Microscopic Optical Potentials from Coupled Cluster Calculations

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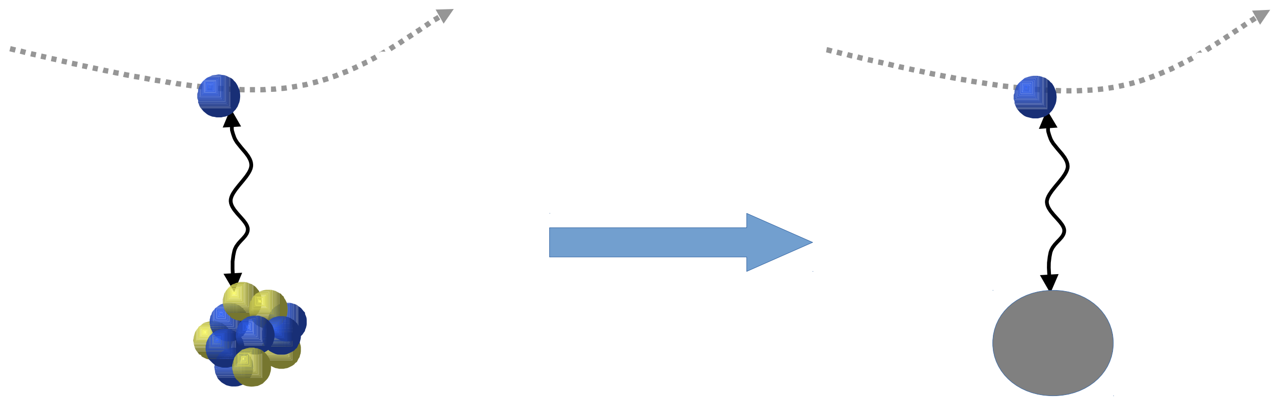
Goals

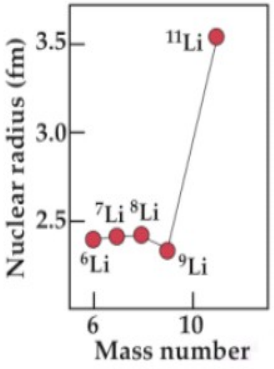
* microscopic construction of optical potentials : nucleons as degrees of freedom, modern realistic n-n, 3n forces...



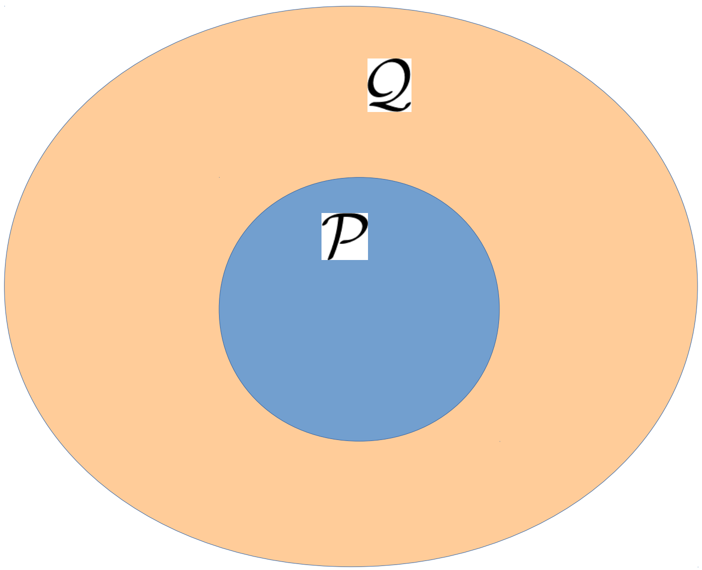
$$H|\Psi(1,\ldots,A)\rangle = E|\Psi(1,\ldots,A)\rangle \qquad H^{eff}|\Psi'(\vec{r})\rangle = E|\Psi'(\vec{r})\rangle$$

* predictive theory for nuclear reactions

* reliable/accurate extrapolations for systems far from stability.



Feshbach projection technique



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

$$\boxed{\begin{aligned} (E - H_{PP})|\Psi_P\rangle &= H_{PQ}|\Psi_Q\rangle \\ (E - H_{QQ})|\Psi_Q\rangle &= H_{QP}|\Psi_P\rangle \end{aligned}}$$

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

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).

Single-particle Green's function

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

$$\eta \to 0$$

Lehman representation

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

<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 :

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

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

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

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

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

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

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

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

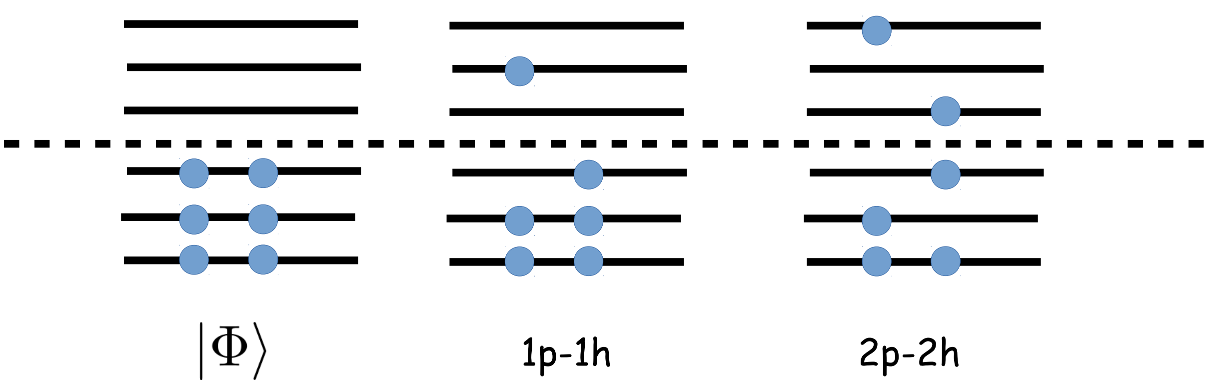
2p-2h operator

Similarity-transformed Hamiltonian

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

Coupled-cluster equations

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



PHYSICAL REVIEW C **86**, 021602(R) (2012)

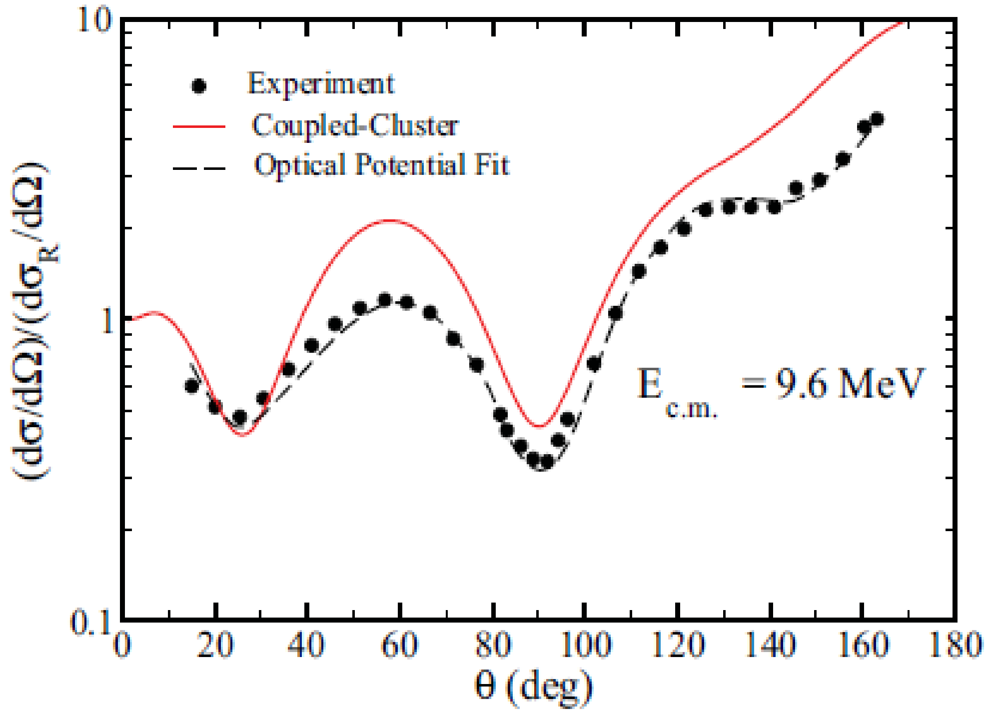
Elastic proton scattering of medium mass nuclei from coupled-cluster theory

G. Hagen[1,2] and N. Michel[2]
[1]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
(Received 11 June 2012; revised manuscript received 24 July 2012; published 13 August 2012)

One-nucleon overlap function

$$O_A^{A+1}(lj;kr) = \sum_n \langle A+1||\tilde{a}^\dagger_{nlj}||A\rangle \phi_{nlj}(r)$$

$^{40}Ca(p,p)^{40}Ca$



NN interaction: N^2LO_{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,[1,2] G. Baardsen,[1] C. Forssén,[3] G. Hagen,[4,5] M. Hjorth-Jensen,[1,2,6] G. R. Jansen,[4,5] R. Machleidt,[7] W. Nazarewicz,[5,4,8] T. Papenbrock,[5,4] J. Sarich,[9] and S. M. Wild[9]

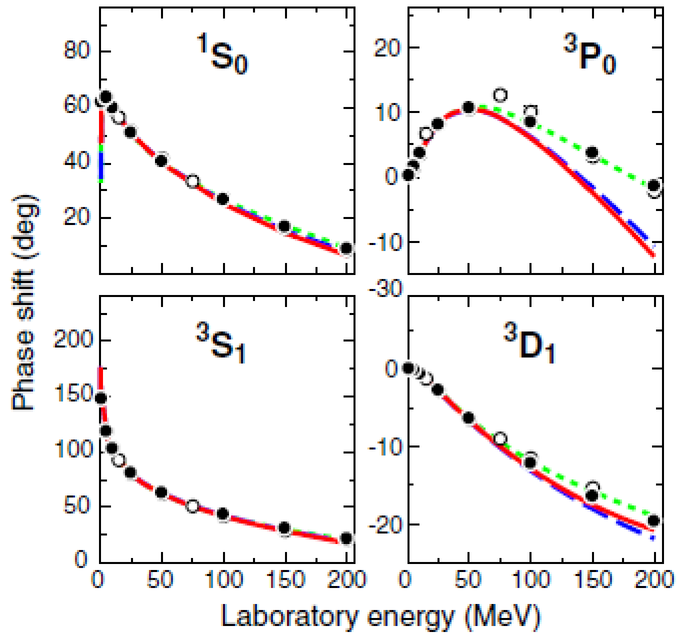
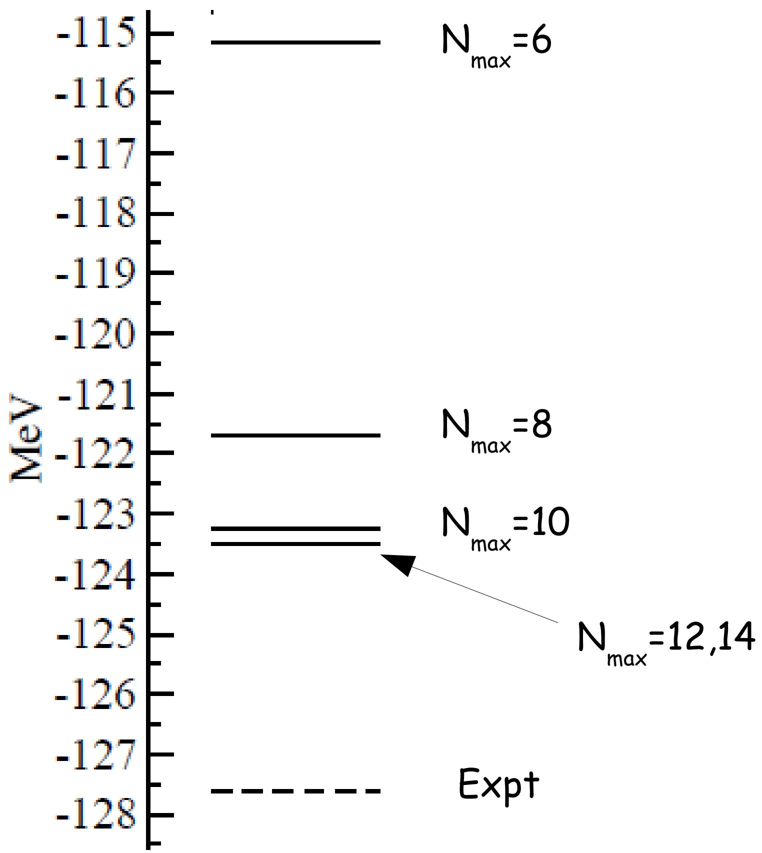


FIG. 1 (color online). Computed *np* phase shifts of the optimized NNLO potential of this work (solid, red line), the NNLO potential of Ref. [3] (dashed, blue line), and the N^3LO potential [4] (green, dotted line) compared with the Nijmegen phase shift analysis [18] (solid dots) and the VPI/GWU analysis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

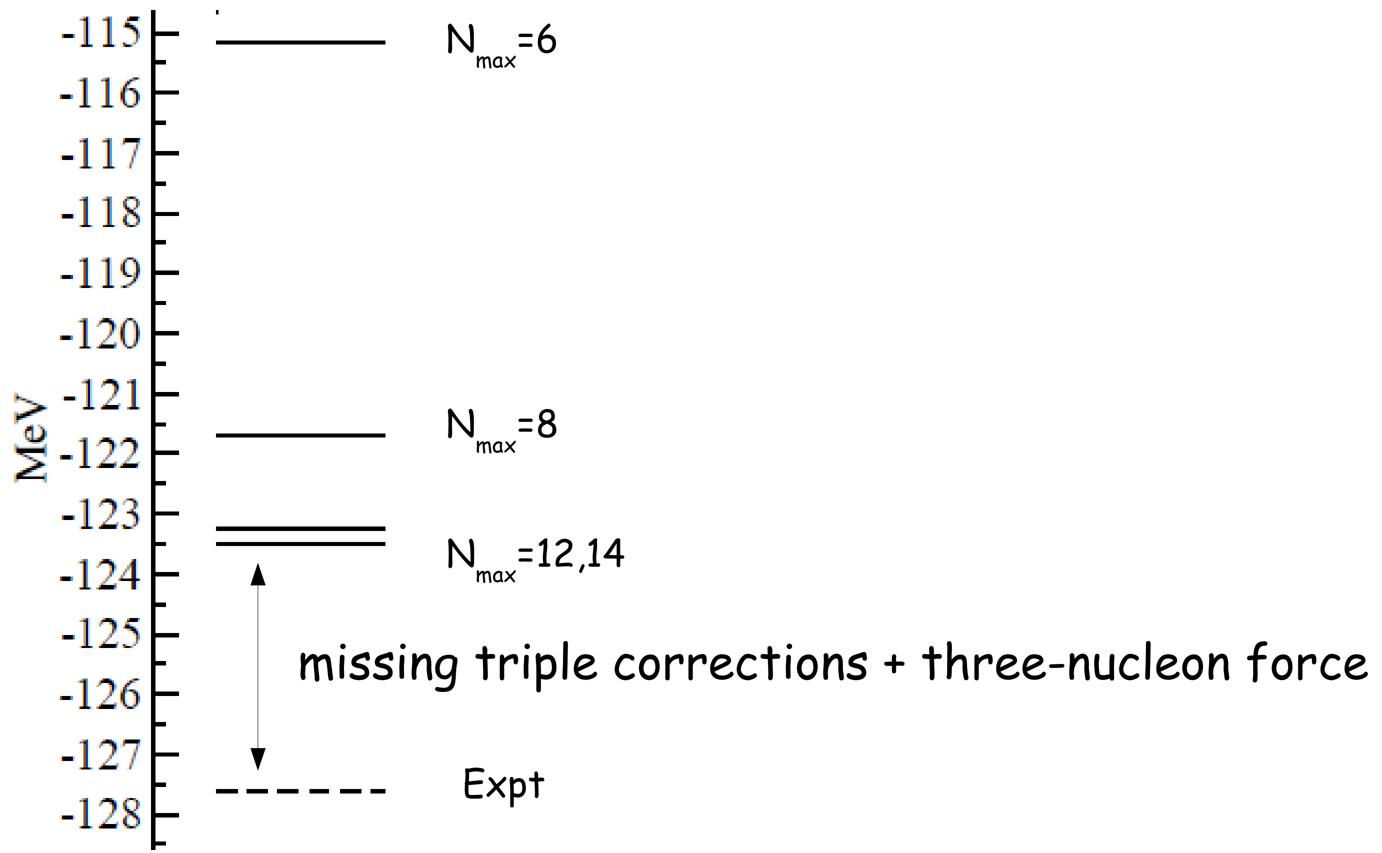
Coupled Cluster (SD) for ^{16}O and ^{17}O with N^2LO_{opt}

^{16}O ground state



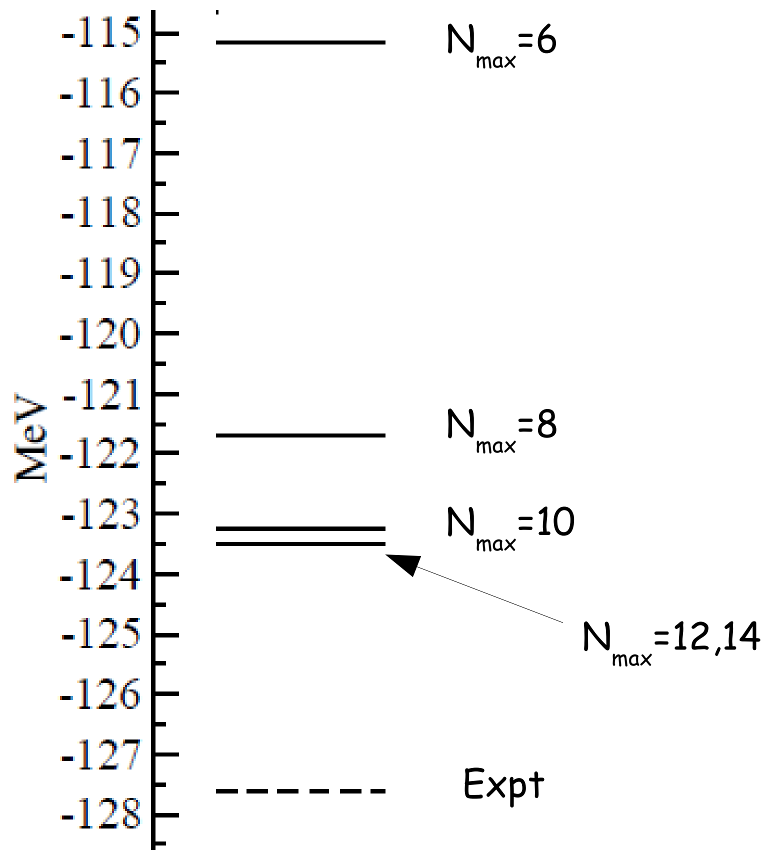
Coupled Cluster (SD) for ^{16}O and ^{17}O with N^2LO_{opt}

^{16}O ground state

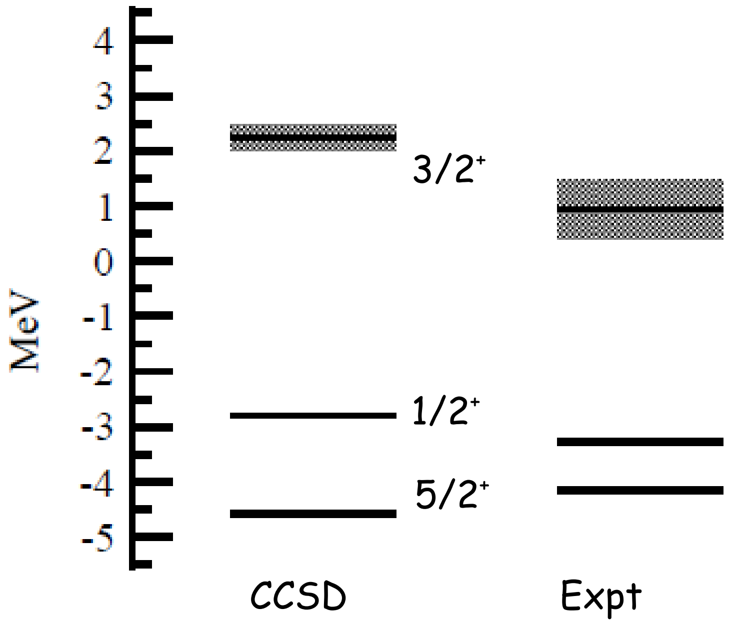


Coupled Cluster (SD) for ^{16}O and ^{17}O with N^2LO_{opt}

^{16}O ground state



^{17}O



Coupled Cluster Green's function

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

→ similarity-transformed operators :

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

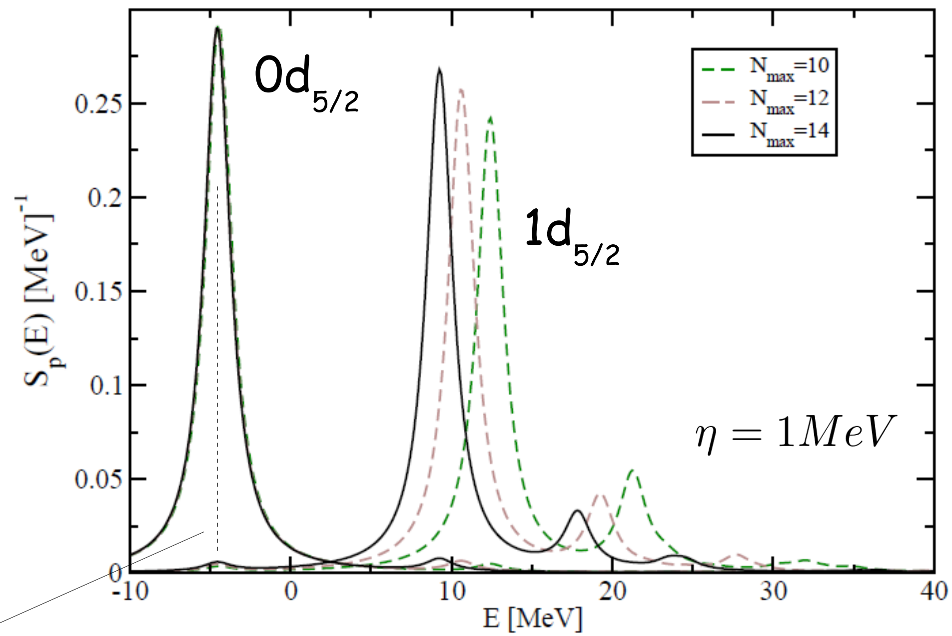
→ Inversion of the (similarity-transformed) Hamiltonian in the Lanczos basis :

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

Particle spectral function in ^{17}O

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

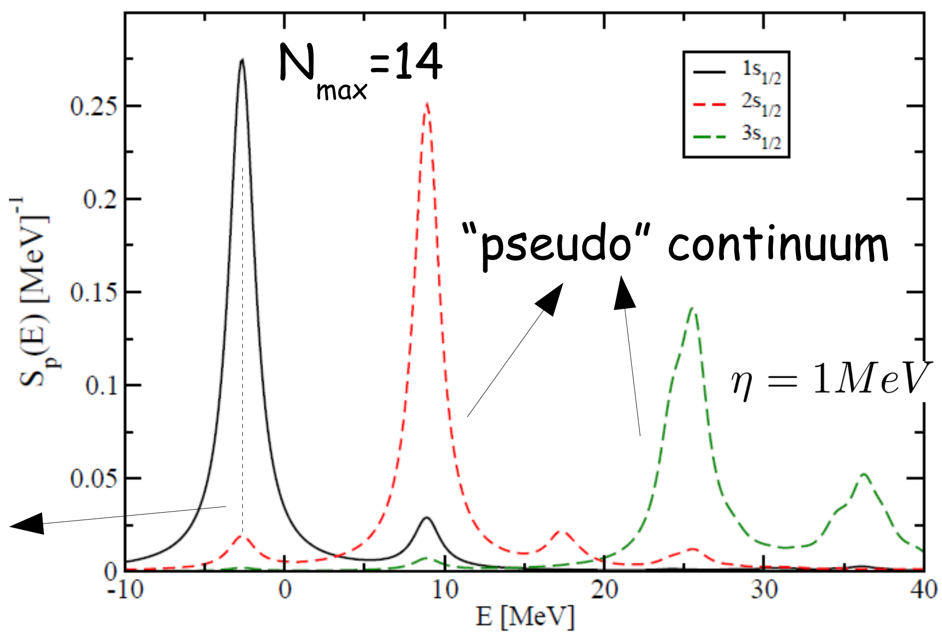
CCSD (Single-Double):
-> H.O. basis with $\hbar\omega$=20 MeV.



ground state

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

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



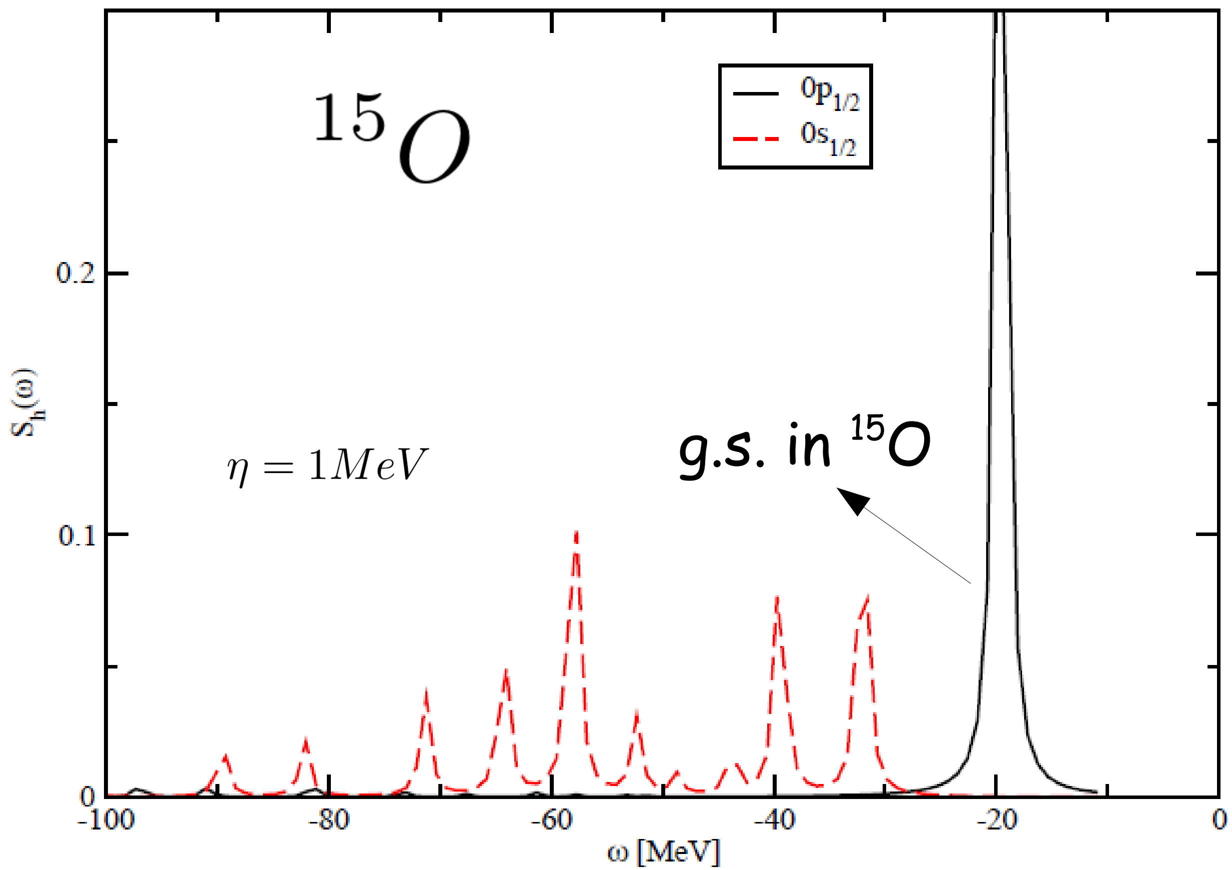
1^{st} excited state

$E^{ccsd}(1/2^+)$=-2.670 MeV

Hole spectral function in ^{15}O

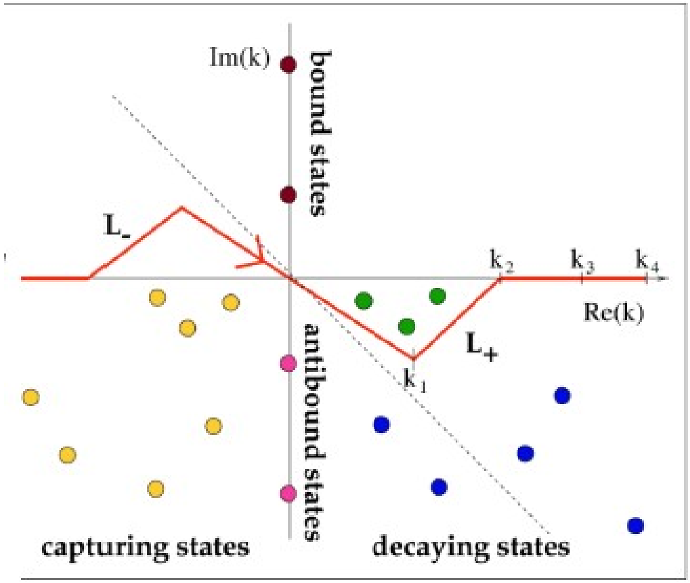
CCSD (Single-Double):

-> H.O. basis with ħω=20 MeV
-> N_{max}=14



Green's function in the Berggren Basis

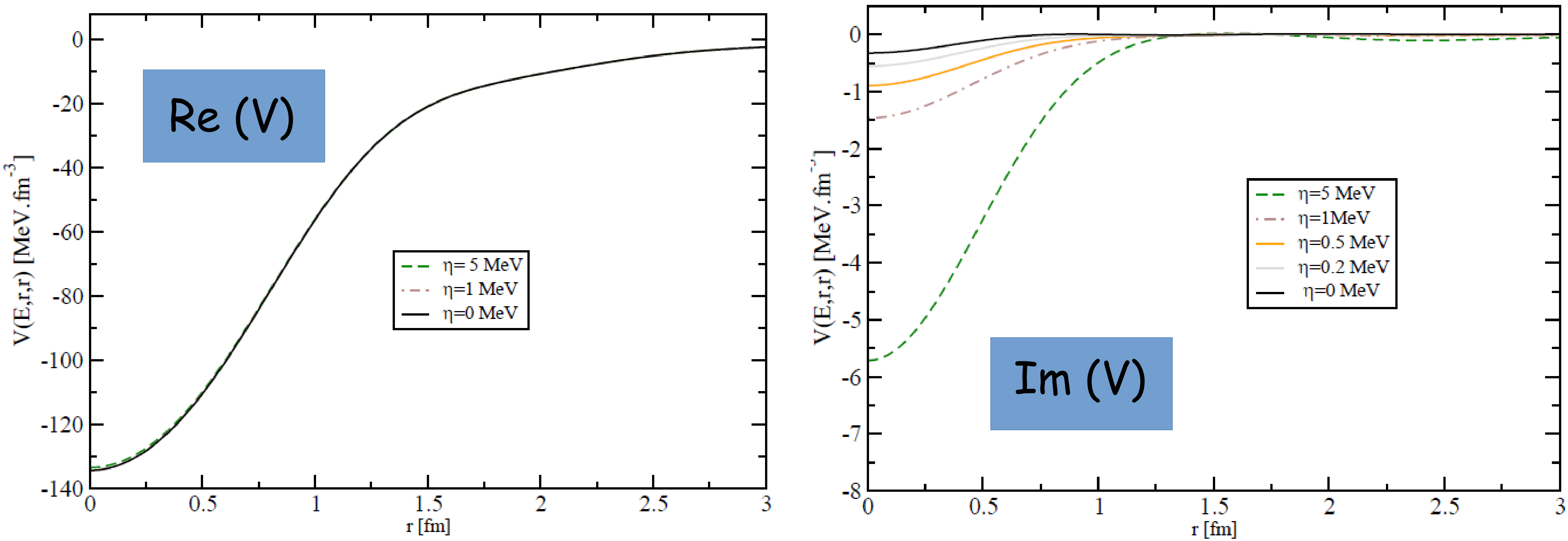
$$G(\alpha,\beta;E) = \sum_n \frac{\langle\Psi_0^A|a_\alpha|\Psi_n^{A+1}\rangle\langle\Psi_n^{A+1}|a_\beta^\dagger|\Psi_0^A\rangle}{E-[\tilde{E}_n^{A+1}-E_0^A]+i\eta} + \sum_m \frac{\langle\Psi_0^A|a_\beta^\dagger|\Psi_m^{A-1}\rangle\langle\Psi_m^{A-1}|a_\alpha|\Psi_0^A\rangle}{E-[E_0^A-\tilde{E}_m^{A-1}]-i\eta}$$



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

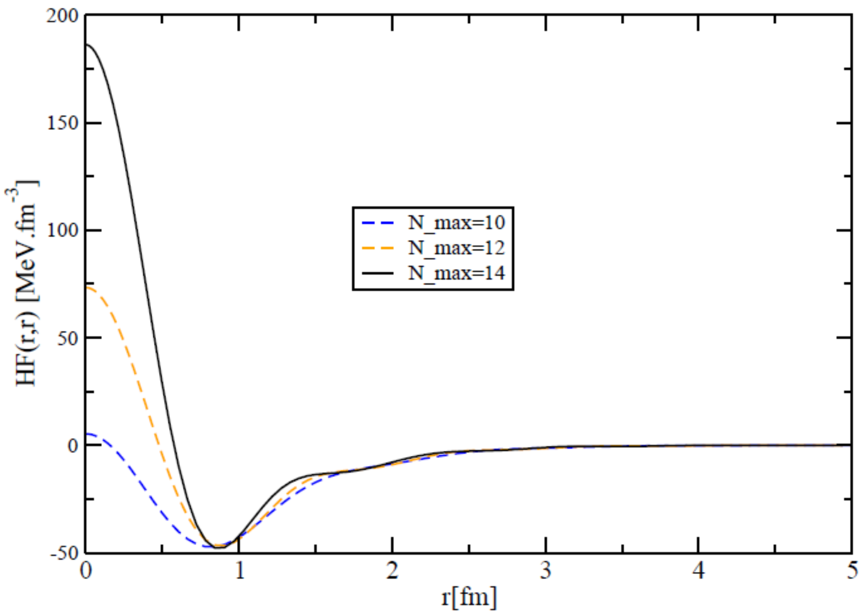
Berggren basis (T. Berggren, NPA 109 (1968))

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

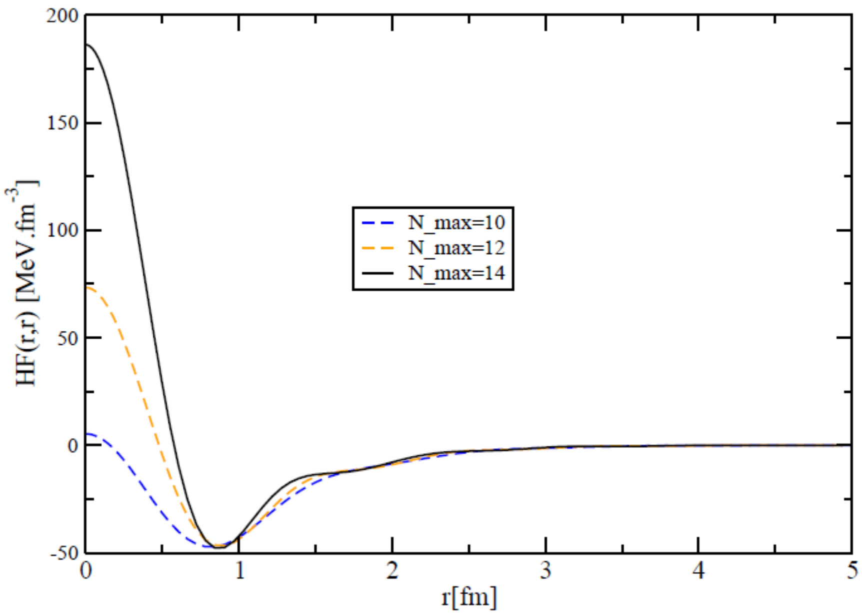


Mixed basis: H.O. shells (N_{max} =10) +40 s-wave **complex** continuum

Convergence of the Hartree-Fock potential

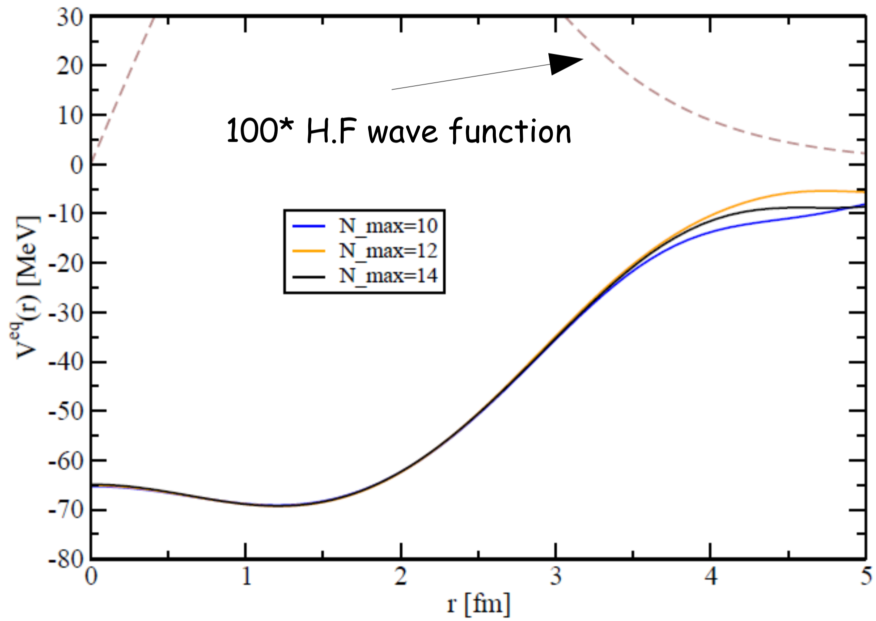


Convergence of the Hartree-Fock potential

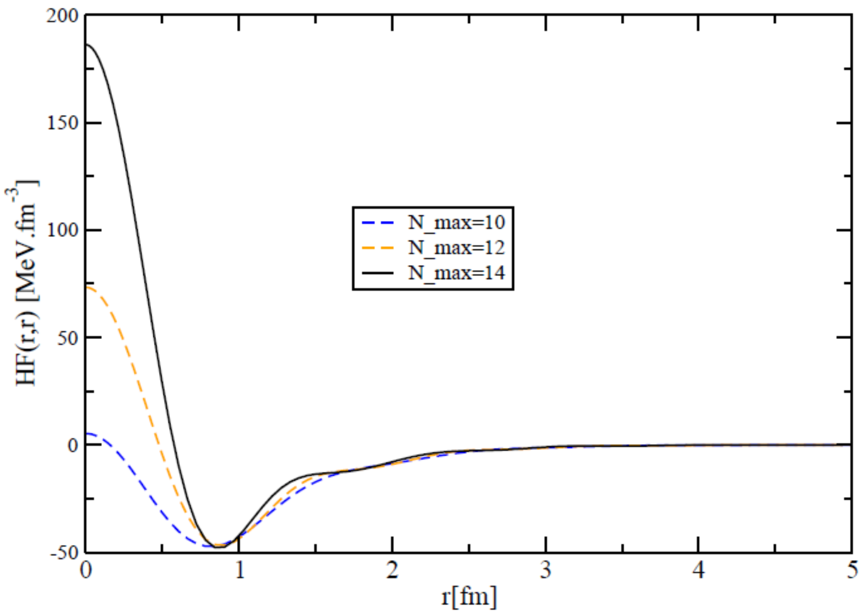


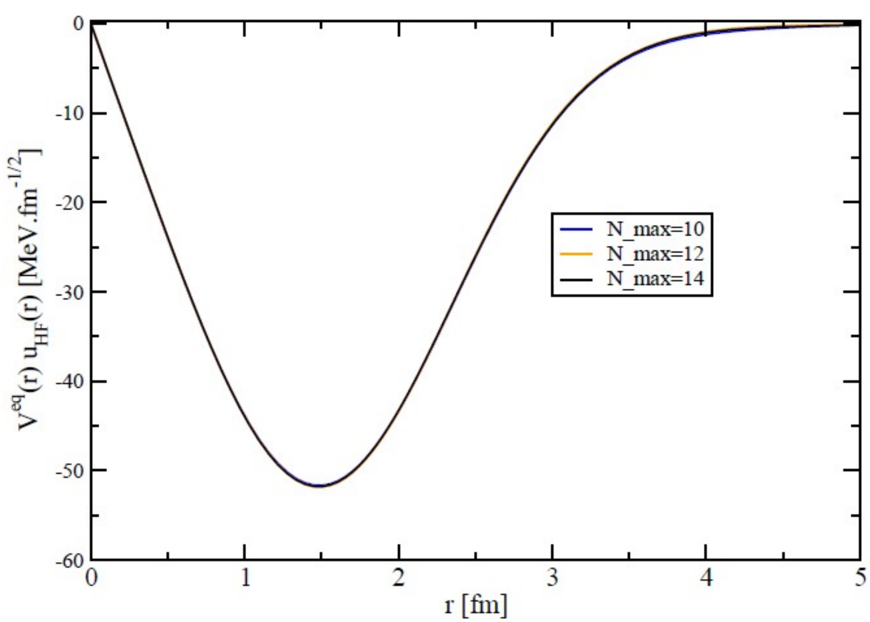
Equivalent Potential

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



Convergence of the Hartree-Fock potential





Equivalent Potential

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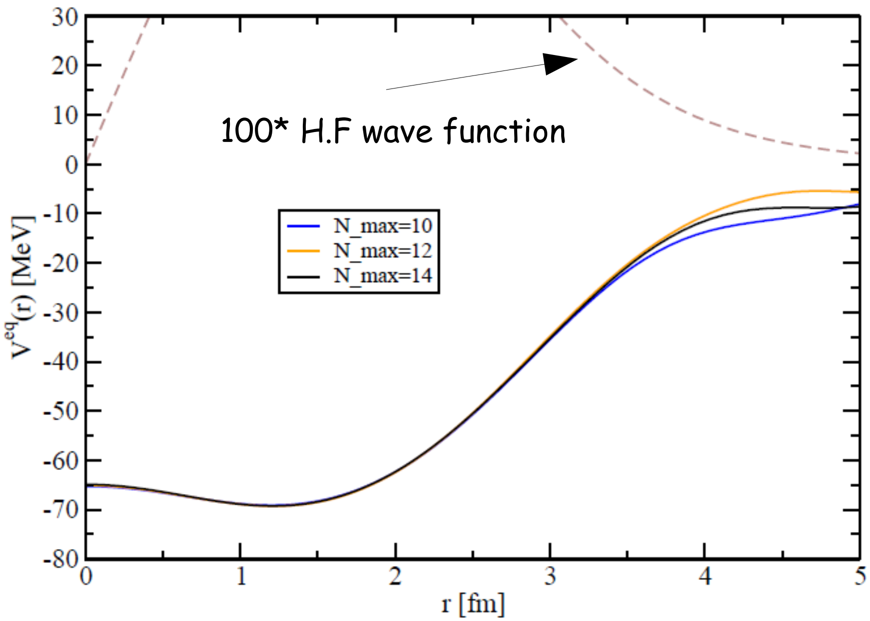
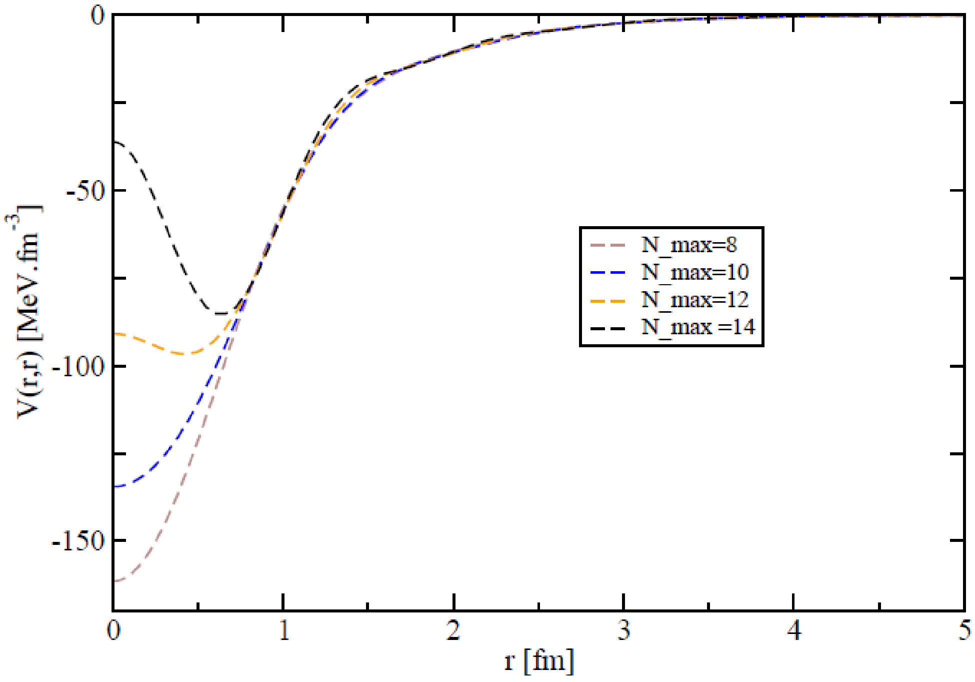
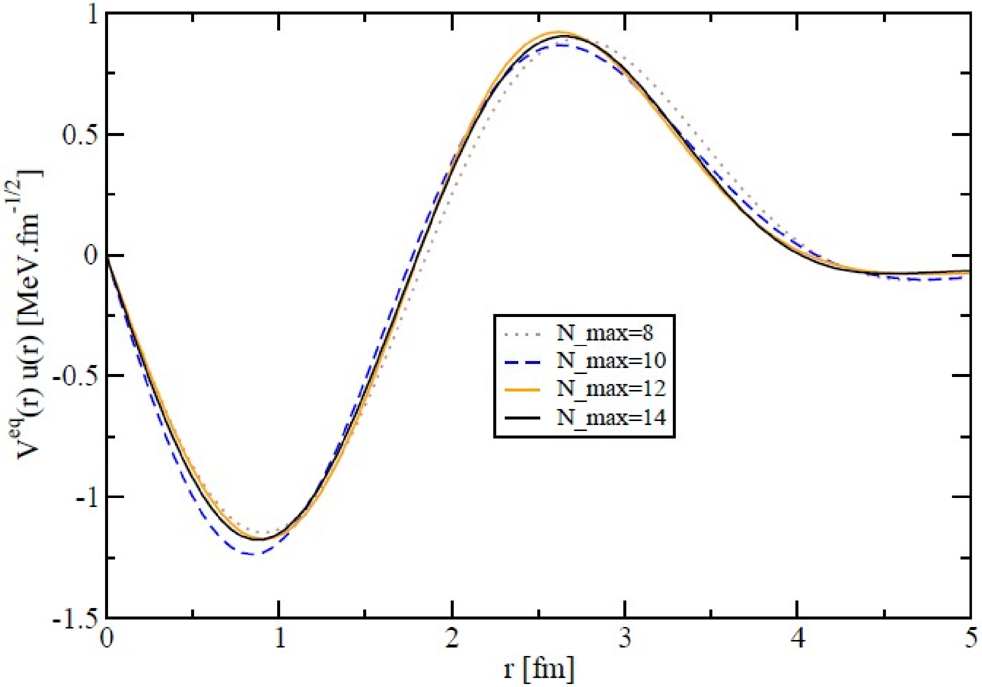


Convergence of the optical potential

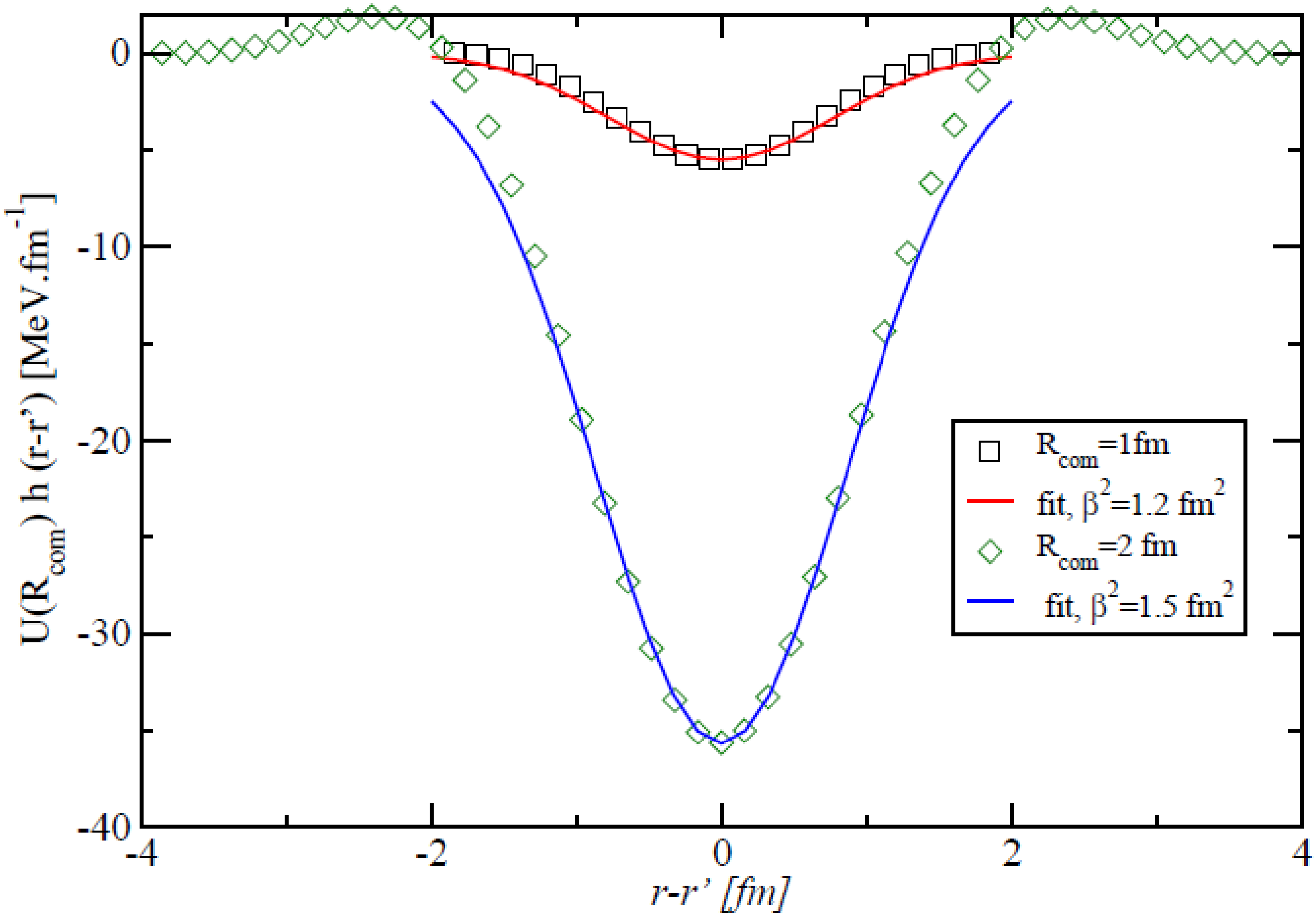
S-wave neutron potential at 10 MeV





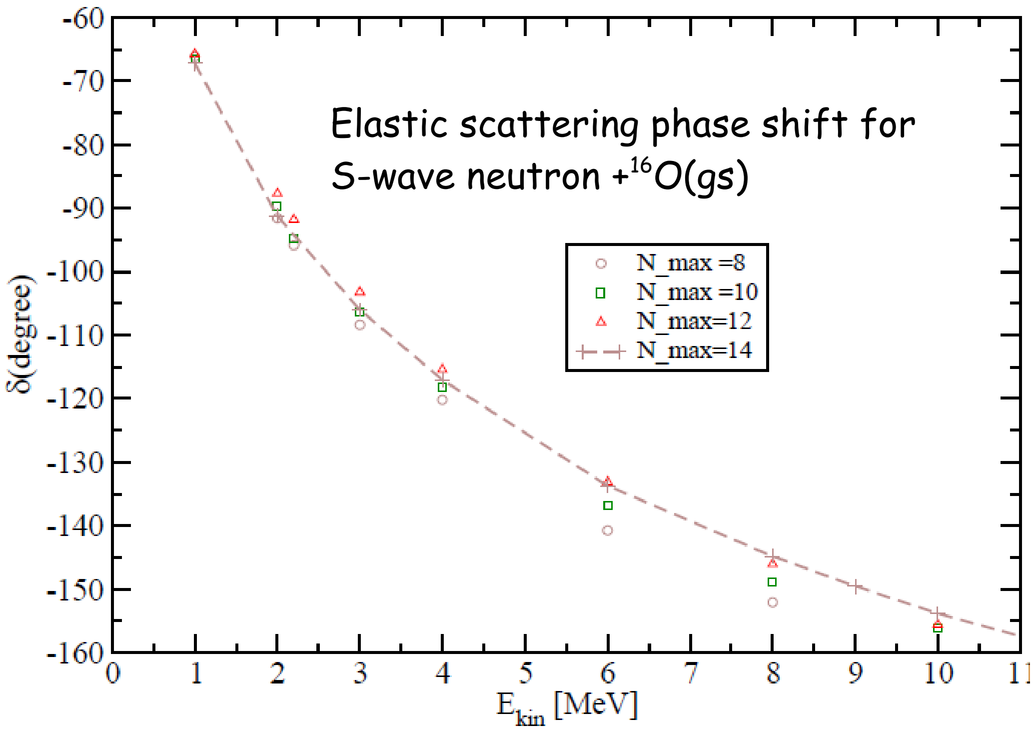
"Picture" of the non-locality

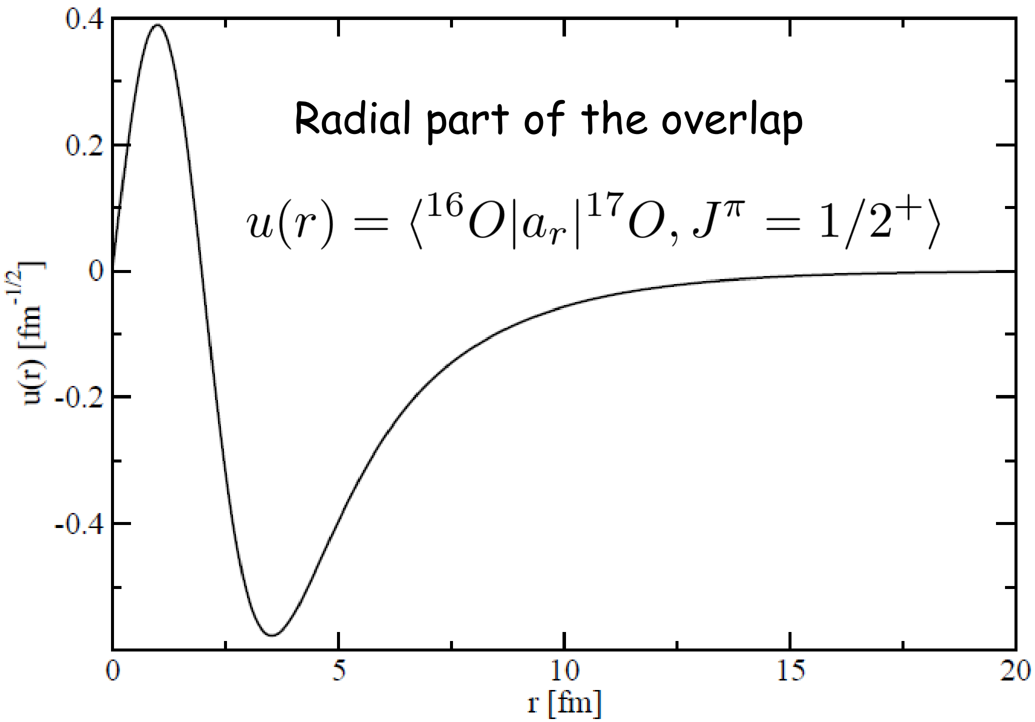
$$V(r,r') \equiv \frac{U(\frac{r+r'}{2})h(r-r')}{rr'}$$



$d_{5/2}$-wave neutron potential at 1 MeV

S-wave neutron

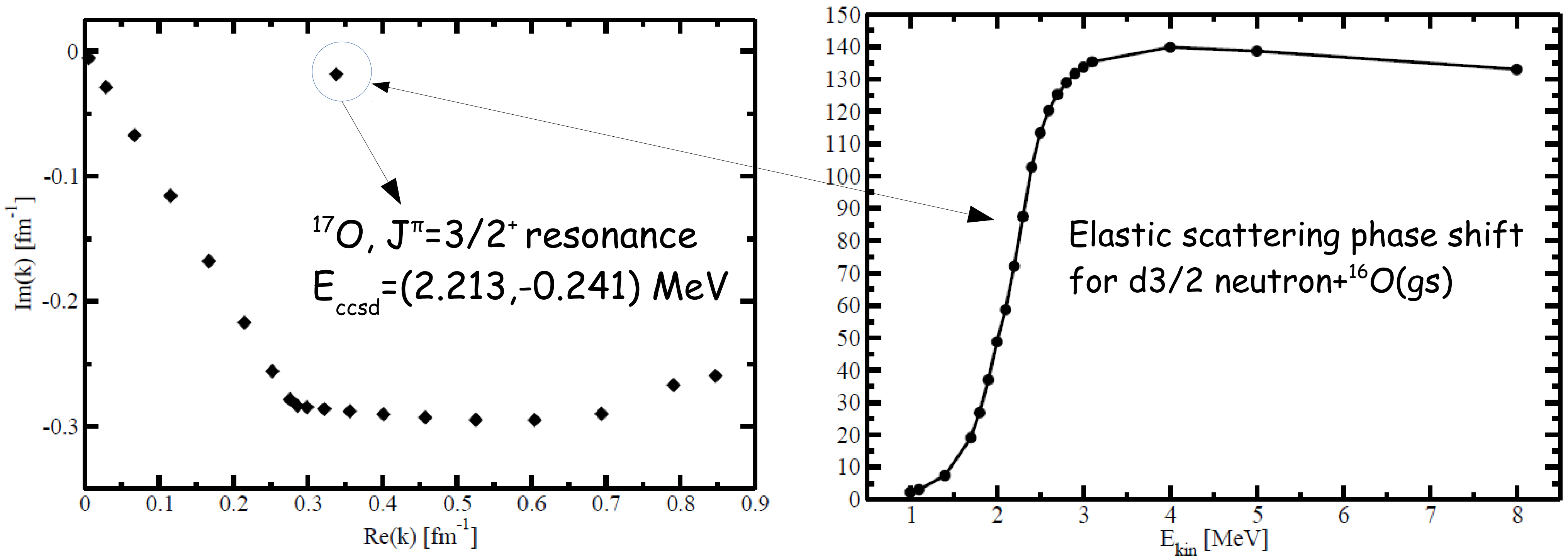




<u>Mixed basis: H.O. shells +40 s-wave **complex** continuum shells</u>

$d_{3/2}$ neutron

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



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

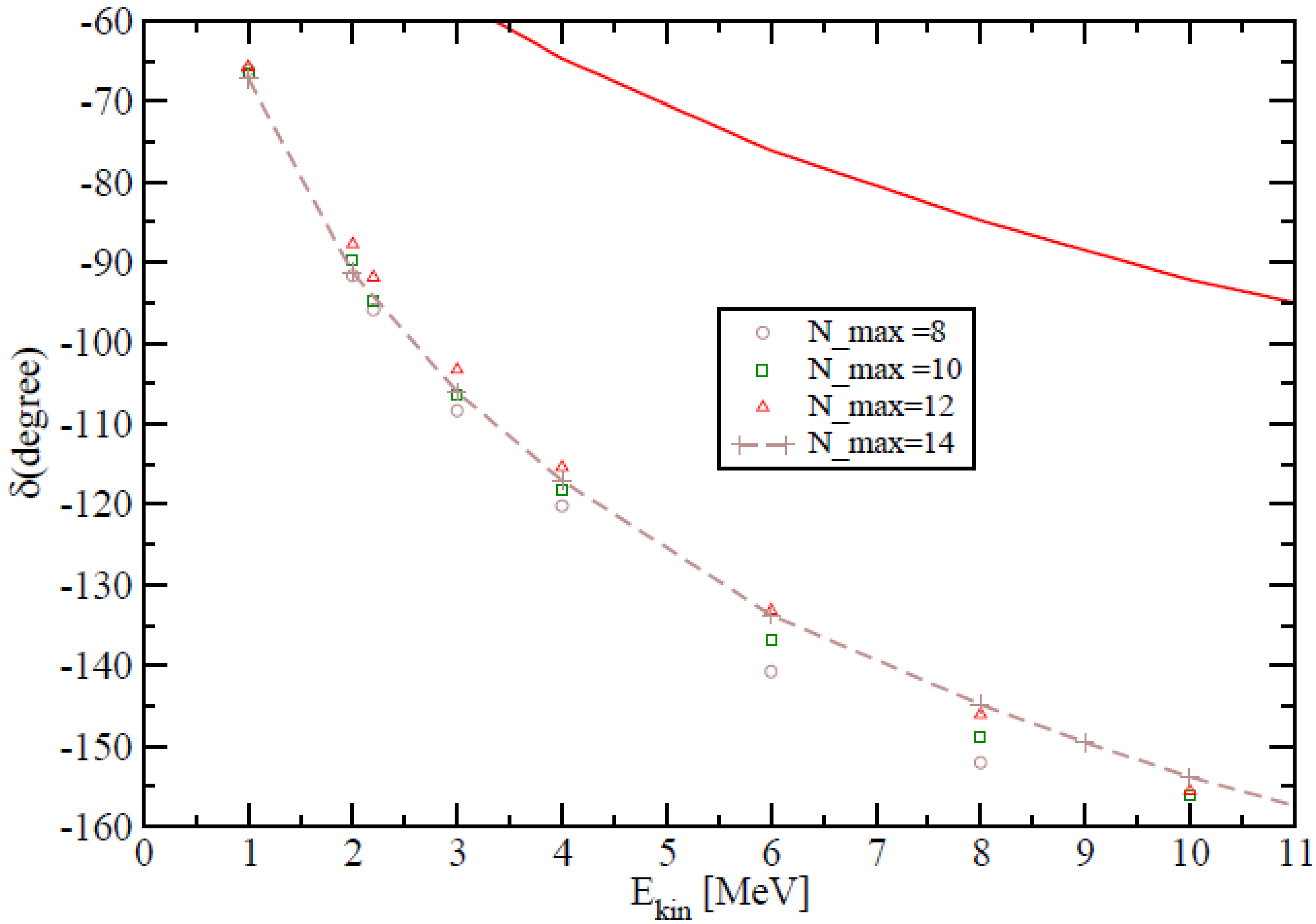
<u>Mixed basis:H.O. shells (N_{max}=10) + 40 $d_{3/2}$-wave **complex** continuum</u>

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



δ(degree)
E_kin [MeV]
N_max =8
N_max =10
N_max=12
N_max=14
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
0
1
2
3
4
5
6
7
8
9
10
11

Phenomenological Optical Potential

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

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

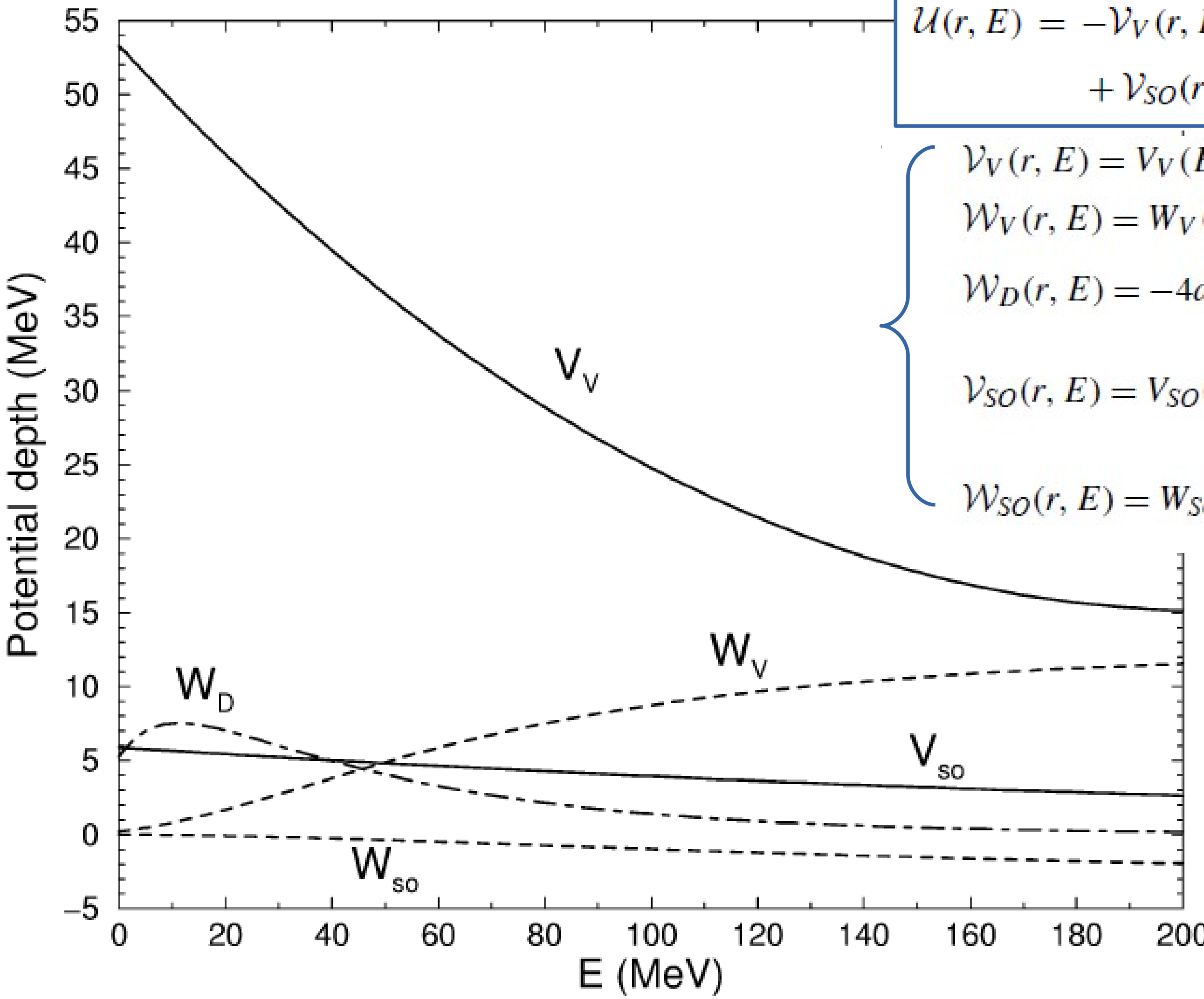
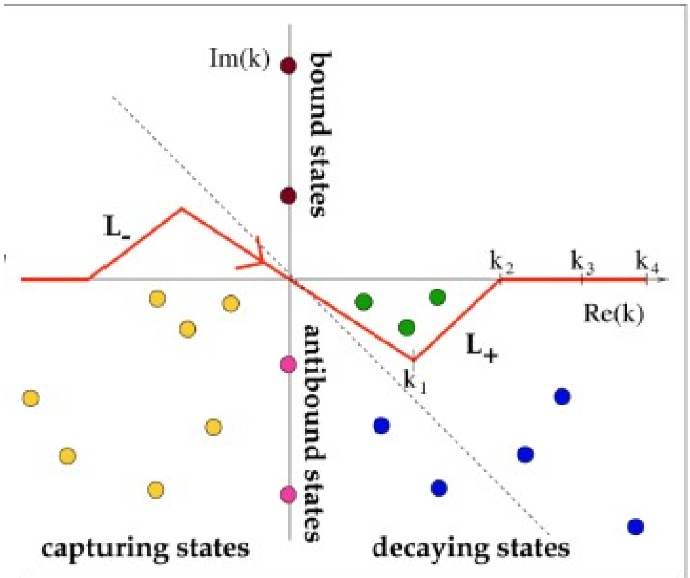


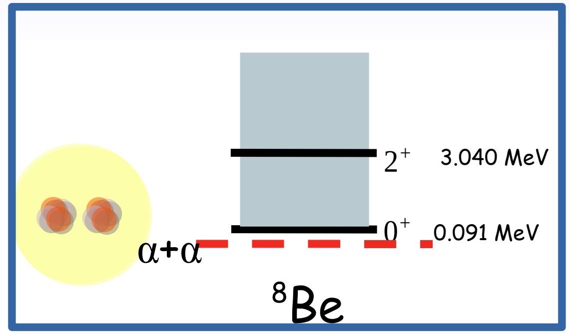
Fig. 1. The various potential well depths as a function of incident (laboratory) energy, see Eq. (7). As an example, the values for neutrons incident on ^{56}Fe are plotted.

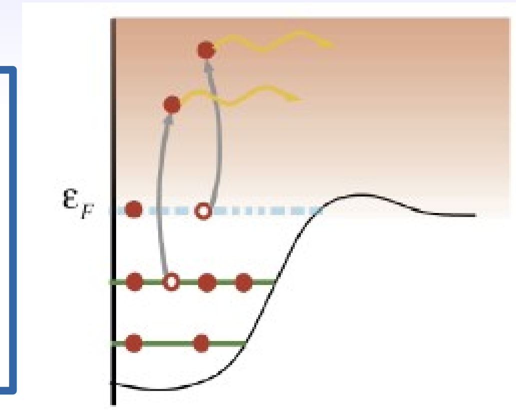
A.J Koning, J. P. Delaroche, NPA 713 (2003)

Berggren basis

Physics of nuclei at the edges of stability







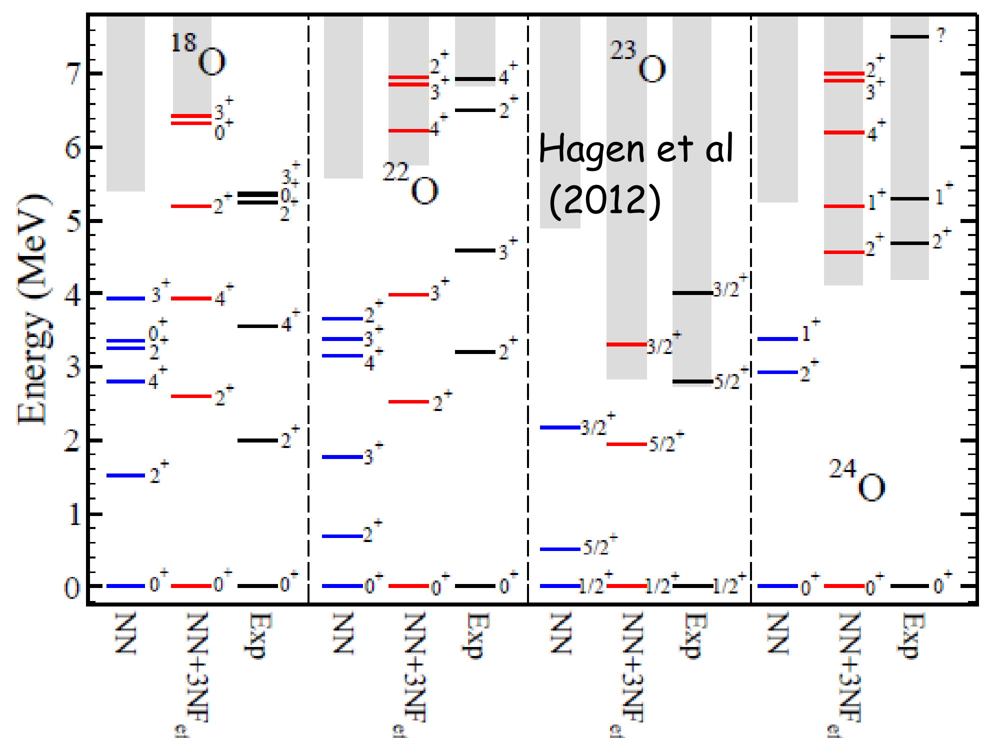
*coupling to the continuum is an essential feature of systems far from stability.
*taken into account by using the Berggren basis which includes bound, resonant and scattering states.

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).



Convergence pattern with the number of Lanczos iterations