

# Microscopic Optical Potentials from Coupled Cluster Calculations

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In collaboration with:

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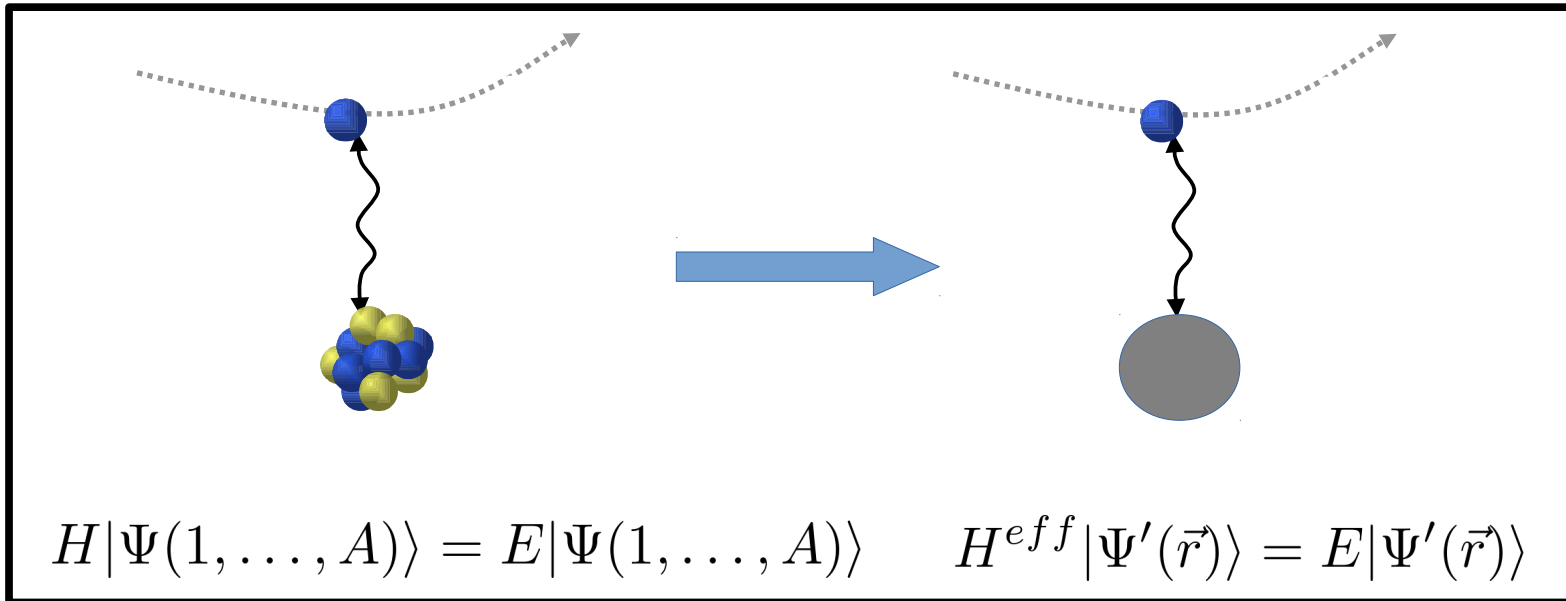
T. Papenbrock



"Towards consistent approaches for nuclear structure and reactions", ECT\*, June 2016.

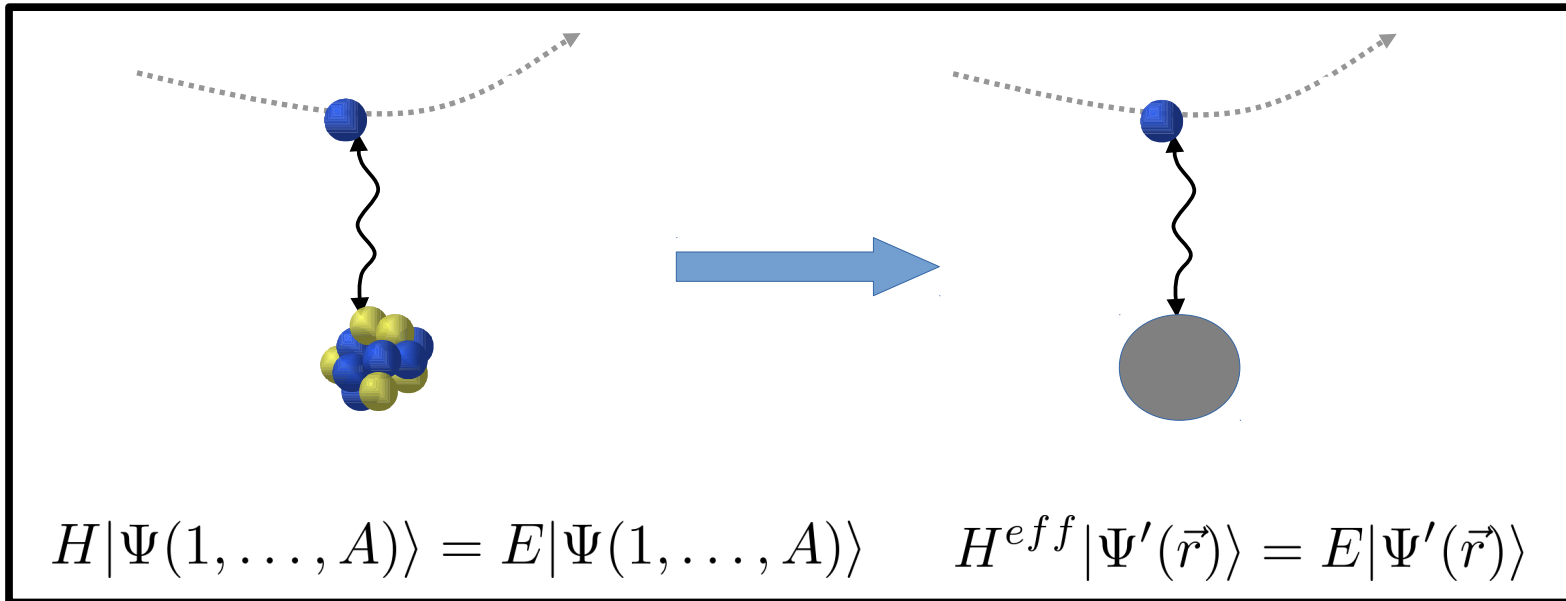
# Goals

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



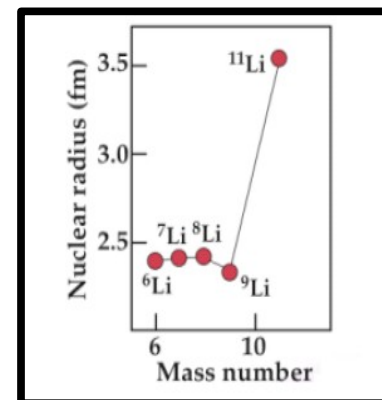
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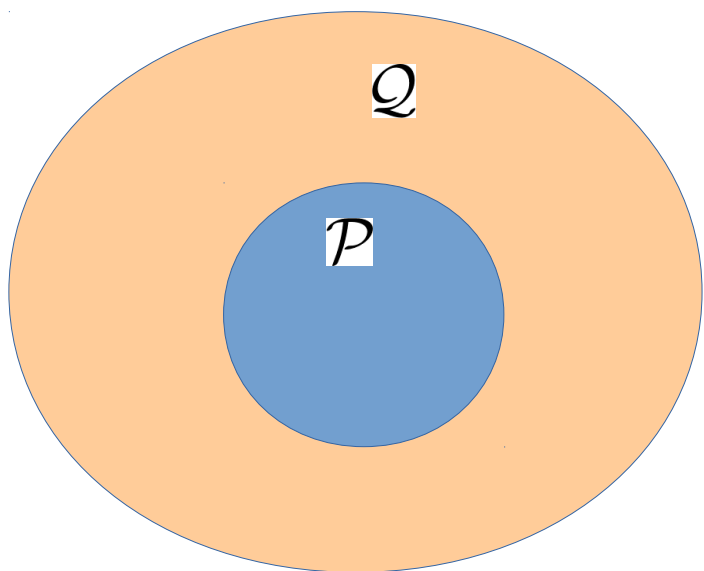


\* predictive theory for nuclear reactions

\* reliable/accurate extrapolations for systems far from stability.



# Feshbach projection technique



$$\left\{ \begin{array}{l} |\Psi\rangle = |\Psi_P\rangle + |\Psi_Q\rangle \\ H = H_{PP} + H_{PQ} + H_{QP} + H_{QQ} \end{array} \right.$$

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

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

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

Effective (optical) potential:

- energy-dependent, non local
- complex (open quantum system)

Continuum Shell 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

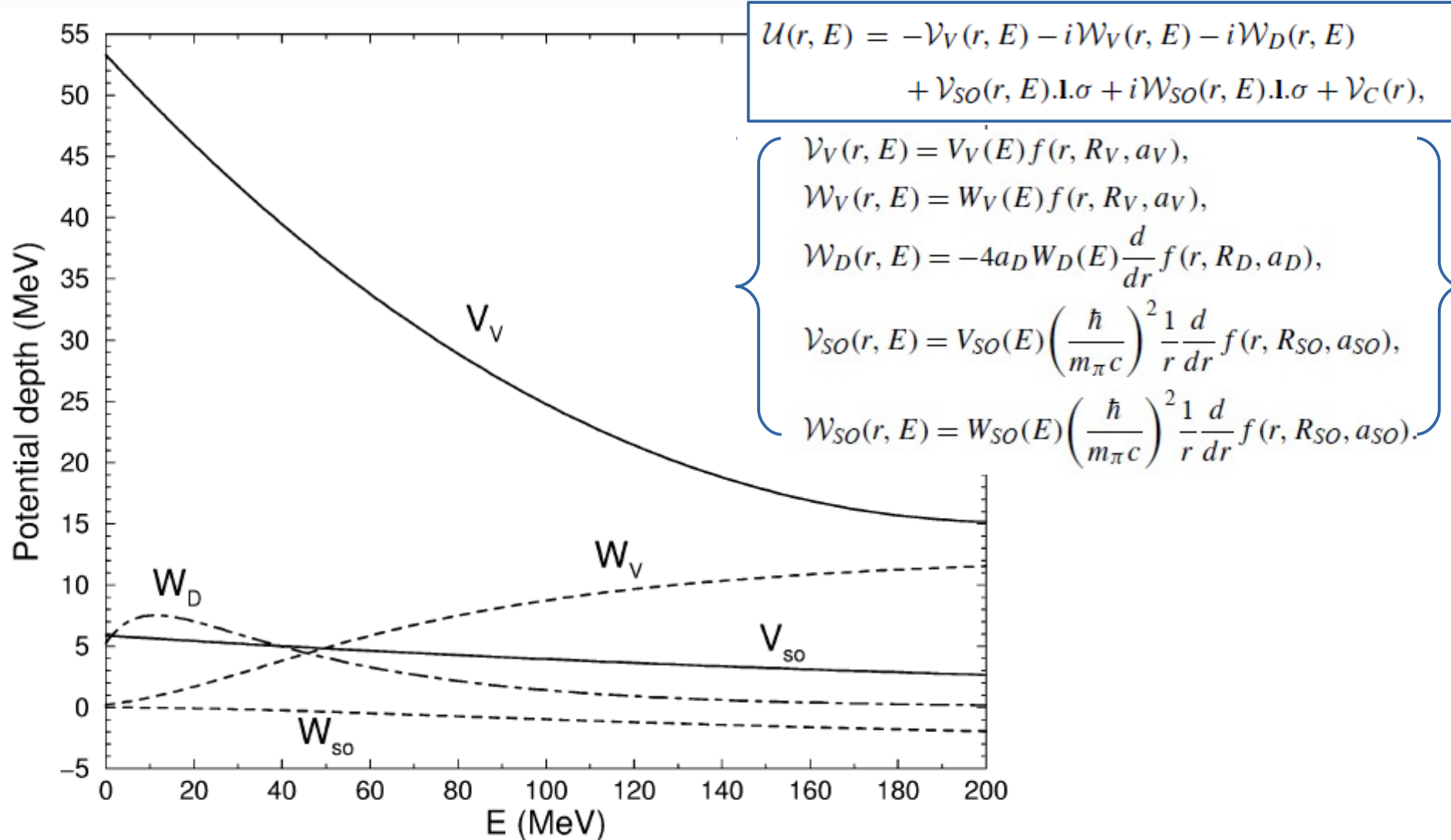


Fig. 1. The various potential well depths as a function of incident (laboratory) energy, see Eq. (7). As an example, the values for neutrons incident on  $^{56}\text{Fe}$  are plotted.

# Single-particle Green's function

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

$$\eta \rightarrow 0$$

# 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 :

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

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

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

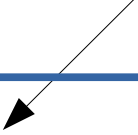
$$E \geq \epsilon_F^+ = E_0^{A+1} - E_0^A$$

“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

$$z_n^{A-1}(r) = \langle \Psi_n^{A-1} | a_r | \Psi_0^A \rangle$$

$$\xi_{E+}^c(r) = \langle \Psi_0^A | a_r | \Psi_{E+}^c \rangle$$

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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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.

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

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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)

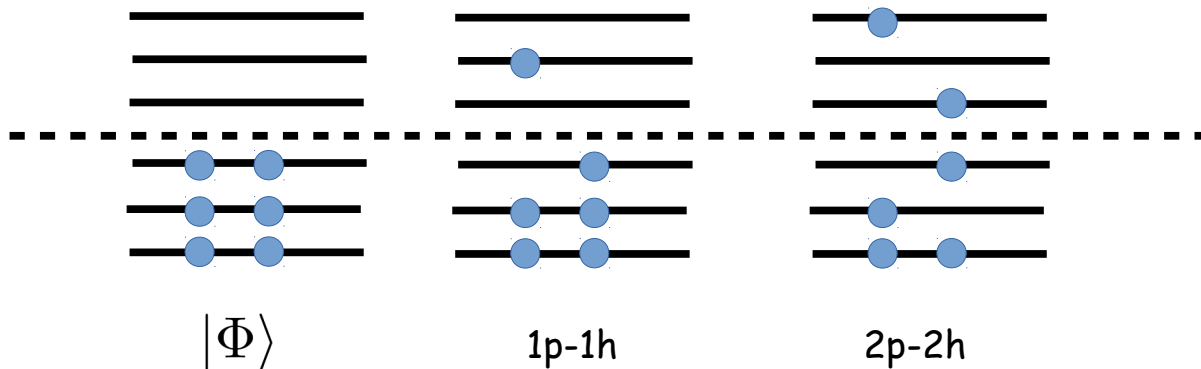
Similarity-transformed Hamiltonian

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

1p-1h operator

$$T = T_1 + T_2 + \dots$$

2p-2h operator



Coupled-cluster equations

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

# NN interaction: $N^2LO_{\text{opt}}$

PRL 110, 192502 (2013)

PHYSICAL REVIEW LETTERS

week ending  
10 MAY 2013

## Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order

A. Ekström,<sup>1,2</sup> G. Baardsen,<sup>1</sup> C. Forssén,<sup>3</sup> G. Hagen,<sup>4,5</sup> M. Hjorth-Jensen,<sup>1,2,6</sup> G. R. Jansen,<sup>4,5</sup> R. Machleidt,<sup>7</sup>  
W. Nazarewicz,<sup>5,4,8</sup> T. Papenbrock,<sup>5,4</sup> J. Sarich,<sup>9</sup> and S. M. Wild<sup>9</sup>

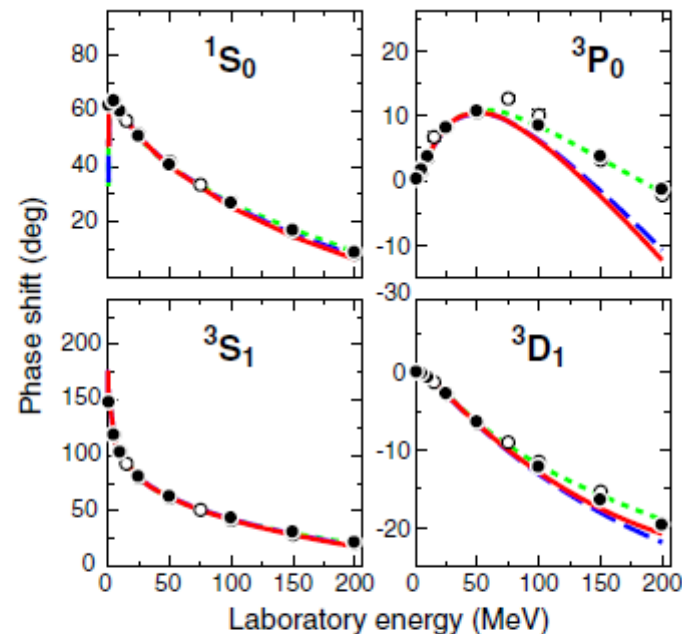
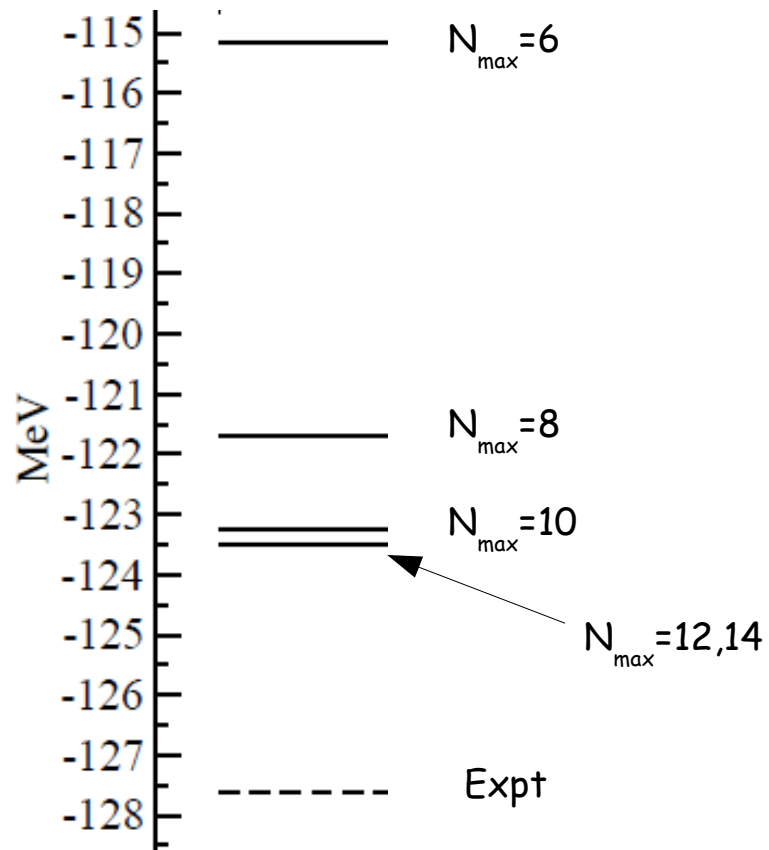


FIG. 1 (color online). Computed  $np$  phase shifts of the optimized NNLO potential of this work (solid, red line), the NNLO potential of Ref. [3] (dashed, blue line), and the N<sup>3</sup>LO potential [4] (green, dotted line) compared with the Nijmegen phase shift analysis [18] (solid dots) and the VPI/GWU analysis SM99 [43] (open circles).

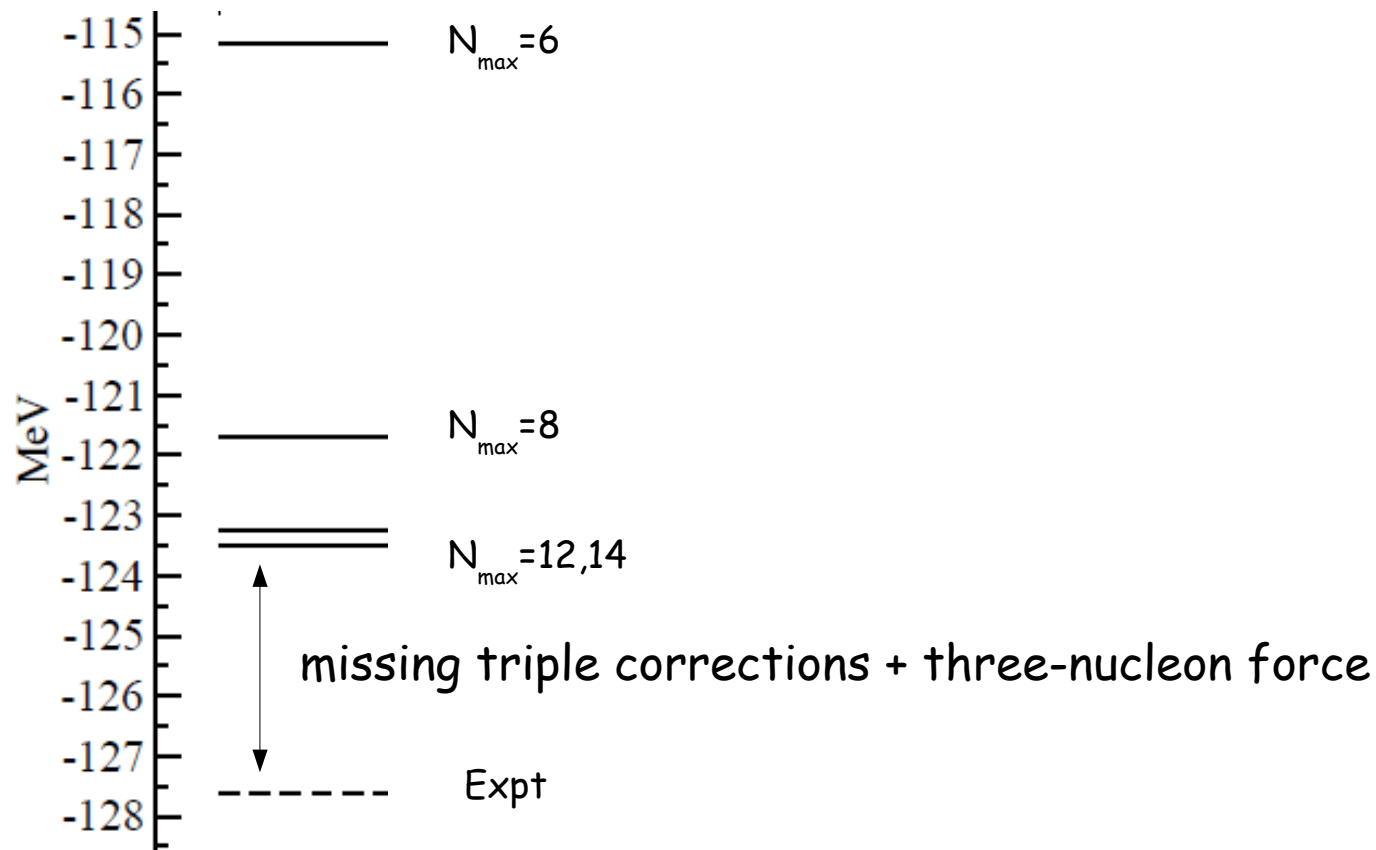
# Coupled Cluster (SD) for $^{16}\text{O}$ and $^{17}\text{O}$ with $\text{N}^2\text{LO}_{\text{opt}}$

$^{16}\text{O}$  ground state



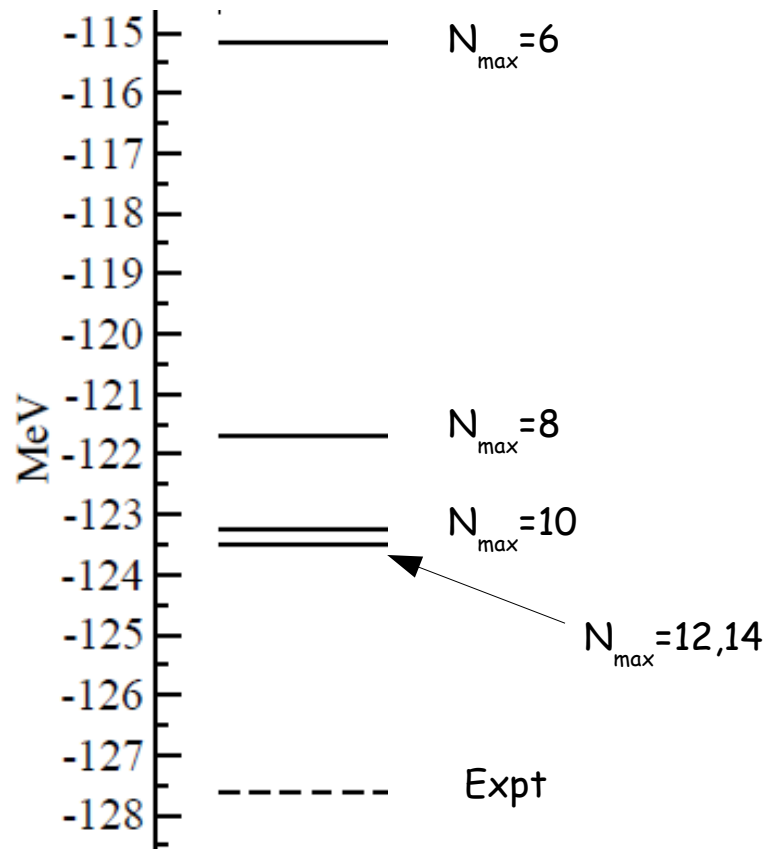
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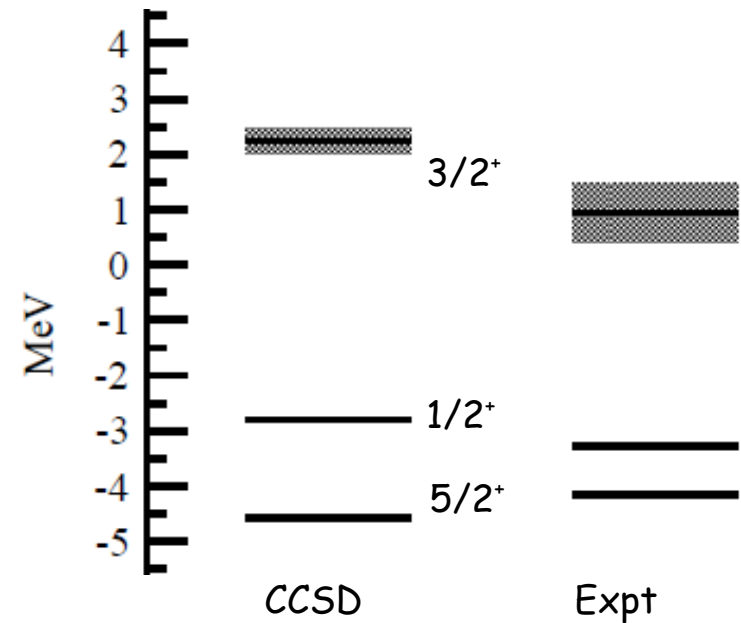


# Coupled Cluster (SD) for $^{16}\text{O}$ and $^{17}\text{O}$ with $\text{N}^2\text{LO}_{\text{opt}}$

$^{16}\text{O}$  ground state



$^{17}\text{O}$





# 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 :

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

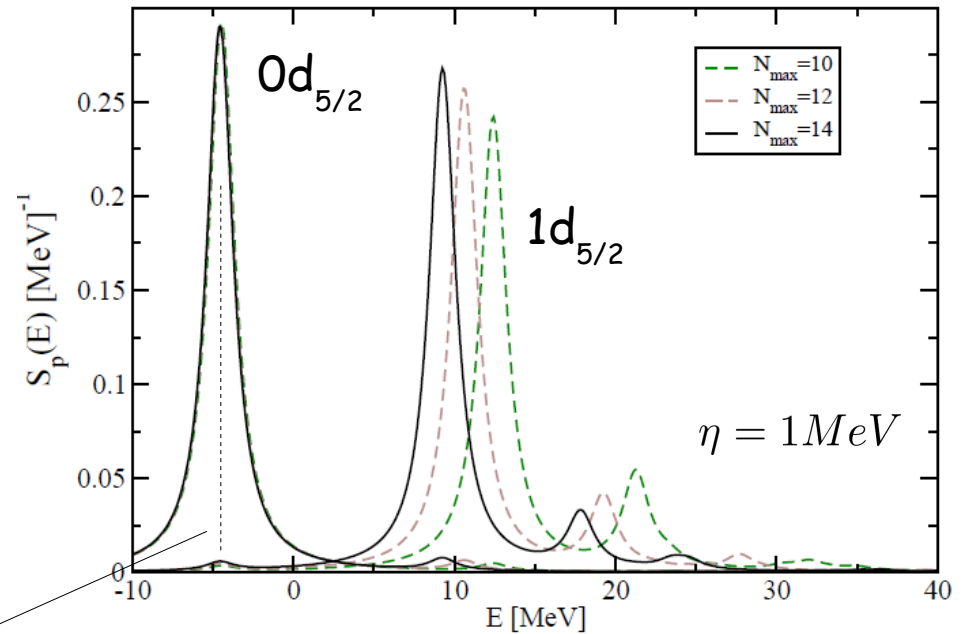
→ Inversion of the (similarity-transformed) Hamiltonian in the Lanczos basis :

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

# Particle spectral function in $^{17}\text{O}$

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

CCSD (Single-Double):  
 -> H.O. basis with  $\hbar\omega=20$  MeV.



ground state

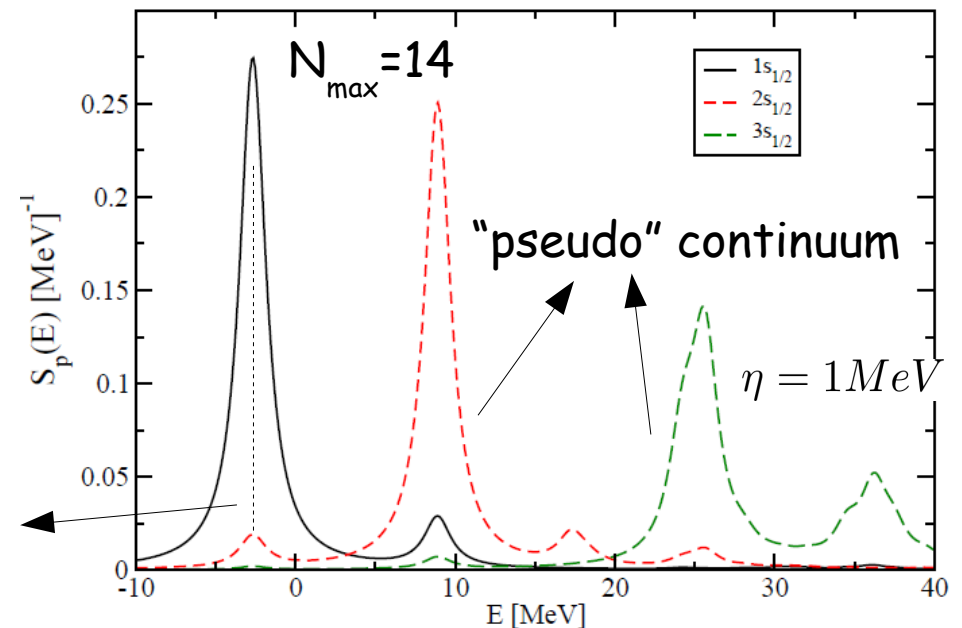
$$E^{\text{ccsd}}(5/2^+) = -4.557 \text{ MeV}$$

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

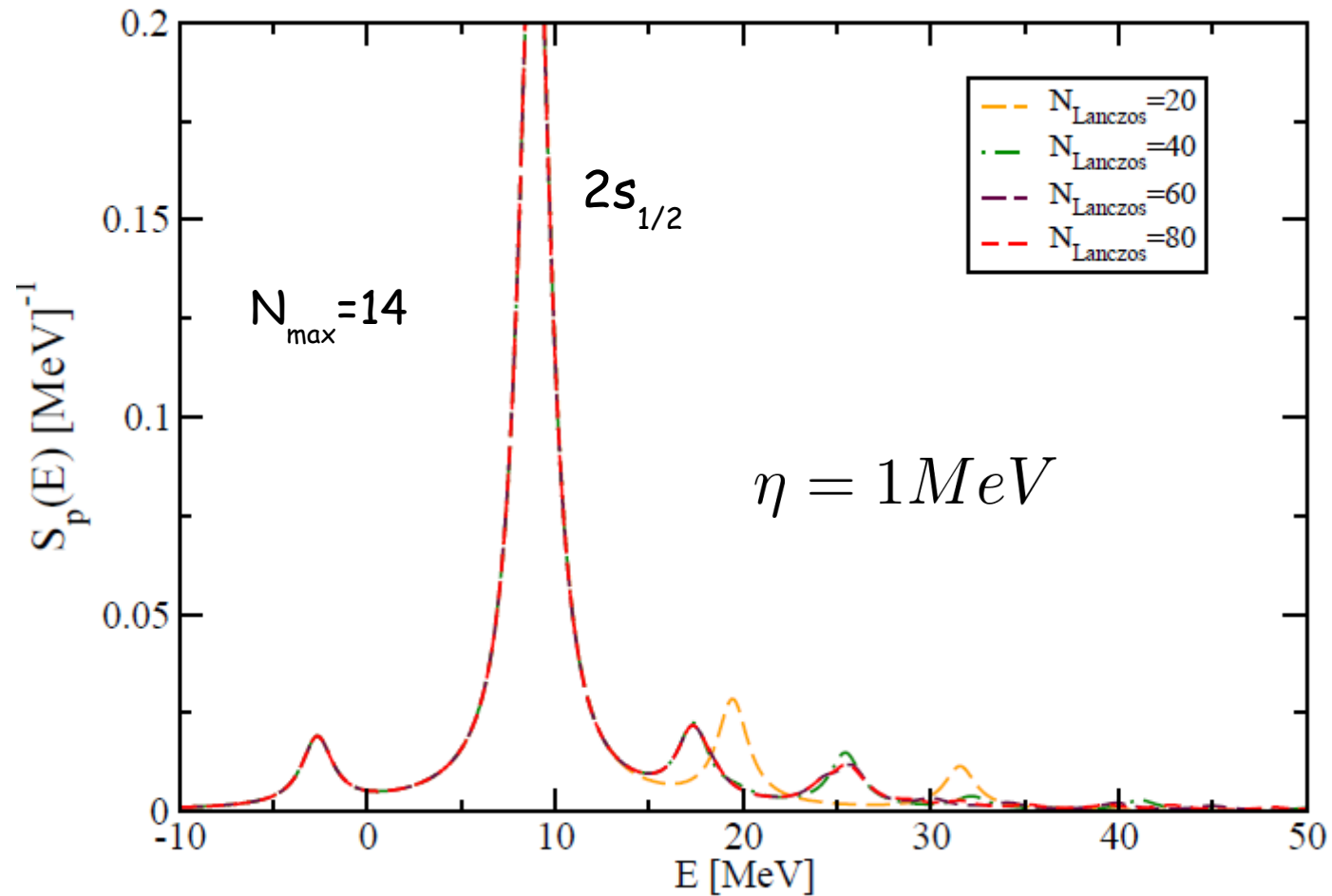
$$E^{\text{exp}}(1/2^+) = -3.272 \text{ MeV}$$

1<sup>st</sup> excited state

$$E^{\text{ccsd}}(5/2^+) = -2.670 \text{ MeV}$$



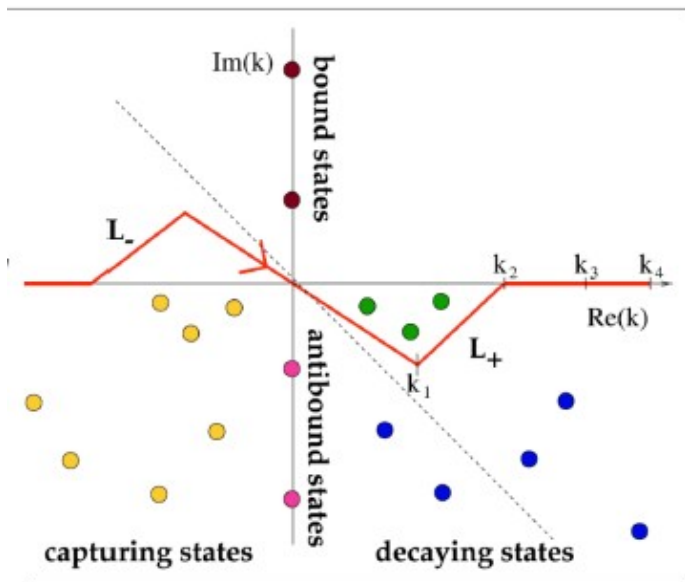
# Convergence pattern with the number of Lanczos iterations



# Green's function in the Berggren Basis

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

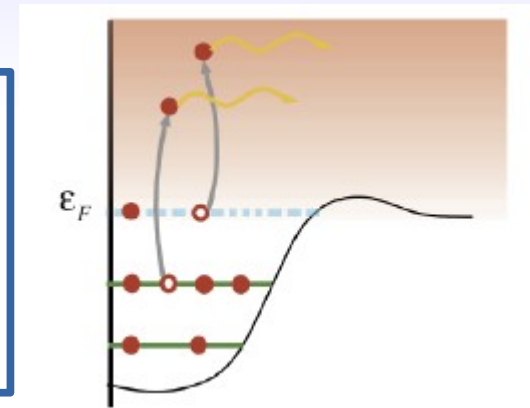
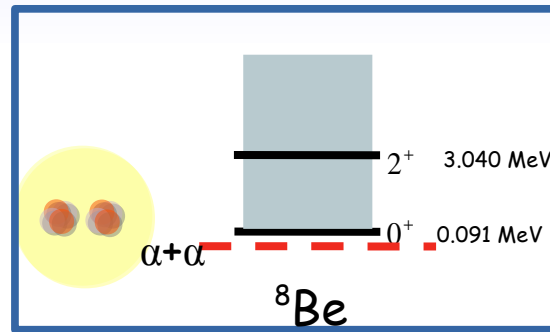
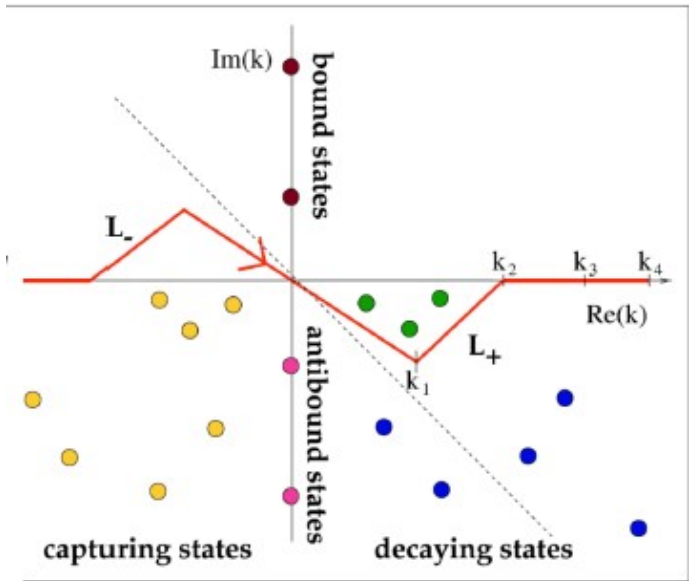
$$+ \sum_m \frac{\langle \Psi_0^A | a_\beta^\dagger | \Psi_m^{A-1} \rangle \langle \Psi_m^{A-1} | a_\alpha | \Psi_0^A \rangle}{E - [E_0^A - \tilde{E}_m^{A-1}] - i\eta}$$



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

# Berggren basis

Physics of nuclei at the edges of stability



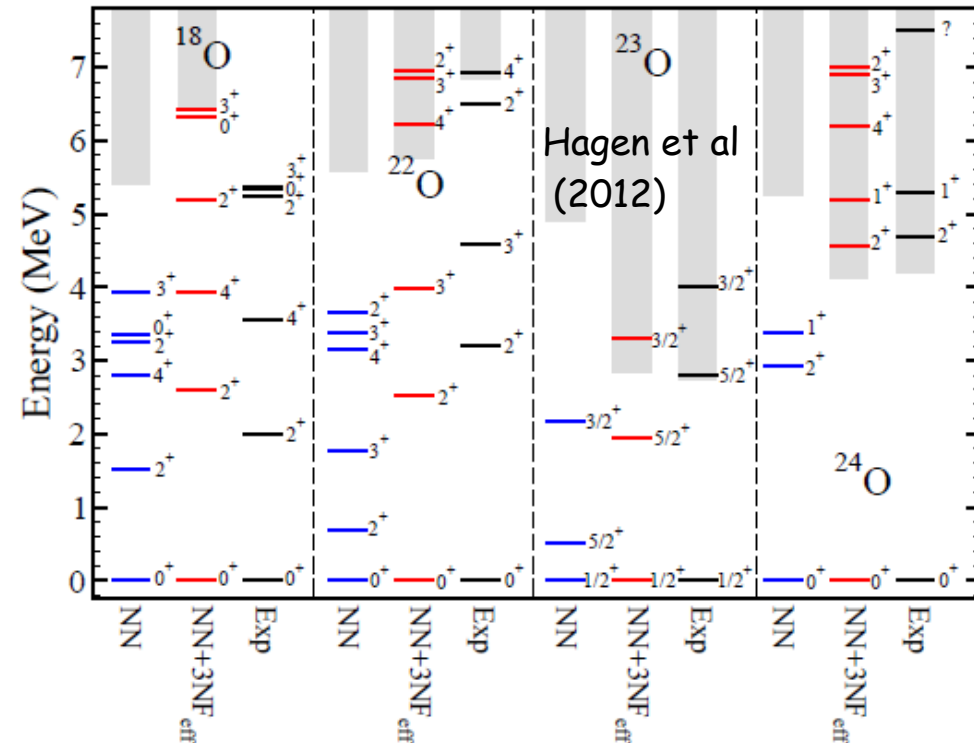
\*coupling to the continuum is an essential feature of systems far from stability.  
 \*taken into account by using the Berggren basis which includes bound, resonant and scattering states.

## Gamow (complex-energy) Shell Model :

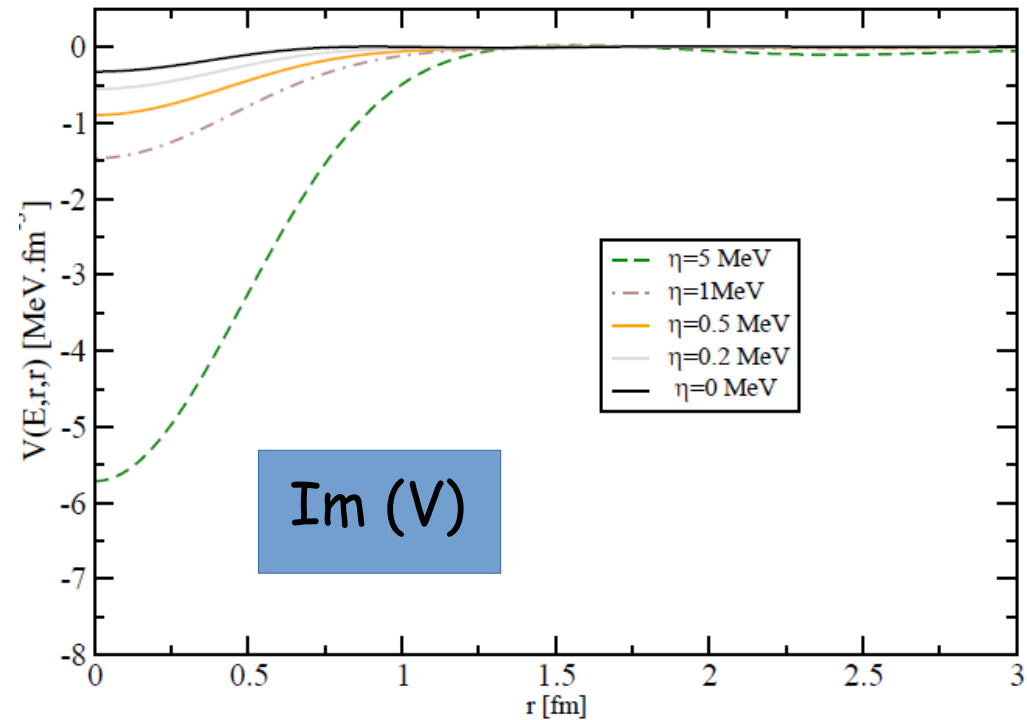
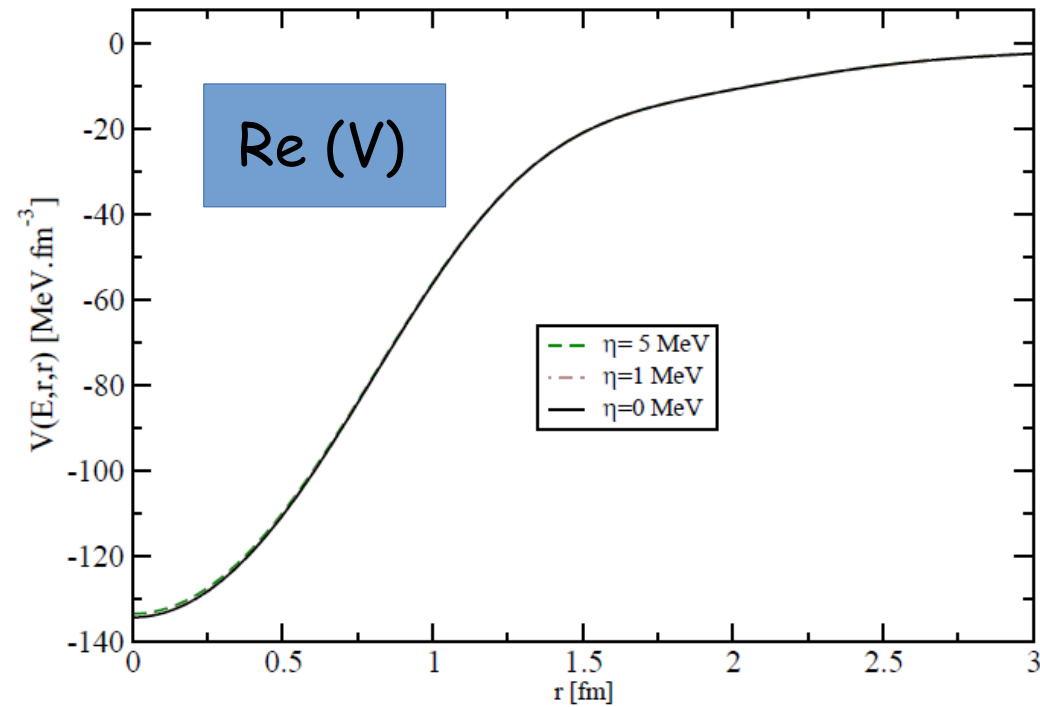
N. Michel et al, PRL (2002) ; G. Hagen et al, PRC (2005) ;  
 J.R et al, PRL (2006) ; N. Michel et al, JPG (2009); G.  
 Papadimitriou et al, PRC (2014); Y. Jaganathen et al, JP  
 (2012) ; K. Fosseiz et al, PRA (2015).

## Coupled Cluster in the Gamow Basis:

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

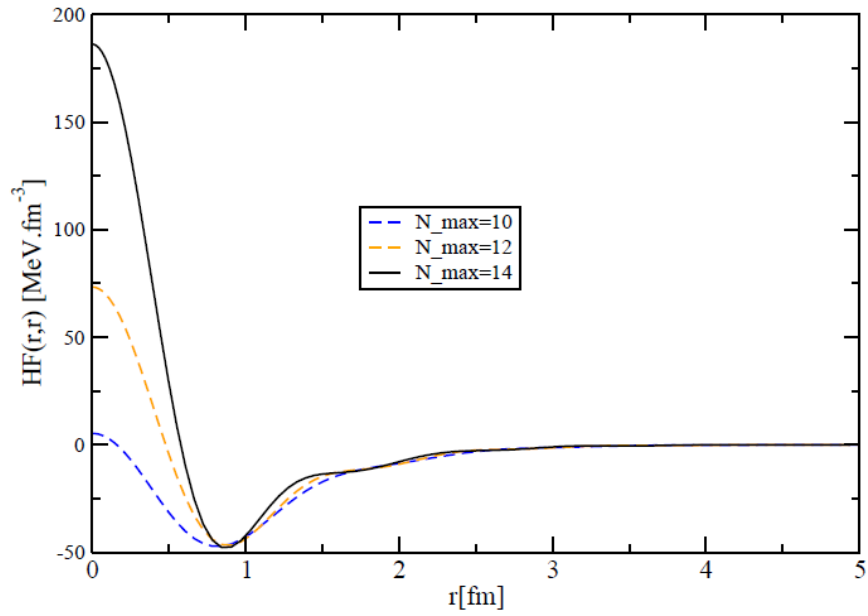


# Optical Potential for S-wave neutron elastic scattering at 10 MeV

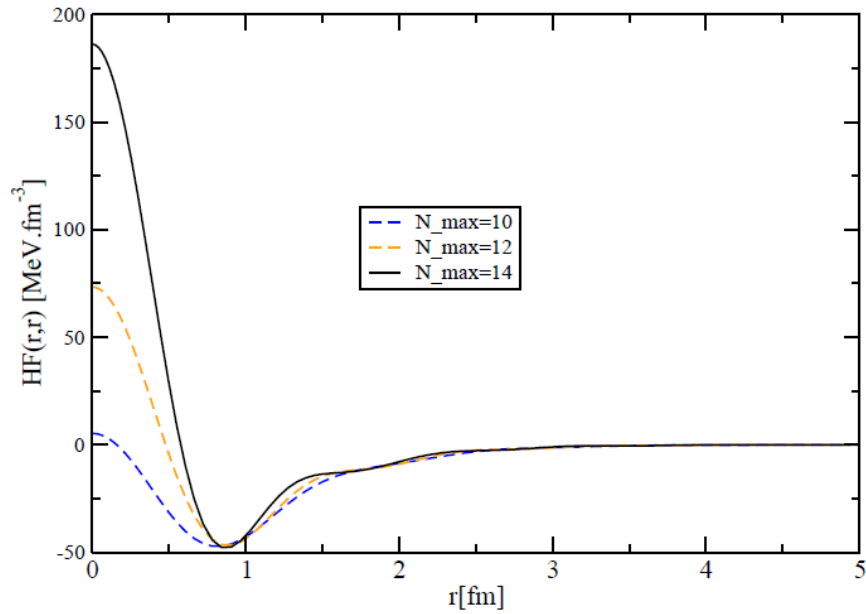


Mixed basis: H.O. shells ( $N_{\text{max}} = 10$ ) + 40 s-wave complex continuum

# Convergence of the Hartree-Fock potential

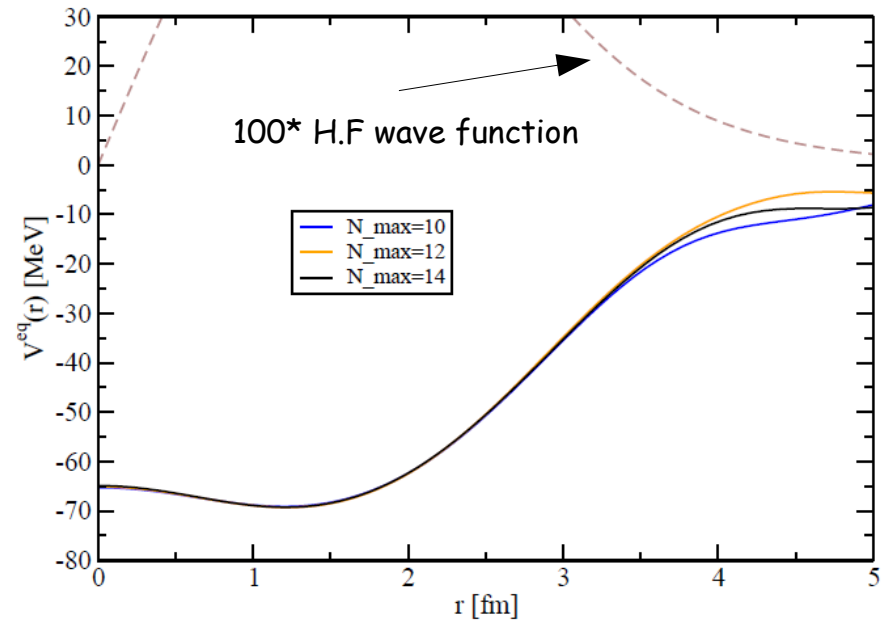


# Convergence of the Hartree-Fock potential



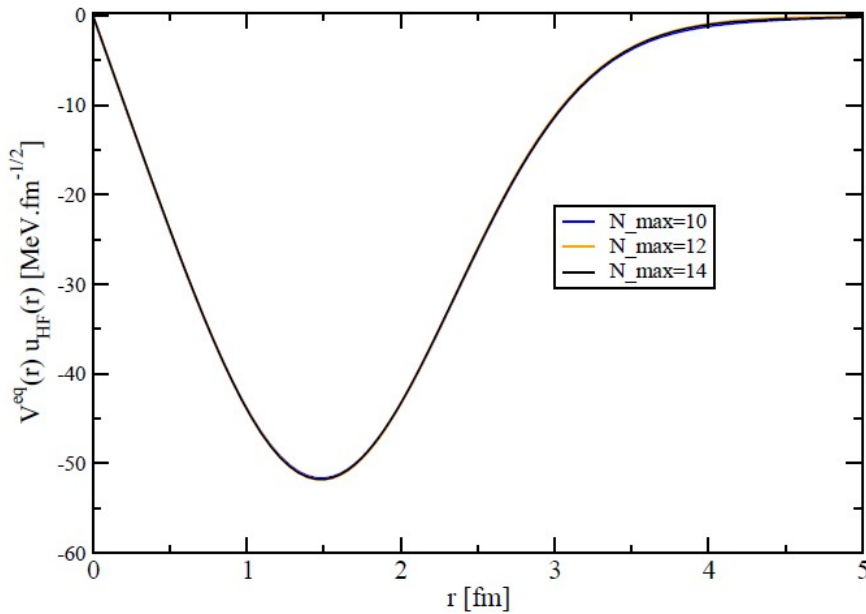
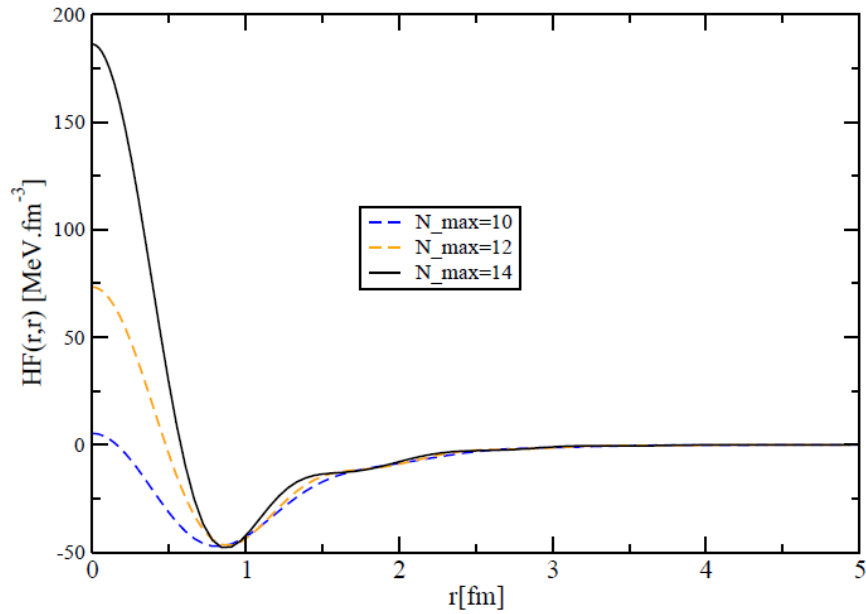
## Equivalent Potential

$$V^{eq}(r) = r \int \frac{r' dr' V^{HF}(r, r') u_{HF}(r')}{u_{HF}(r)}$$



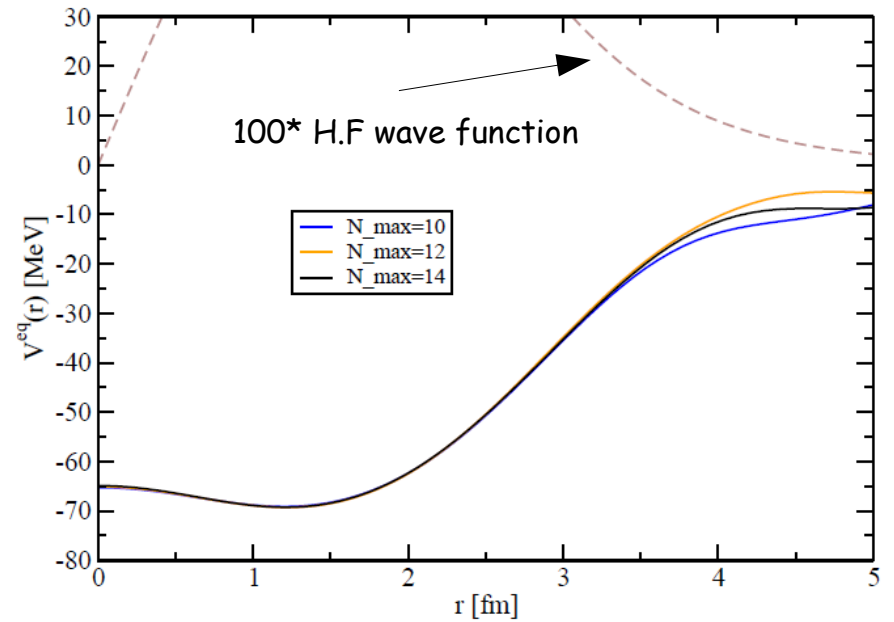


# Convergence of the Hartree-Fock potential



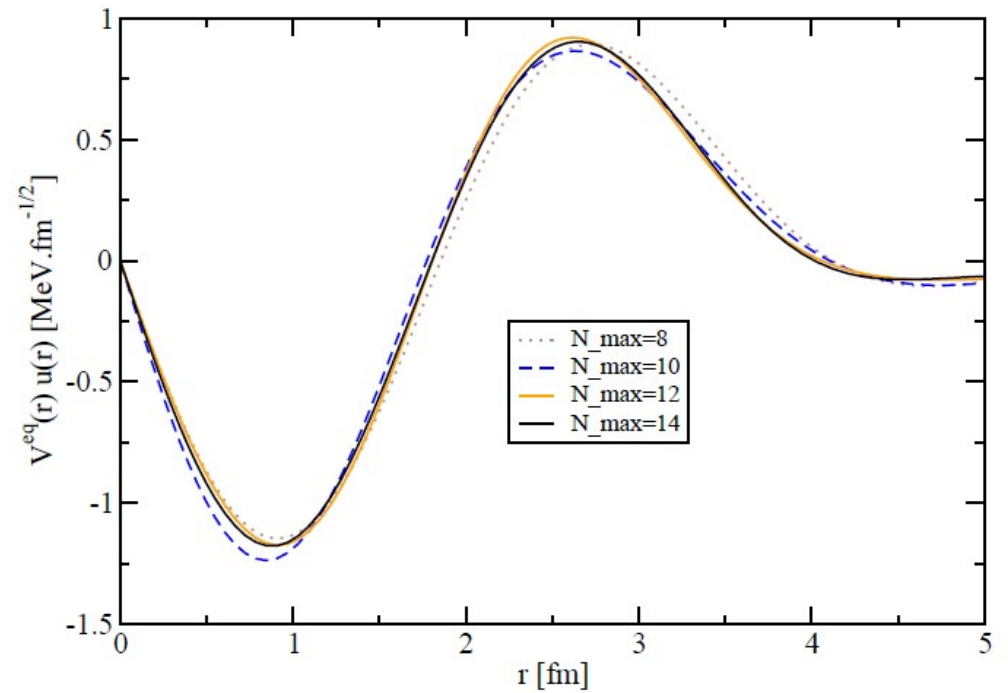
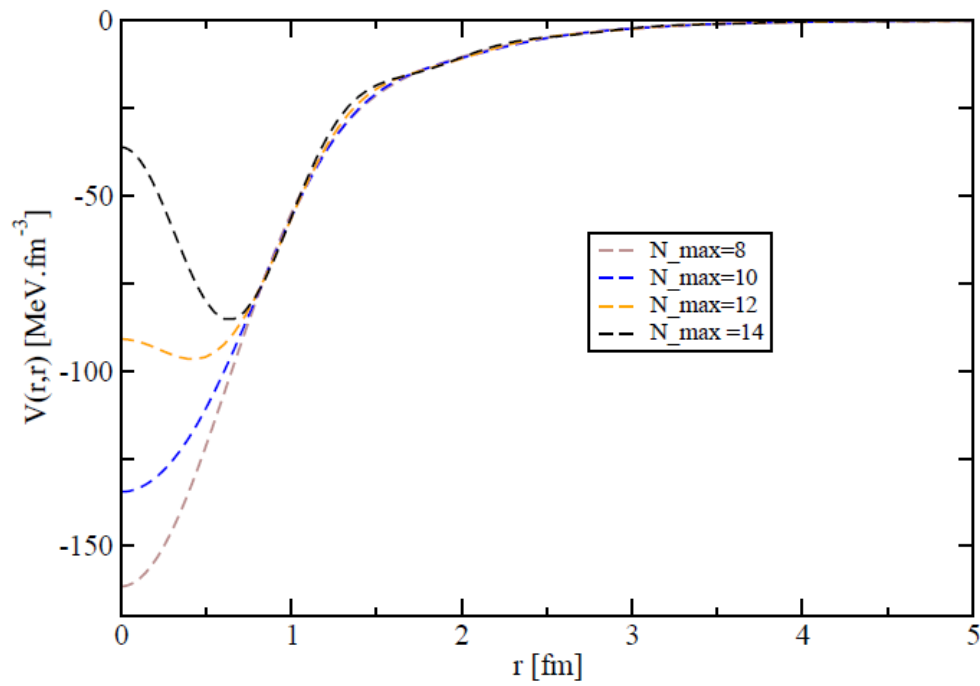
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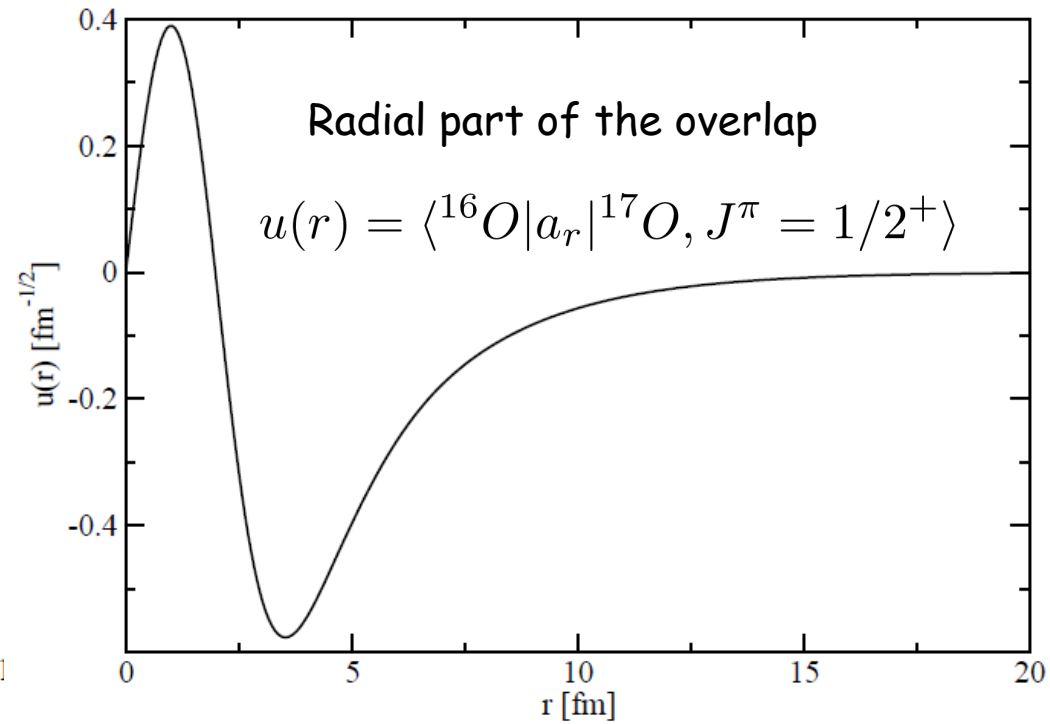
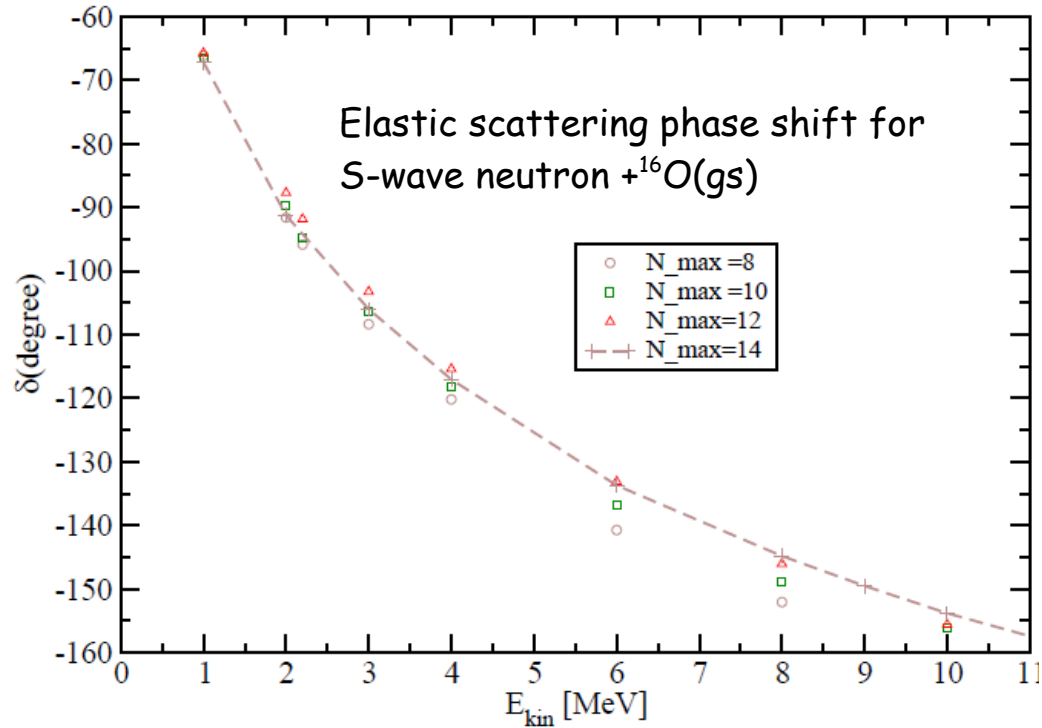


# Convergence of the optical potential

## S-wave neutron potential at 10 MeV



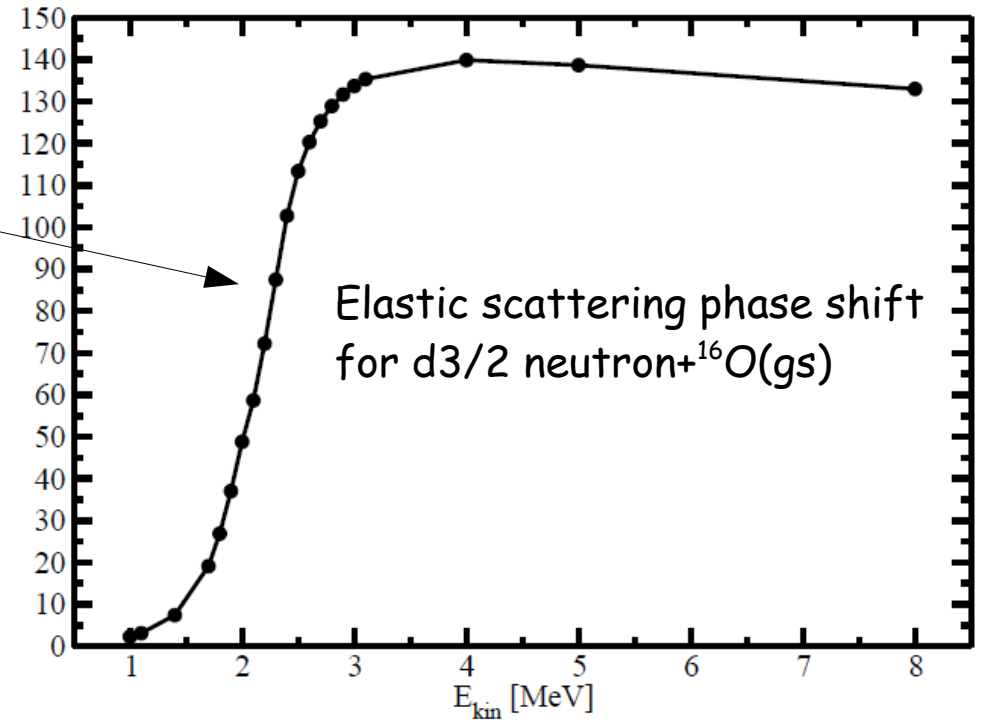
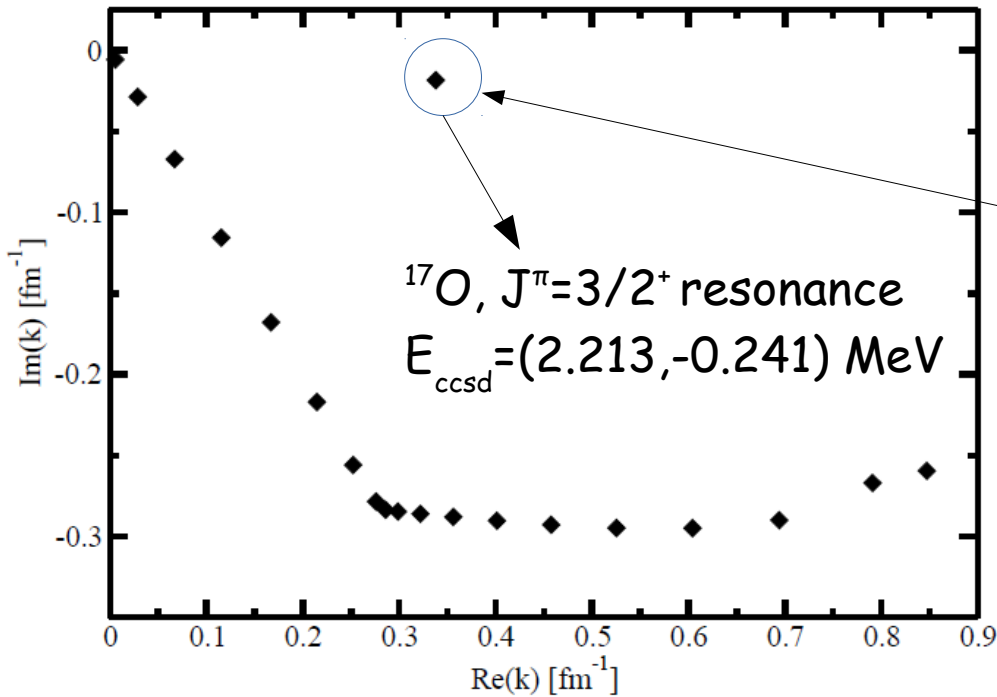
# S-wave neutron



Mixed basis: H.O. shells +40 s-wave **complex** continuum shells

# $d_{3/2}$ neutron

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



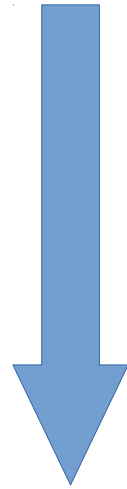
$$E^{\text{exp}}(3/2^+) = (0.943, -0.48) \text{ MeV}$$

Mixed basis: H.O. shells ( $N_{\text{max}}=10$ ) + 40  $d_{3/2}$ -wave complex continuum

# 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

