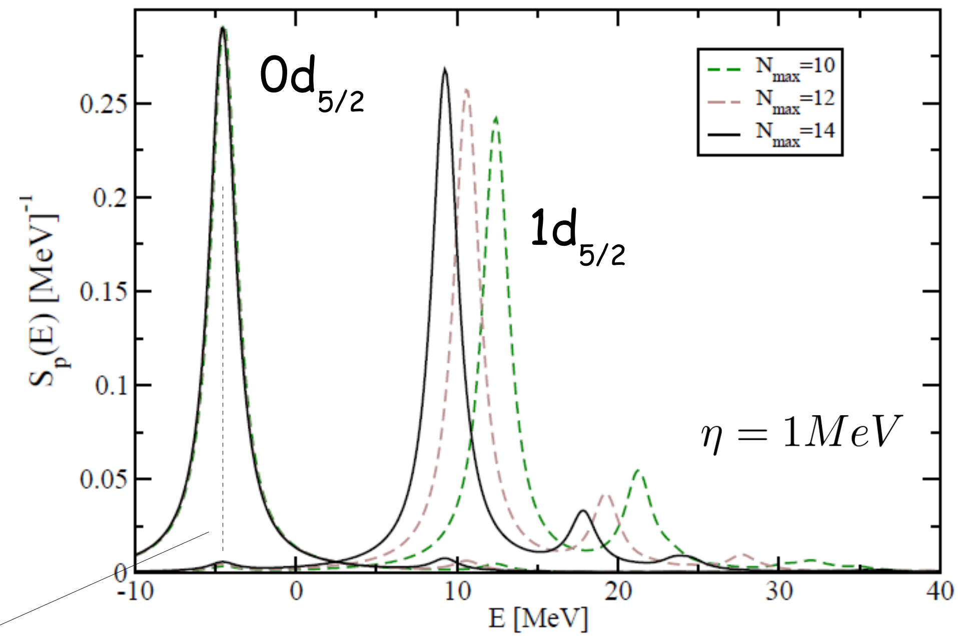
→ Inversion of the (similarity-transformed) Hamiltonian in the Lanczos basis :

$$\{\langle\Phi_L|\bar{a}_\alpha, \langle\Phi_L|\bar{a}_\alpha\bar{H}, \langle\Phi_L|\bar{a}_\alpha\bar{H}^2, \ldots, \bar{H}^2\bar{a}_\beta^\dagger|\Phi\rangle, \bar{H}\bar{a}_\beta^\dagger|\Phi\rangle, a_\beta^\dagger|\Phi\rangle\}$$

Particle spectral function in ^{17}O

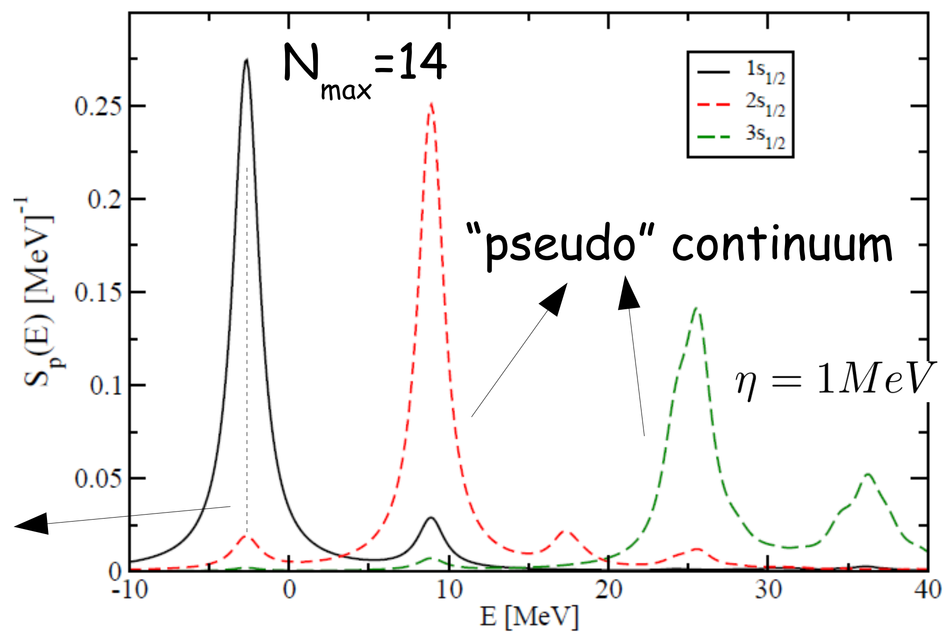
$$S_p(\alpha; E) = -\frac{1}{\pi}\text{Im } G(\alpha, \alpha; E)$$

CCSD (Single-Double):
-> H.O. basis with ħω=20 MeV.
→ Interaction : N^2LO_{opt}
(A. Ekström et al, PRL 110 [2013])



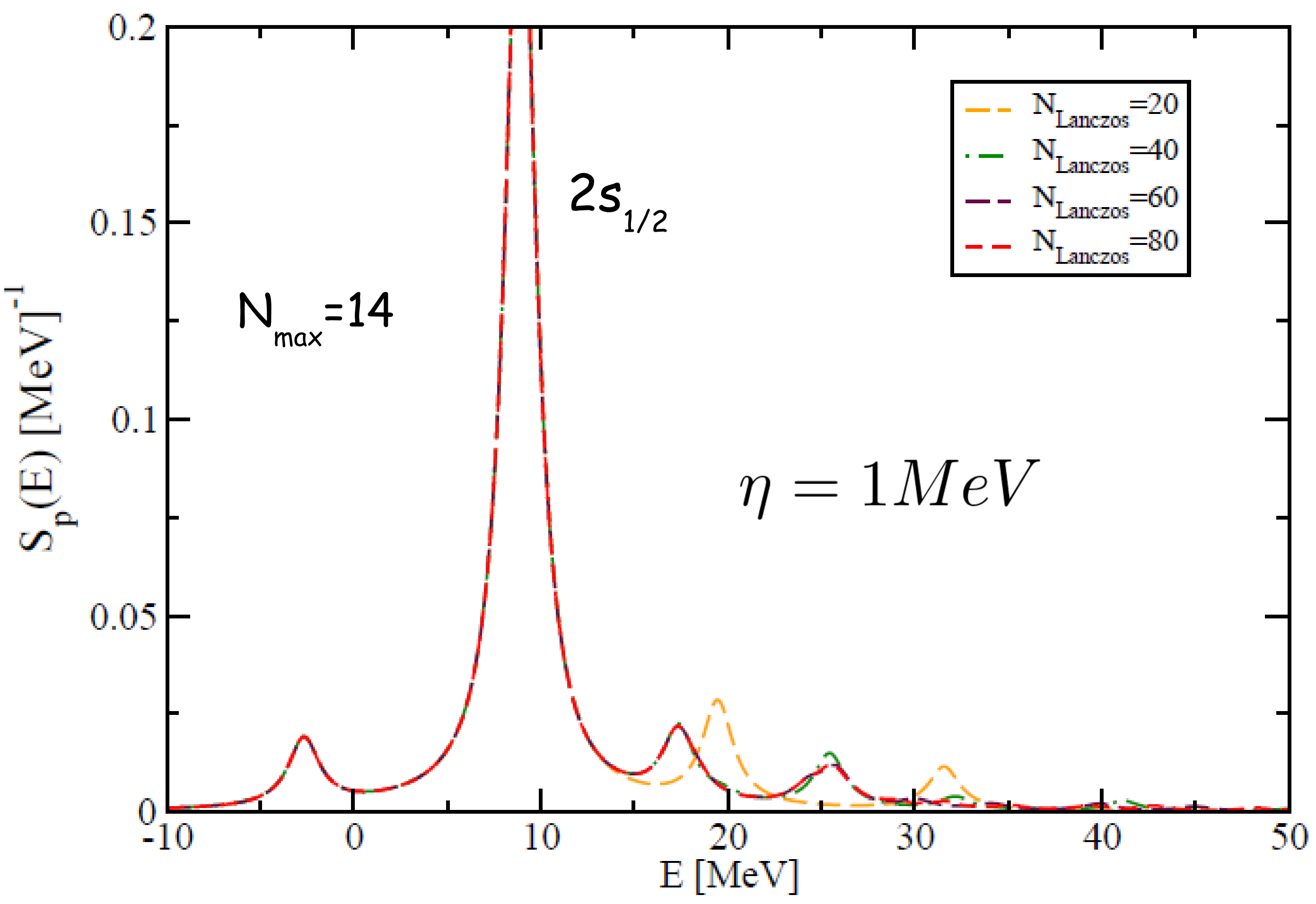
ground state
(E_{ccsd}=-4.557 MeV)

$E^{exp}(5/2^+)$ =-4.142 MeV
$E^{exp}(1/2^+)$ =-3.272 MeV



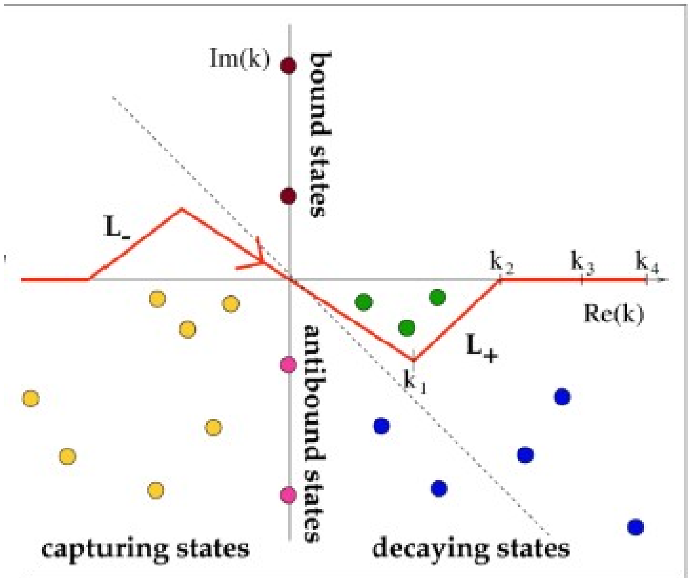
1^{st} excited state
(E_{ccsd}=-2.670 MeV)

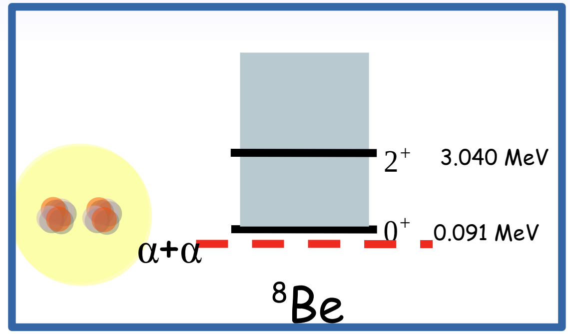
Convergence pattern with the number of Lanczos iterations

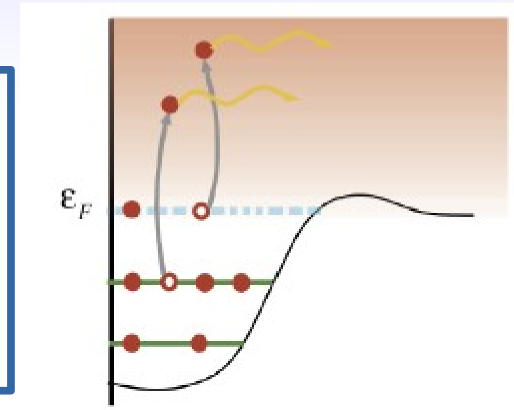


Berggren basis

Physics of nuclei at the edges of stability







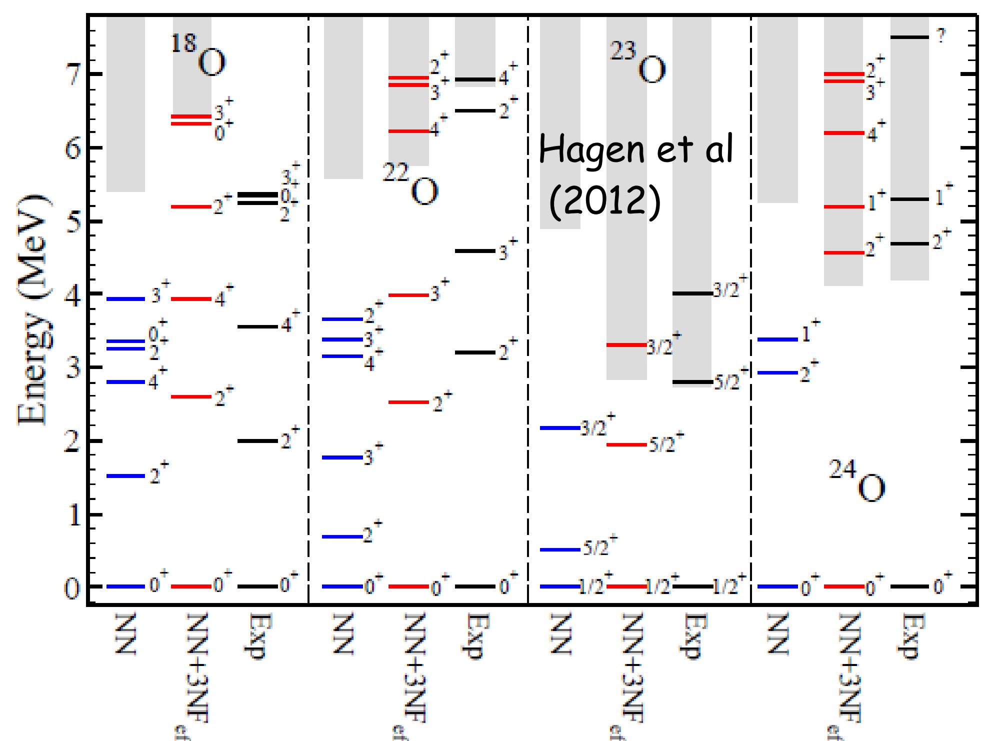
*coupling to the continuum is an essential feature of systems far from stability.
*taken into account by using the Berggren basis which includes bound, resonant and scattering states.

Gamow (complex-energy) Shell Model :

N. Michel et al, PRL (2002) ;G. Hagen et al, PRC (2005) ; J.R et al, PRL (2006) ; N. Michel et al, JPG (2009); G. Papadimitriou et al, PRC (2014); Y. Jaganathen et al, JP (2012) ; K. Fossez et al,PRA (2015).

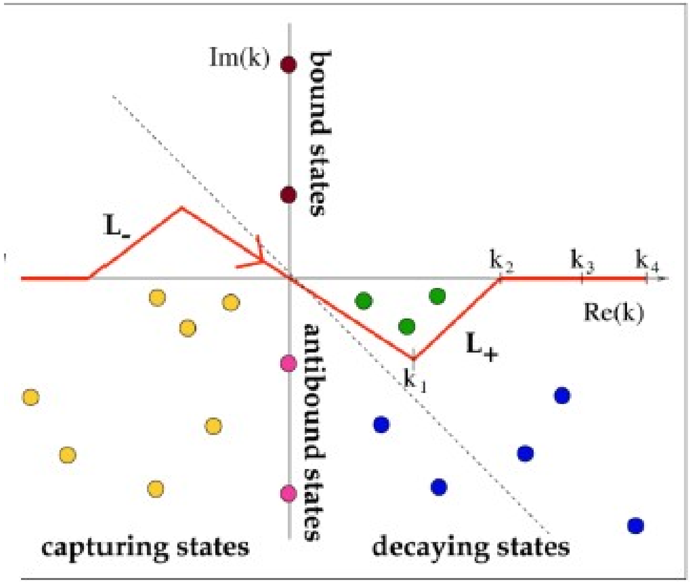
Coupled Cluster in the Gamow Basis:

G. Hagen et al;PLB (2007),PRC (2009), PRL (2010),PRL (2012), RPP (2014).



Green's function in the Berggren Basis

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



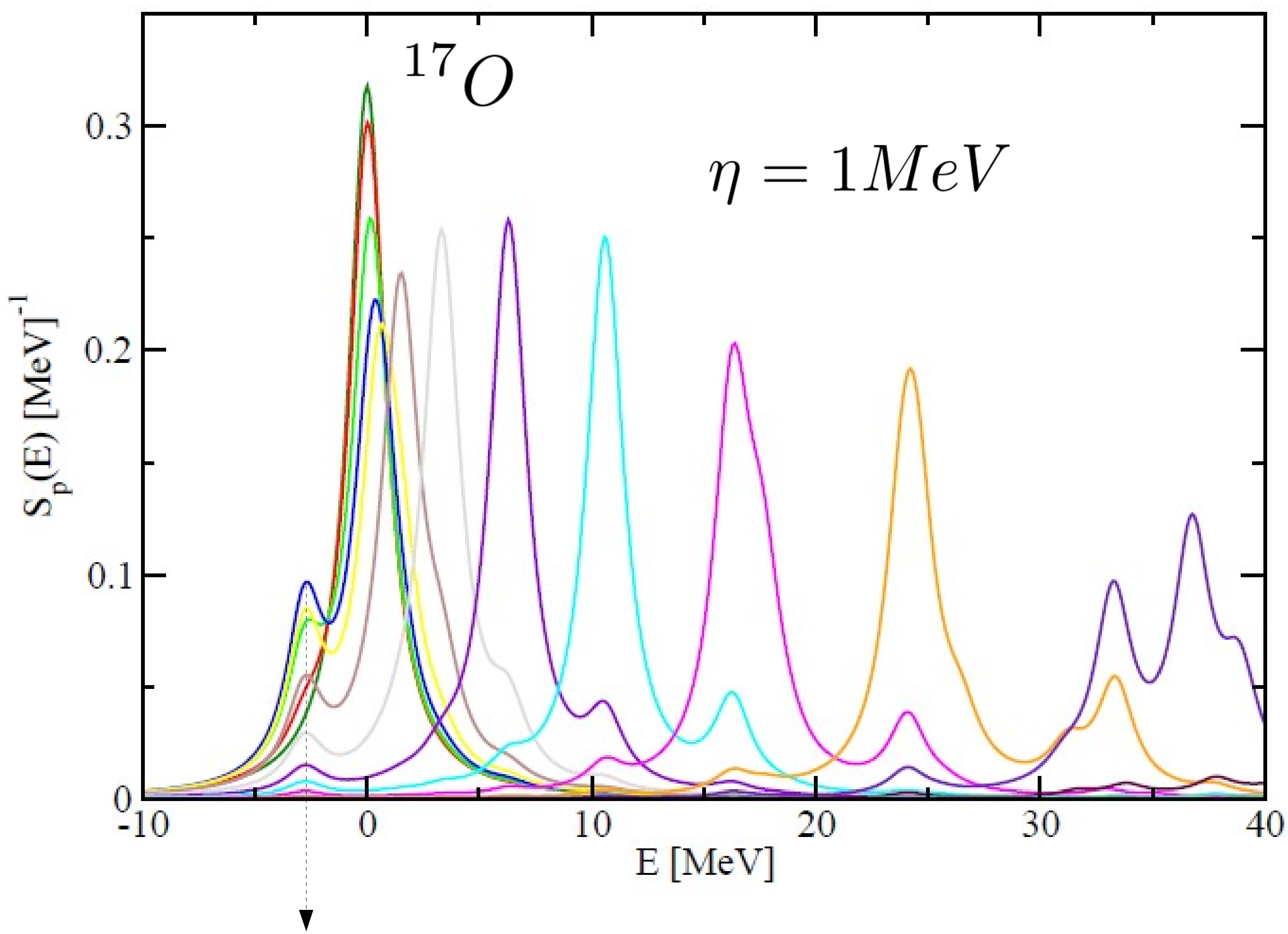
→ with the complex-continuum the (numerical) Green's function behaves smoothly as η goes to 0.

Particle spectral function in ^{17}O

CCSD:

→ H.O. Shells (N_{max} =14)
→ 40 s-wave (**real**) continuum shells

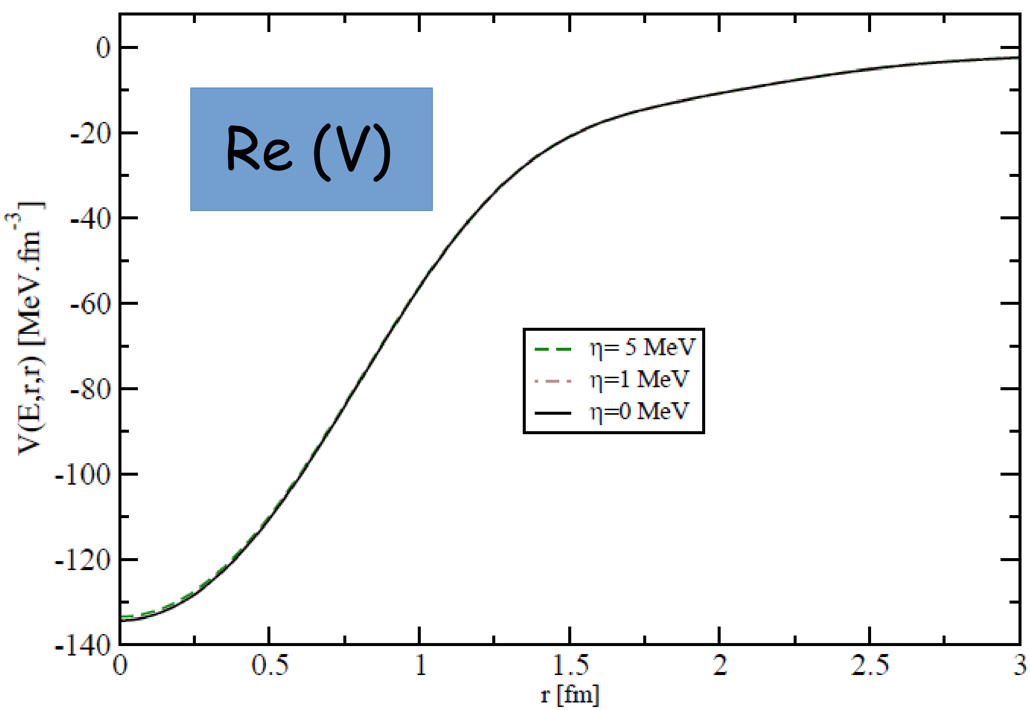
→ Interaction : N^2LO_{opt}

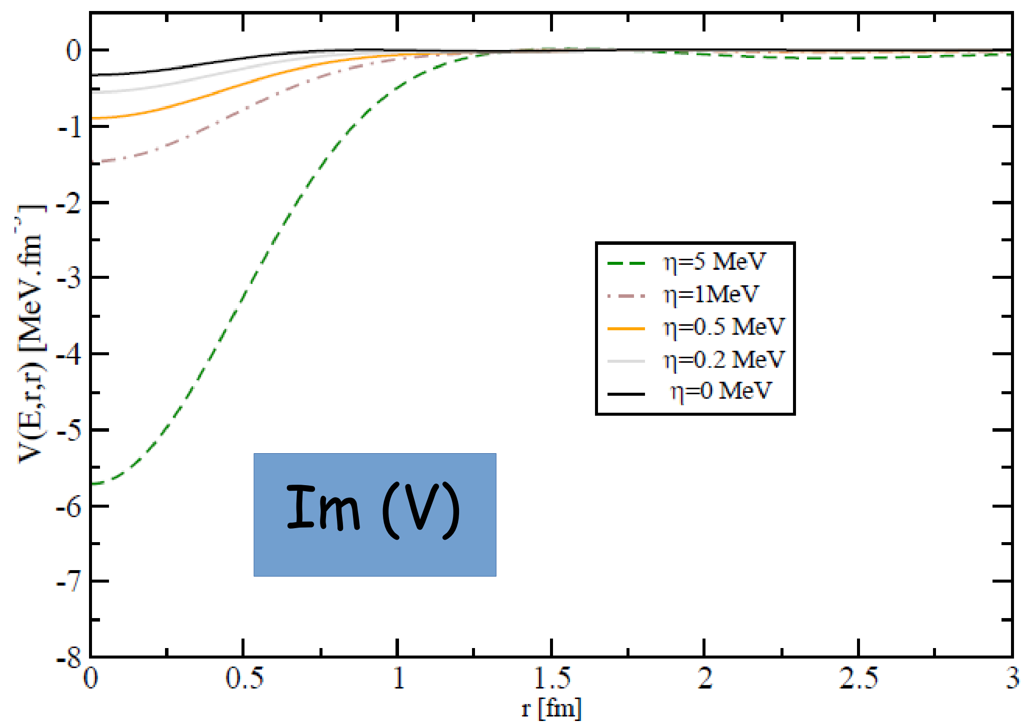


$1/2^+$ bound state in ^{17}O

(E_{ccsd}=-2.761 MeV)

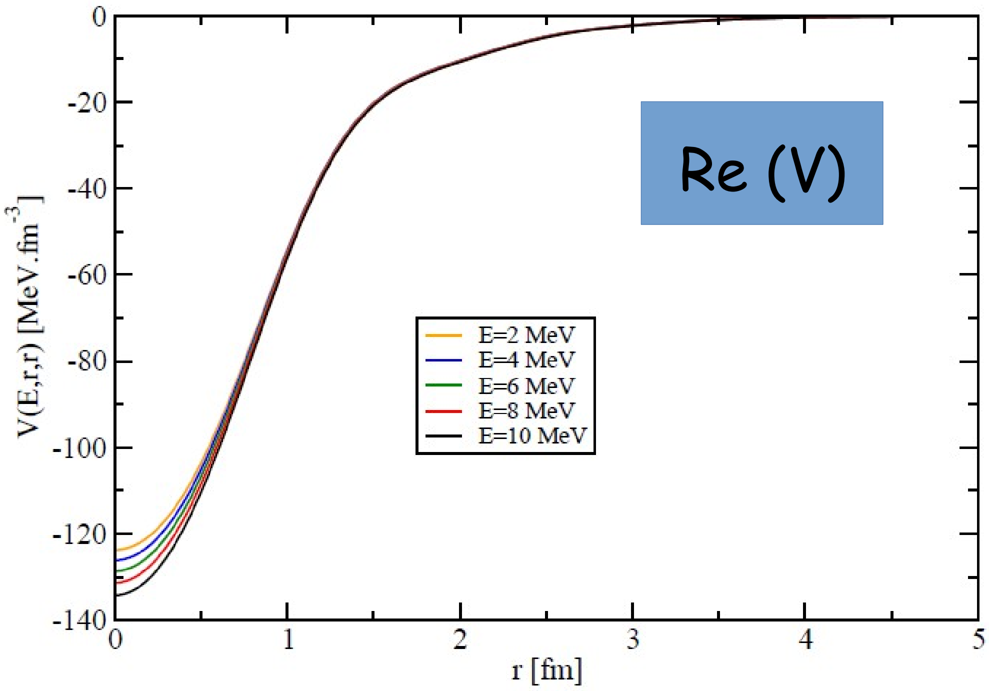
Optical Potential for S-wave neutron elastic scattering at 10 MeV

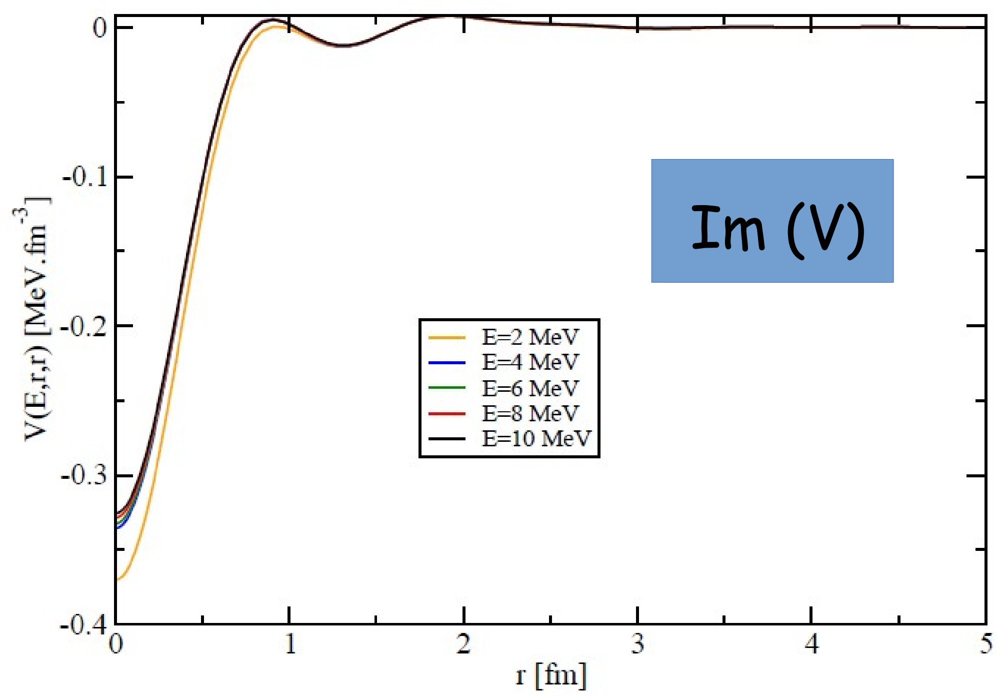




H.O. shells (N_{max} =10) +40 s-wave **complex** continuum

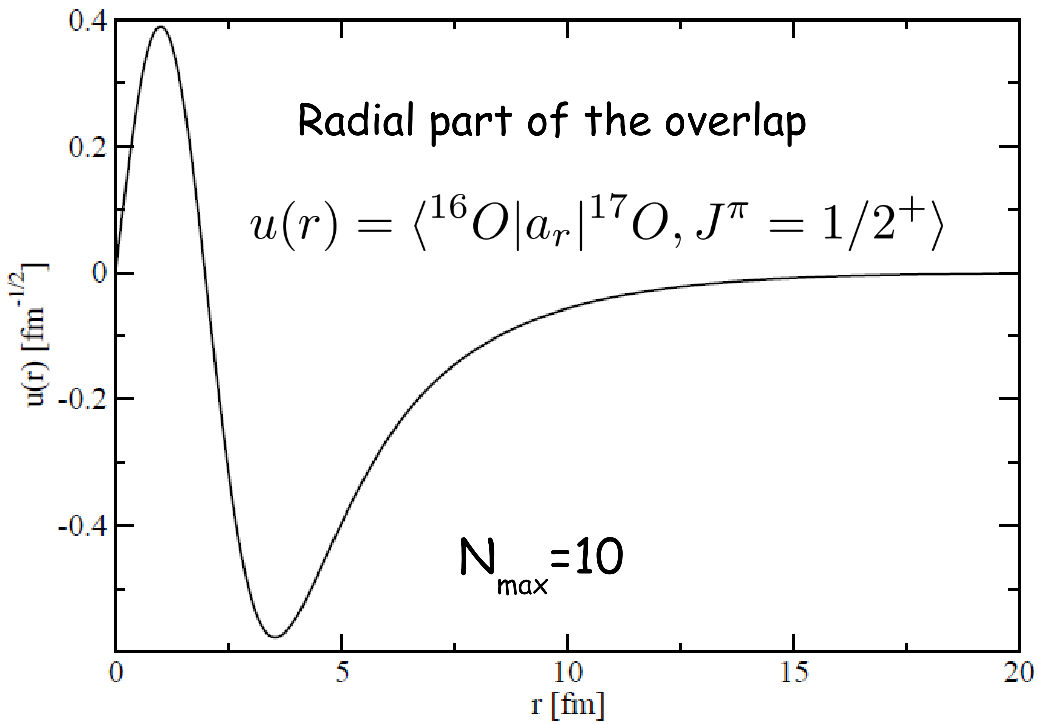
Optical Potential for S-wave neutron elastic scattering

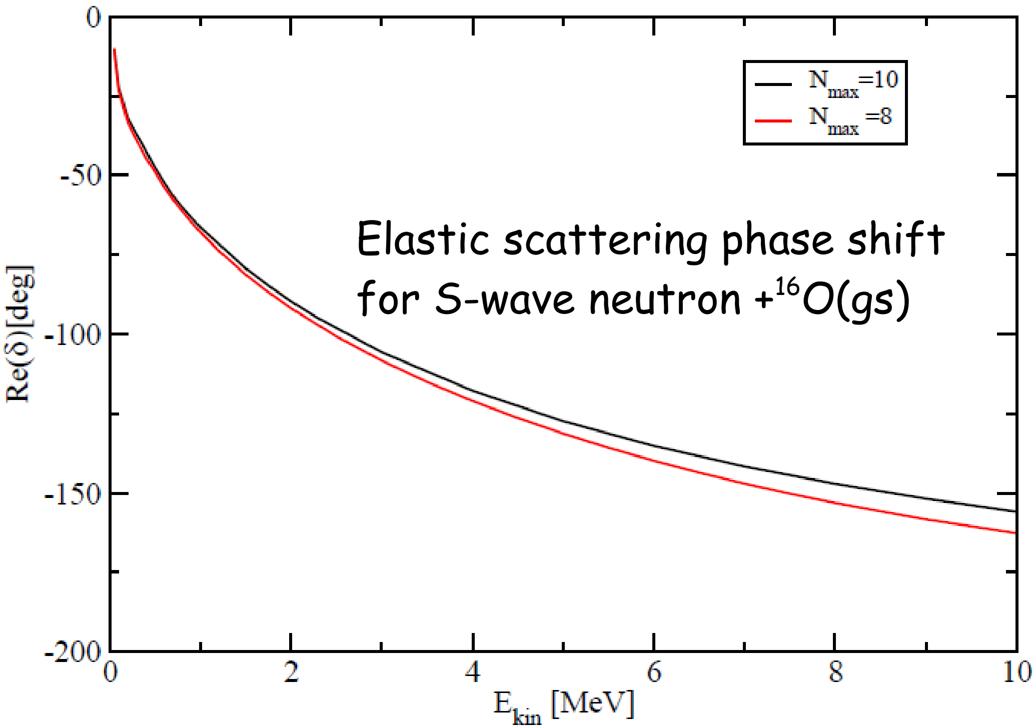




<u>H.O. shells (N_{max} =10) +40 s-wave **complex** continuum</u>

S-wave neutron

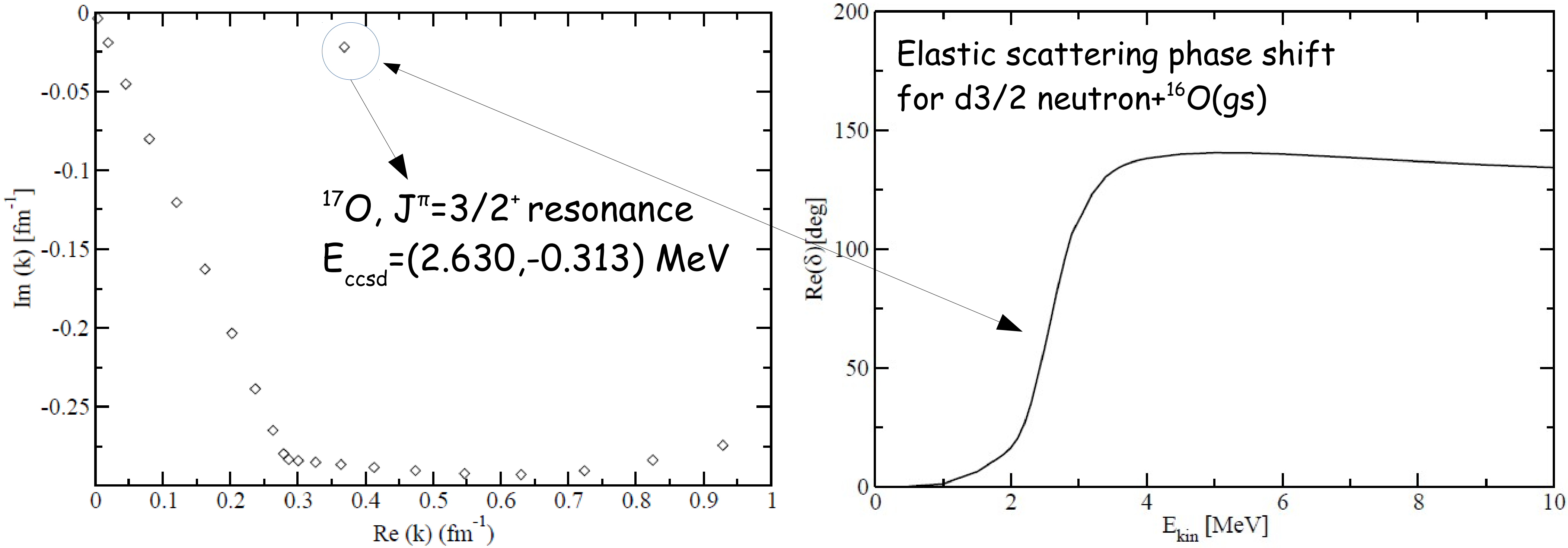




<u>H.O. shells +40 s-wave **complex** continuum shells</u>

$d_{3/2}$ neutron

CCSD spectrum in k-space for $J^{\pi}=3/2^{+}$



$E^{exp}(3/2^{+})$ =(0.943,-0.48) MeV

<u>H.O. shells (N_{max}=10) + 40 $d_{3/2}$-wave **complex** continuum</u>

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