Towards Optical Potentials from Coupled Cluster Calculations

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Collaborators:
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F. Nunes
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Theory for open-shell nuclei near the limits of stability, MSU, May 11-29 2015

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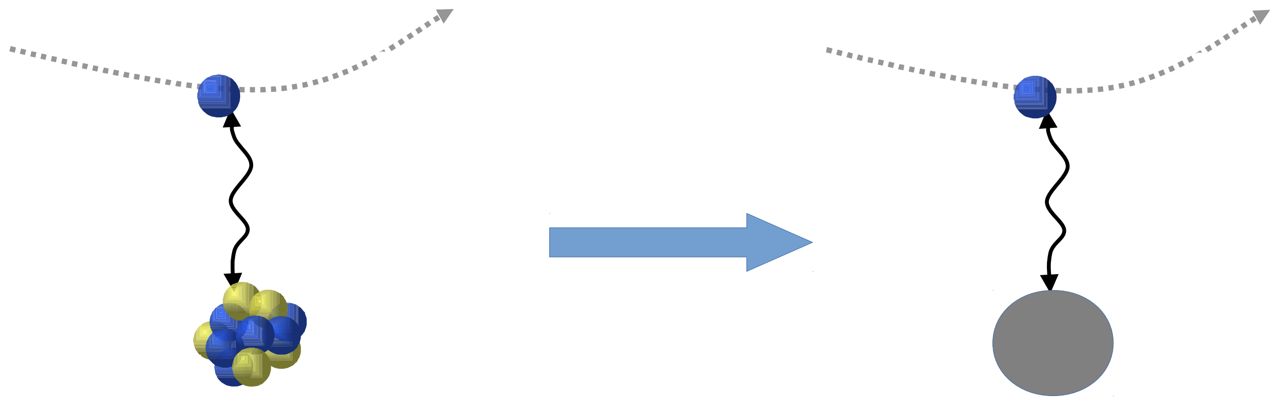
Theory for open-shell nuclei near the limits of stability, MSU, May 11-29 2015

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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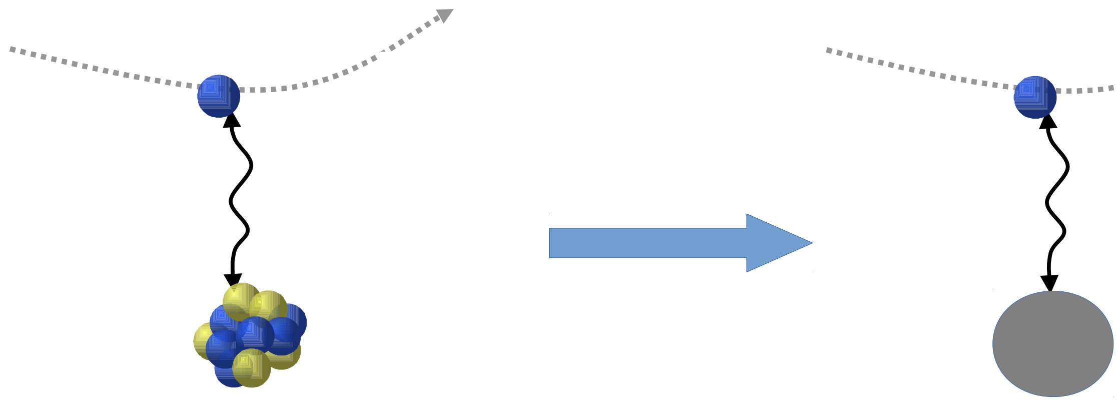
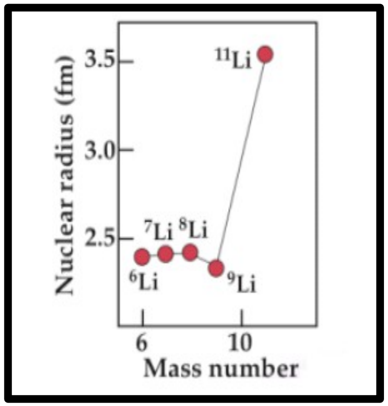


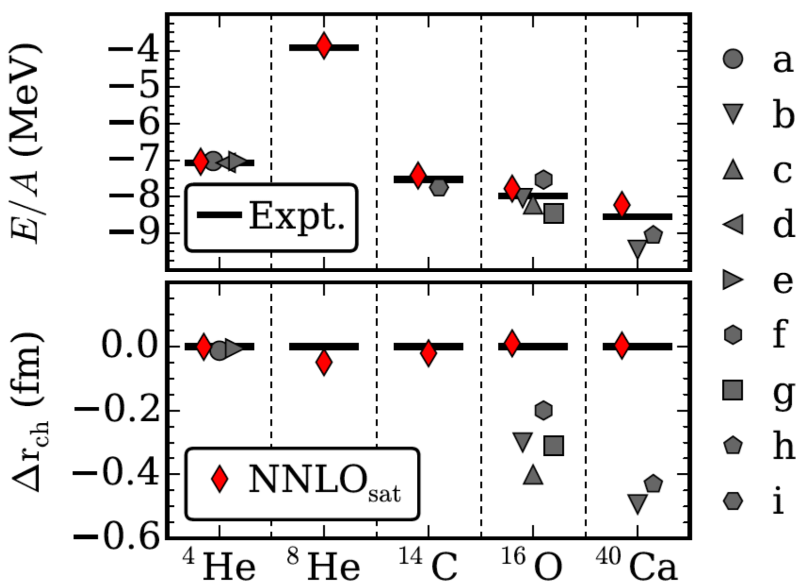
$$H|\Psi(1,\ldots,A)\rangle = E|\Psi(1,\ldots,A)\rangle \qquad H^{eff}|\Psi'(\vec{r})\rangle = E|\Psi'(\vec{r})\rangle$$

* predictive theory for nuclear reactions
* reliable/accurate extrapolations for systems far from stability.



Our approach:

Coupled Cluster combined with the Green's function method



Coupled Cluster calculations of g.s. energies and charge radii (taken from A. Ekström et al, 2015)

Other approaches:

Phenomenological potentials, Dispersive Optical Model (see talk by M.H. Mahzoon), Green's function, Gorkov-Green's function, No-Core Shell Model with continuum, full-folding optical potentials....

Green's function

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

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

<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 :

$$\boxed{E \le \epsilon_F^-}$$

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

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

$$\boxed{E \ge \epsilon_F^+}$$

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

Dyson equation

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

Irreducible self-energy = Optical potential

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

$$\boxed{\xi^c_{E+}(r) = \langle\Psi^A_0|a_r|\Psi^c_{E+}\rangle}$$

eigensolution of the one-body Schrödinger
equation with the irreducible energy.

Our approach : calculate the Greens' function with the Coupled cluster approach
and then extract the optical potential.

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

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

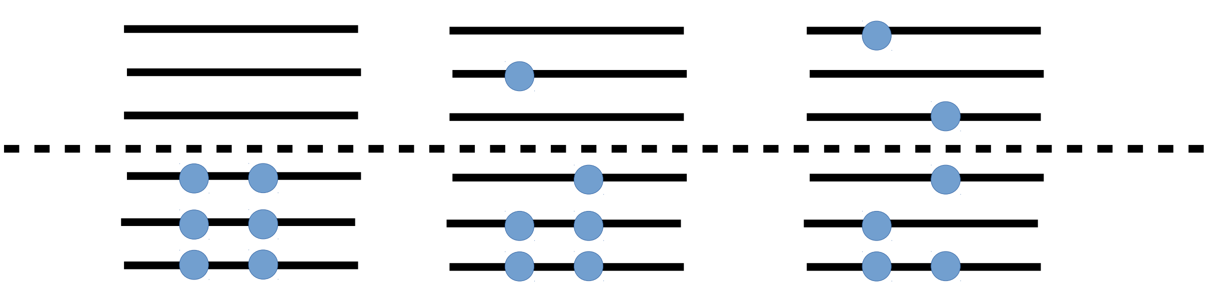
1p-1h operator

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

2p-2h operator

Coupled-cluster equations

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

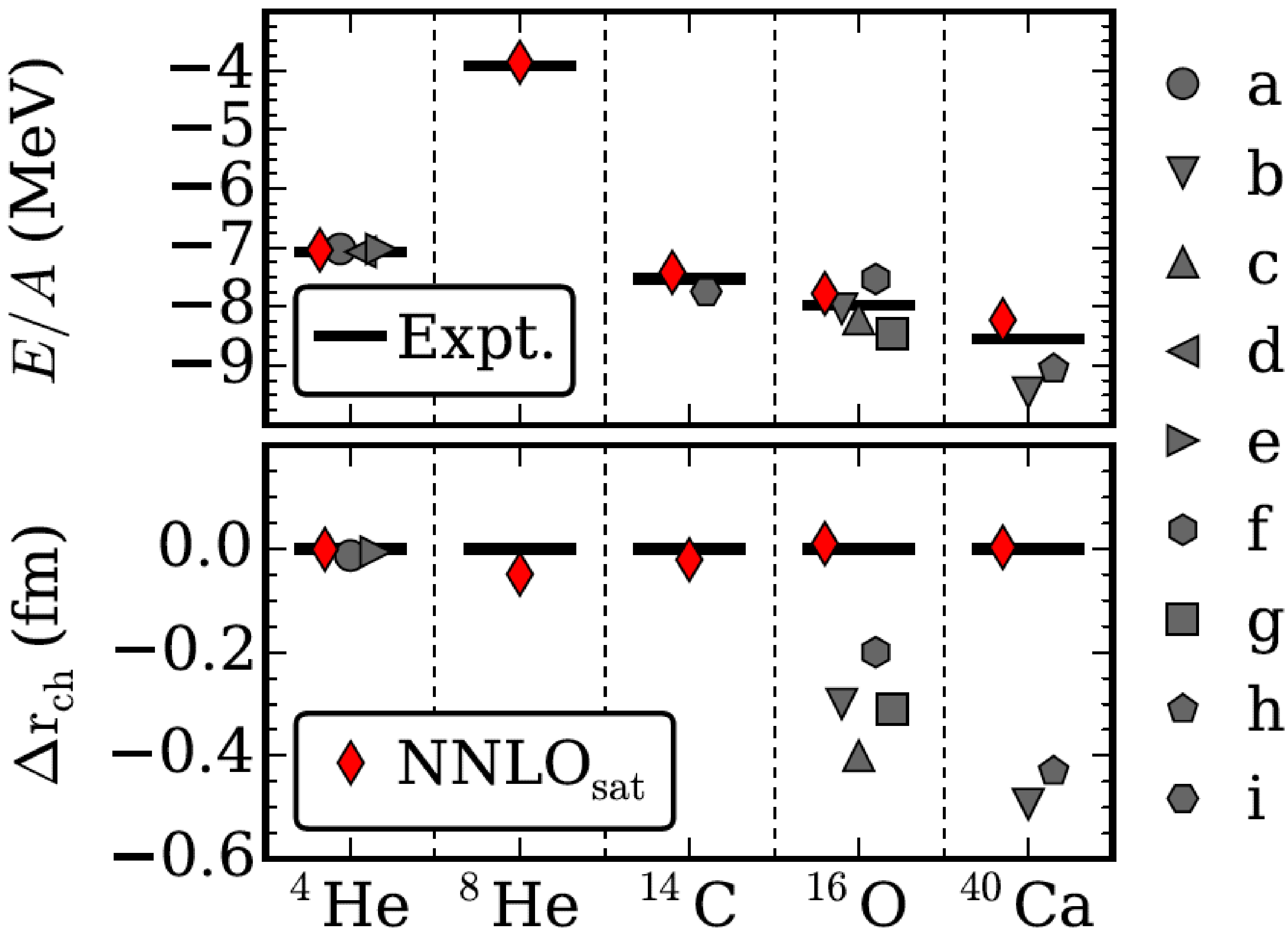


$|\Phi\rangle$ 1p-1h 2p-2h

Coupled cluster (ii)

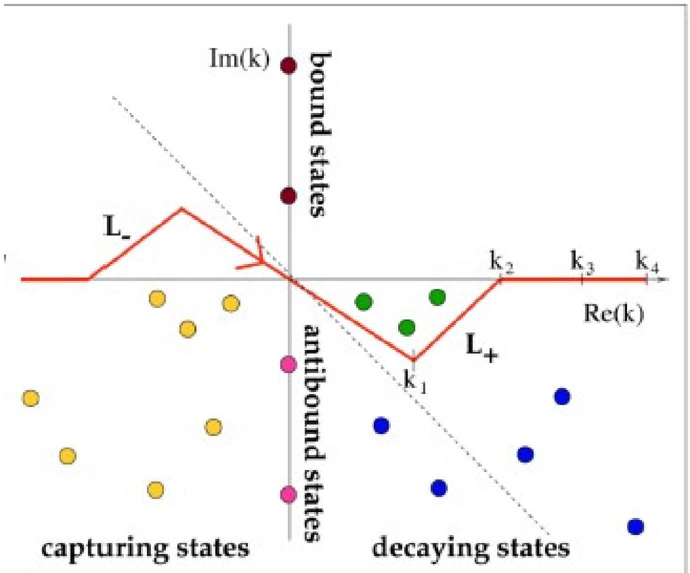
Accurate binding energies and radii from a chiral interaction

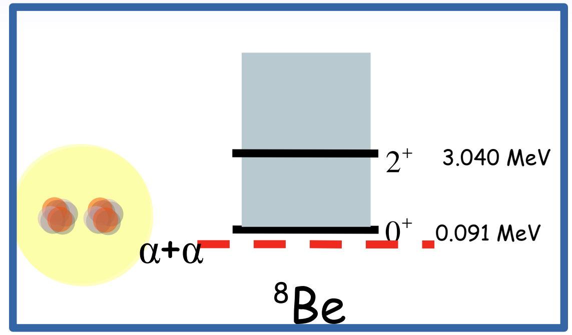
A. Ekström, G. R. Jansen, K. A. Wendt, G. Hagen, T. Papenbrock, B. D. Carlsson, C. Forssén, M. Hjorth-Jensen, P. Navrátil and W. Nazarewicz (2015)



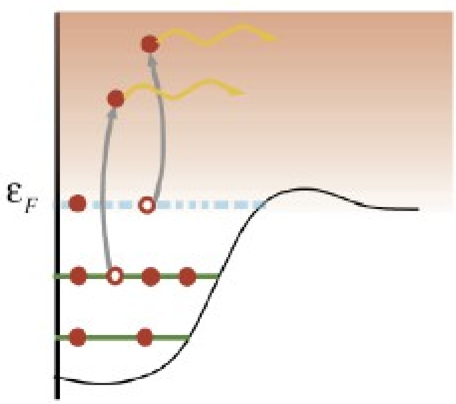
Coupled cluster (iii)

Physics of nuclei at the edges of stability

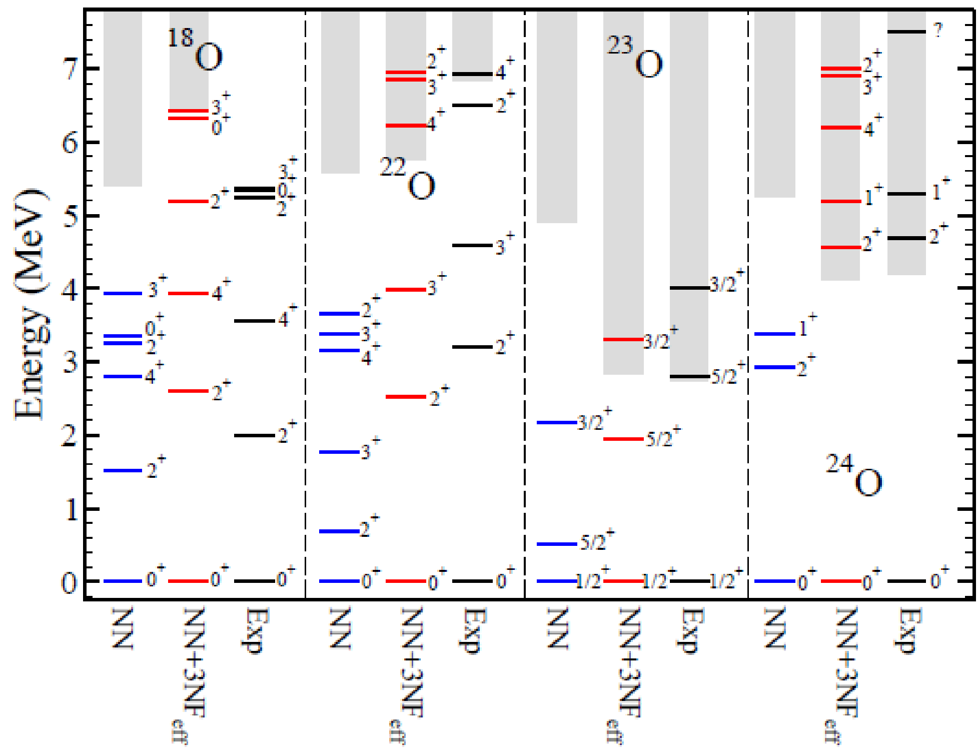




*coupling to the continuum is an essential feature of systems far from stability.
*taken into account by using the Berggren basis which includes bound, resonant and scattering states.



Hagen et al (2012)



(see also applications of the Berggren basis to nuclear systems in review by N. Michel et al (2009) and talks by G. Papadimitriou and K. Fossez)

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

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

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

Particle spectral function

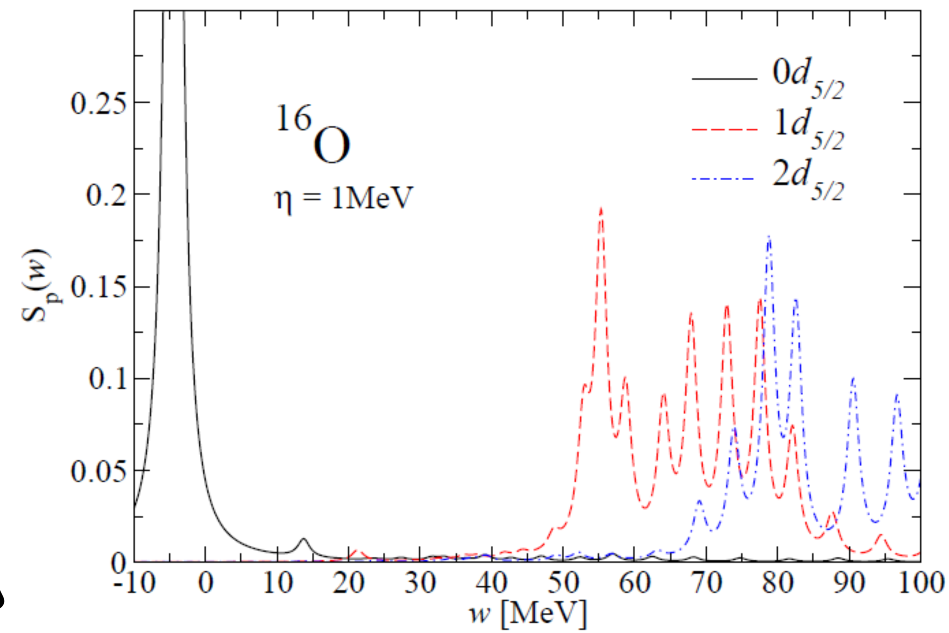
$$S_p(\alpha; E) = -\frac{1}{\pi}\mathrm{Im}\ G(\alpha, \alpha; E)$$

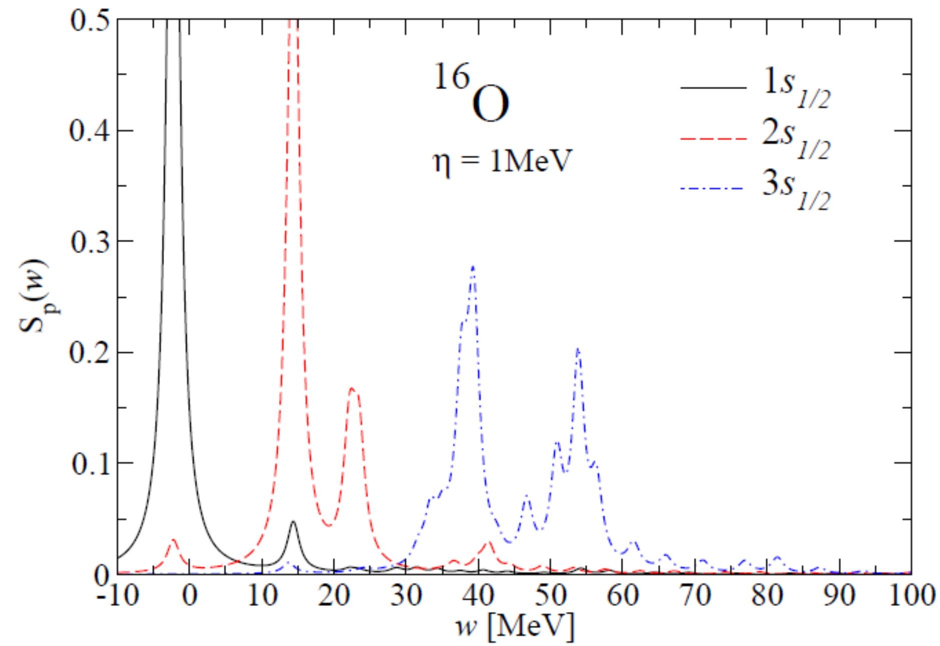
CCSD
Harmonic Oscillator basis:
N_{max} =10, hw=22 MeV.

Interaction : N^2LO_{opt}

(A. Ekström et al (2013))

Preliminary





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