Construction of microscopic optical potentials

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Optical potentials

Fig. 2. Comparison of predicted neutron total cross sections and experimental data, for nuclides in the Mg–Ca mass region, for the energy range 10 keV–250 MeV. For more details, see Section 4.1.

FIG. 5. The angular distribution of the differential cross section divided by the Rutherford cross section for elastic proton scattering from $^6$He, $^8$He, and $^{12}$C at 200 MeV laboratory kinetic energy as a function of the momentum transfer and the c.m. angle calculated with the NNLO optical chiral interaction [37]. The lines follow the same notation as Fig. 3. All calculations employ $\hbar! = 20$ with $N_{\text{max}} = 18$ for $^6$He, $N_{\text{max}} = 14$ for $^8$He and $N_{\text{max}} = 10$ for $^{12}$C. The data for $^6$He are taken from Ref. [49], and for $^{12}$C from Ref. [50].

Koning, Delaroche, NPA713, 231 (2002)
Fig. 1.1 Propagation of Drunken Man
(Reproduced with the kind permission of The Encyclopedia of Physics)

\[
P(2,1) = P_0(2,1) + P_0(A,1)P(A)P_0(2,A) + P_0(B,1)P(B)P_0(2,B) + \cdots
\]

\[
+ P_0(A,1)P(A)P_0(B,A)P(B)P_0(2,B) + \cdots.
\]
Green’s functions

\[ g_{\alpha\beta}(\omega + i\eta) = \sum_n \frac{\langle \psi_0^A|c_\alpha|\psi_n^{A+1}\rangle\langle \psi_n^{A+1}|c_\beta^+|\psi_0^A\rangle}{\omega - E_n^{A+1} + E_0^A + i\eta} \]

\[ + \sum_i \frac{\langle \psi_0^A|c_\alpha^+|\psi_i^{A-1}\rangle\langle \psi_i^{A-1}|c_\beta|\psi_0^A\rangle}{\omega - E_0^A + E_i^{A-1} - i\eta} \]

Unperturbed case

\[ g^0 (\omega + i\eta) = \sum_i \frac{1}{E - \epsilon_i^{base} \pm i\eta} \]
Green’s functions

\[ g_{\alpha\beta}(\omega + i\eta) = \sum_n \frac{\langle \psi_0^A | c_\alpha | \psi_n^{A+1} \rangle \langle \psi_n^{A+1} | c_\beta^+ | \psi_0^A \rangle}{\omega - E_n^{A+1} + E_0^A + i\eta} + \sum_i \frac{\langle \psi_0^A | c_\alpha^+ | \psi_i^{A-1} \rangle \langle \psi_i^{A-1} | c_\beta | \psi_0^A \rangle}{\omega - E_0^A + E_i^{A-1} - i\eta} \]

Unperturbed case

\[ g^0(\omega + i\eta) = \sum_i \frac{1}{E - \epsilon_i^{base} \pm i\eta} \]

self-consistent Green’s functions method finds spectra of the Hamiltonian operator

\[ H(A) = T - T_{c.m.}(A + 1) + V + W \]
Green’s functions as many-body method

Dyson Equation

\[ g(\omega + i\eta) = g^0(\omega + i\eta) + g^0(\omega + i\eta)\Sigma^*(\omega + i\eta)g(\omega + i\eta) \]

“Dressed” (with correlation)

\[ H(A) = T - T_{c.m.}(A + 1) + V + W \]
Green’s functions as many-body method

Dyson Equation

\[ g(\omega + i\eta) = g^0(\omega + i\eta) + g^0(\omega + i\eta)\Sigma^*(\omega + i\eta)g(\omega + i\eta) \]

“Dressed” (with correlation)

Particle Propagator

Interaction between the particle and the system (physical choice)

Fragments and changes energy of the “bare” state

\[ \Sigma_{\alpha\beta}(\omega + i\eta) = \sum_r \frac{m^r_{\alpha}m^r_{\beta}}{\omega - E_r + i\eta} \]
Nucleon elastic scattering

The irreducible self-energy is a nucleon-nucleus optical potential*

\[ \Sigma^*_\alpha\beta (r, r'; \omega) = \Sigma^{\infty}_{\alpha\beta} + \sum_i \frac{m^i_\alpha m^{i*}_\beta}{\omega - \epsilon_i \pm i\eta} \]

correlated mean-field

resonances beyond mean-field

\[ \Sigma^{\infty} \]

\[ \Sigma^{A+1} \]

\[ \Sigma^{A-1} \]

This provides *consistent* many-body and scattering wave functions

Green’s functions as optical potentials

Dyson Equation

\[ g(\omega + i\eta) = g^0(\omega + i\eta) + g^0(\omega + i\eta)\Sigma^*(\omega + i\eta)g(\omega + i\eta) \]

Equation of motion

\[ \left( E + \frac{\hbar^2}{2m} \nabla^2 \right) g(r, r'; E, \Gamma) = \delta(r - r') + \int dr'' \Sigma^*(r, r''; E, \Gamma)g(r'', r; E, \Gamma) \]

Corresponding Hamiltonian

\[ H(r, r') = -\frac{\hbar^2}{2m} \nabla_r^2 + \Sigma^*(r, r'; E, \Gamma) \]

\( \Sigma \) corresponds to the Feshbach’s generalized optical potential
Why optical potentials?

- Optical potentials **reduce many-body complexity** decoupling structure contribution and reactions dynamics.
- Often fitted on elastic scattering data (locally or globally)

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**1 particle transfer**

A.I. et al. PRC 92, 031304 (2015)

Koning, Delaroche, NPA713, 231 (2002)
Green functions and Dyson equation

\[ g_{\alpha\beta}(\omega) = g_{\alpha\beta}^0(\omega) + \sum_{\gamma\delta} g_{\alpha\gamma}^0(\omega) \Sigma_{\gamma\delta}^*(\omega) g_{\delta\beta}(\omega) \]

HF

ADC(1)

\[ \sum^* \]

\[ = \sum_{\gamma\delta} \]

Faddeev RPA

ADC(3)

Particle hole 'polarization' propagator (ph-RPA)

Particle-particle (pp-RPA) two-body correlation 'ladder' propagator
Källén–Lehmann spectral representation

\[ H(A) = T - T_{c.m.}(A + 1) + V + W \]

\[
g_{\alpha, \beta}(E, \Gamma) = \sum_n \frac{\langle \Psi_0^A | c_{\alpha} | \Psi_n^A+1 \rangle \langle \Psi_n^A+1 | c^\dagger | \Psi_0^A \rangle}{E - E_n^{A+1} + E_0^A + i\Gamma} + \sum_i \frac{\langle \psi_0^A | c^\dagger_{\alpha} | \Psi_n^{A-1} \rangle \langle \Psi_n^{A-1} | c_{\beta} | \Psi_0^A \rangle}{E - E_0^A + E_i^{A-1} + i\Gamma},
\]

Overlaps of A+1 and A-1 states

Excited states calculated from Dyson equation

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Volume integrals

\[ J^l_W(E) = 4\pi \int dr r^2 \int dr' r'^2 \text{Im} \sum_0^l \langle r, r' \rangle \langle E \rangle \]

\[ \Sigma_{n_a, n_b}^{\ell_j} (E) = \sum_r \frac{m_{n_a}^r m_{n_b}^r}{E - \varepsilon_r \pm i\eta} \]

Non local potential

\[ |J_W/A| (\text{MeV/A fm}^3) \]

\[ \begin{array}{c@{, }c}
40\text{Ca} & 40\text{Ca} \\
48\text{Ca} & 48\text{Ca} \\
52\text{Ca} & 52\text{Ca} \\
54\text{Ca} & 54\text{Ca} \\
60\text{Ca} & 60\text{Ca} \\
\end{array} \]

\[ E (\text{MeV}) \]

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Overlap function

\[ \Psi_i(r) = \sqrt{A} \int dr_1 \ldots dr_A \Phi^+_i(r_1, \ldots, r_{A-1}) \Phi_i(r_1, \ldots, r_A) \]

Proton particle-hole gap

EM results from A. Cipollone PRC 92, 014306 (2015)
- Solve Dyson equation in HO Space, find \( \Sigma_{n,n'}^{l,j*}(E) \)
- diagonalize in full continuum momentum space \( \Sigma^{l,j*}(k, k', E) \)

\[
\frac{k^2}{2\gamma m} \psi_{l,j}(k) + \gamma^3 \int dk' k'^2 \left( \Sigma_{n,n'}^{l,j*}(\gamma k, \gamma k', \gamma E) \right) \psi_{l,j}(k') = E \psi_{l,j}(k)
\]
$n + {}^{16}\text{O (g.s.)}$

Navrátíl, Roth, Quaglioni, PRC82, 034609 (2010)

Al, Barbieri, Navrátíl
PRL 123, 092501
NNLO_{sat} \quad n + ^{16}\text{O} \ (g.s. + exc)

<table>
<thead>
<tr>
<th>$\varepsilon \ (\text{MeV})$</th>
<th>$5/2^+$</th>
<th>$1/2^+$</th>
<th>$1/2^-$</th>
<th>$5/2^-$</th>
<th>$3/2^-$</th>
<th>$3/2^+$</th>
<th>$5/2^+$</th>
<th>$5/2^-$</th>
<th>$7/2^-$</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp.</td>
<td>-4.14</td>
<td>-3.27</td>
<td>-1.09</td>
<td>-0.30</td>
<td>0.41</td>
<td>0.94</td>
<td>3.23</td>
<td>3.02</td>
<td>3.54</td>
</tr>
<tr>
<td>NNLO_{sat}</td>
<td>-5.06</td>
<td>-3.58</td>
<td>-0.15</td>
<td>-1.23</td>
<td>-2.24</td>
<td>0.91</td>
<td>4.57</td>
<td>3.36</td>
<td>3.37</td>
</tr>
</tbody>
</table>

To conclude, we have benchmarked optical potentials $\text{NNLO}_{sat}$ in $n + ^{16}\text{O}$ elastic scattering. The table compares the experimental data (exp.) with the results from $\text{NNLO}_{sat}$. The $\text{NNLO}_{sat}$ calculations predict the deuteron transition energies well, capturing the observed resonances up to $7/2^-$.

The plots show the differential cross sections for neutron elastic scattering at different energies. The $\varepsilon$ values are derived from the differential cross sections, and the $\text{NNLO}_{sat}$ calculations agree well with the experimental data. The $\text{NNLO}_{sat}$ approach provides a promising description of complex resonance structures, especially beyond the neutron separation threshold in $^{44}\text{Ca}$. The chiral effective field theory used in the $\text{NNLO}_{sat}$ framework achieves a promising description of complex resonance structures, including diffraction minima that are consistent with the experimental data.
neutron elastic scattering from ab initio optical potential

\[ E_n = 3.286 \text{ MeV} \]

\[ E_n = 3.2 \text{ MeV} \]
We investigated this problem by computing total cross sections, comparing the energies of some representative bound and scattering states to the experimental data from $^{40}$Ca at 3.2 MeV. The minima are both predicted as bound states, although experimentally they are found inverted with the 3$^+_2$ resonances, measured between 0.41 and 0.94 MeV for this nucleus.

Note that there are more than 200 experimentally observed resonances, of which a small number correspond to excited states, close to the ones originating from Eq. (16). Broad resonances, measured between 1.55 and 2.82 MeV, that our SCGF calculations do not reproduce even to large energies, so it describes e.g. the different incident states, above the lowest one, for each partial wave.

FIG. 3. Differential cross section for neutron elastic scattering on $^{16}$O (and close to the experiment). The 3$^+_2$ are both predicted as bound states, although experimentally they are found inverted with the 5$^+_1$ resonances in the continuum. We calculate a narrow width for a 5$^+_1$ state, confirming the correct prediction of density matrix elements. The use of a saturating chiral interaction and compared to the empirical data from $^{40}$Ca, confirming the correct prediction of density matrix elements.
Conclusions

- We are developing an interesting tool to study nuclear reactions effectively: a non-local generalized optical potential corresponding to nuclear self energy.
- SCGF provide a rich description of low energy properties.
- \((p-h)\) correlations are related to absorption, \textit{that is missing}
Perspectives

- Use the information of SCGF in the continuum in other contexts: e.g. overlap functions for Knockout
- Explore the effect of different bases and bridge the Energy gap between spectator and GF expansions
- Enrich the description of correlations in ground and excited states: *multiconfiguration with projection*

Thanks to

**Surrey**
- C. Barbieri

**TRIUMF**
- P. Navrátil

**Lund**
- J. Ljungberg
- J. Rotureau
- G. Carlsson
Knockout Spectroscopic Factors

\[ \frac{k^2}{2m} \psi_{l,j}(k) + \int dk' k'^2 \left( \sum_{l,j}^1 (k, k', E) \right) \psi_{l,j}(k') = E \psi_{l,j}(k) \]

\[ SF = \left| \left\langle \Phi_n^{(A-1)} | \Phi_{g.s.}^A \right\rangle \right|^2 \]

Calculated from overlap wavefunctions

Open circles neutrons, closed protons

Separation Energy (MeV)

Spectroscopic Factor (%)
Overlap wavefunctions

\[ \langle A - 1 | A \rangle \]

\[ ^{14}\text{O} \ (1p_{1/2}) \]

\[ ^{16}\text{O} \ (1p_{3/2}) \]

\[ ^{22}\text{O} \ (1p_{3/2}) \]

\[ ^{16}\text{O} \ (2s_{1/2}) \ (\text{neutron}) \]

\[ r \ [\text{fm}] \]

Collaboration with C. Bertulani
Deviation of quasi-free \((p, pn)\) cross section calculation for different wavefunctions 
\[ (\sigma_{GF} - \sigma_{WS})/\sigma_{WS} \]

| Nucleus (state) | \(E_B\) [MeV] | \(\langle r^2\rangle_{WS}^{1/2}\) [fm] | \(\langle r^2\rangle_{GF}^{1/2}\) [fm] | \(C_{WS}\) [fm\(^{-1/2}\)] | \(C_{GF}\) | \(\sigma_{qf}^{WS}\) [mb] | \(\sigma_{qf}^{GF}\) [mb] | \(\sigma_{kn}^{WS}\) [mb] | \(\sigma_{kn}^{GF}\) [mb] | \(C^2 S_{GF}\) |
|----------------|-------------|----------------|----------------|----------------|---------|----------------|---------|----------------|---------|----------------|---------|
| \(^{14}\)O \((\pi 1p_{3/2})\) | 8.877 | 2.856 | 2.961 | 6.785 | 7.172 | 27.38 | 28.60 | 27.19 | 27.42 | 0.548 |

\(|\%\text{ deviation}|<1\%\)

\(|\%\text{ deviation}|5\%\)

Collaboration with C. Bertulani

18/06/2020

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Spectroscopic Factor (%) vs Separation Energy (MeV) for the Oxygen Chain:
- O14
- O16
- O22
- O24

The graph shows the spectroscopic factor (%) on the y-axis and the separation energy (MeV) on the x-axis.
The «Imaginary» Parameter

\[ \Gamma(E) = \frac{1}{\pi} \frac{a (E - E_F)^2}{(E - E_F)^2 - b^2} \]

\[ b = 22.36 \text{ MeV} \]

\(^{16}\text{O}(n,n)^{16}\text{O} \quad E_n=3.286 \text{ MeV} \]

\[
\begin{align*}
\text{d}\sigma/d\Omega \text{ (b/sr)} \\
\theta_{\text{c.m.}} \text{ (deg)}
\end{align*}
\]

- \(a=0.2\ \text{MeV}\) (purple)
- \(a=0.02\ \text{MeV}\) (cyan)
- \(a=0.002\ \text{MeV}\) (orange)

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\[
\delta \text{ (deg)}
\]

\[
E_{c.m.} \text{ (MeV)}
\]

For different values of \(N_{\text{max}}\):
- \(N_{\text{max}} = 7\)
- \(N_{\text{max}} = 9\)
- \(N_{\text{max}} = 11\)
- \(N_{\text{max}} = 13\)

\[
\delta \text{ (deg)}
\]

\[
E_{c.m.} \text{ (MeV)}
\]

For different values of \(d_{3/2}\):
- \(s_{1/2}\)
Different colors to different $l$

$$g_{\alpha \beta}(\omega) = \sum_i \frac{X^i_{\alpha} X^{i*}_{\beta}}{\omega - \epsilon_i \pm i\eta}$$
$^{40}\text{Ca} + n @ 3.2 \text{ MeV}$
Volume integrals

\[ J_{\mathcal{W}}^\ell (E) = 4\pi \int dr \ r^2 \int dr' \ r'^2 \text{Im} \ \Sigma_0^\ell (r, r'; E) \]

\[ J_{\mathcal{V}}^\ell (E) = 4\pi \int dr \ r^2 \int dr' \ r'^2 \text{Re} \ \Sigma_0^\ell (r, r'; E) \]

\[ \tilde{\Sigma}_{n_a, n_b}^{\ell, j} (E) = \sum_r \frac{m_{n_a}^r m_{n_b}^r}{E - \varepsilon_r \pm i\eta} \]

48 Ca protons |\( J_{\mathcal{W}}^\ell \)|

different Fermi energies and particle-hole gap for different interactions

\[ \text{Im} \{ \Sigma (\varepsilon_F) \} = 0 \]

S. Waldecker et al. PRC 84, 034616(2011)
Ca isotopes

neutron and proton volume integrals of self energies.
$^{16}$O and $^{24}$O

NNLO$_{sat}$ proton comparison

NNLO$_{sat}$ neutron comparison