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Ab initio optical potentials and nucleon scattering on medium mass nuclei

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Abstract. We show first results for the elastic scattering of neutrons off oxygen and calcium isotopes obtained from *ab initio* optical potentials. The potential is derived using self–consistent Green's function theory (SCGF) with the saturating chiral interaction NNLO_{sat}. Calculations are compared to available scattering data and show that it is possible to reproduce low energy scattering observables in medium mass nuclei from first principles.

1. Introduction

Recent years have seen considerable advances in the theory of optical potentials. Non locality effects have been shown to be crucial for describing three-body processes [1, 2], the importance of both scattering and bound states in the coupling to breakup channels has been explored [3], and global dispersive optical potentials have been developed [4].

The greatest challenge remains, however, the one of describing the nuclear structure and scattering consistently, from the same theory. Many-body Green's function methods are particularly suited to attempt this for medium and large nuclei since their central quantity, the self-energy, is naturally linked to the Feshbach theory of optical potentials [5, 6]. In particular, the particle part of the self-energy is equivalent to the original formulation of Feshbach, while its hole part describes the structure of the target [7]. Nuclear field theory is one of the first (semi phenomenological) attempts to build such a theory for atomic nuclei [8, 9] and it has been extended to nuclear transfer reactions [10, 11]. Another incarnation of Green's function related theories is the dispersive optical model (DOM) [12], which is a data driven formulation of global (local and non local) potentials constructed as the best possible parameterization of the microscopic self-energy [13, 4]. Finally, in the last years the nuclear structure method (NSM) followed by the authors of Ref. [14] obtained good reproduction of ^{40}Ca scattering based on the Gogny D1S interaction.

For transfer reactions, such as (d, p), it would be particularly important to have an optical potential that is deduced consistently from the same Hamiltonian used in the proton-neutron channel [2]. To do so, one needs *realistic* nuclear interactions and *ab initio* calculations of elastic nucleon-nucleus scattering. The no-core shell model with continuum (NCSMC) has been successful to calculate scattering and transfer reactions for light targets [15, 16, 17]. On the other hand, the self consistent Green's function (SCGF) formalism [18, 19] can calculate the *ab initio* optical potential directly even for havier nuclei. This approach has been used to calculate phase shifts [20] and to investigate analytical properties of DOMs [21]. However, these calculations were limited to two-body forces and a direct comparison to the experiment has been hindered by

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the lack of realistic interactions capable to reproduce accurately nuclear radii. Coupled cluster theory has also been recently employed [22], in combination with a Green function approach, to calculate phase shifts for ^{16}O.

Three-body interactions have been recently implemented for SCGF in [23, 24, 25]. Moreover, the introduction of the NNLO$_{\rm sat}$ interaction [26] has allowed a good reproduction of nuclear saturation and, hence, of radii and binding energies across the oxygen [27] and calcium chains [28]. Although this interaction has limitations regarding the symmetry energy in neutron rich nuclei, we are now in the position to make a meaningful comparison of first principle approaches to scattering data. Here, we perform state of the art SCGF calculations to test the quality of current *ab initio* methods and of the NNLO$_{\rm sat}$ Hamiltonian in predicting elastic scattering.

2. The microscopic optical potential

The irreducible self-energy, $\Sigma^\star(\omega)$, has the following general spectral representation,

$$\Sigma^\star_{\alpha\beta}(E) = \Sigma^{(\infty)}_{\alpha\beta} \; + \; \sum_{i,j} \mathbf{M}^\dagger_{\alpha,i} \left[\frac{1}{E - (\mathbf{K}^> + \mathbf{C}) + i\eta} \right]_{i,j} \mathbf{M}_{j,\beta}$$
$$+ \; \sum_{r,s} \mathbf{N}_{\alpha,r} \left[\frac{1}{E - (\mathbf{K}^< + \mathbf{D}) - i\eta} \right]_{r,s} \mathbf{N}^\dagger_{s,\beta} \; , \qquad (1)$$

where α and β label the single particle quantum numbers and $\Sigma^{(\infty)}$ is the correlated and energy independent mean field. We perform calculations with the third order algebraic diagrammatic construction [ADC(3)] method, where the matrices $\mathbf{M}$ ($\mathbf{N}$) couple single particle states to intermediate 2p1h (2h1p) configurations, $\mathbf{C}$ ($\mathbf{D}$) are interaction matrices among these configurations and $\mathbf{K}$ are their unperturbed energies [29, 30].

We use a spherical harmonic oscillator basis consisting of $N_{\rm max}$+1 oscillator shells, so the optical potential for a given partial wave (l, j) is expressed in terms of the oscillator radial functions $R_{n,l}(r)$ as

$$\Sigma^{\star\, l,j}(r, r'; E) = \sum_{n,n'} R_{n,l}(r)\, \Sigma^{\star\, l,j}_{n,n'}(E)\, R_{n',l}(r') \; , \qquad (2)$$

which is non local and energy–dependent. We solve the corresponding scattering problem in the full one-body space (so that, even if the many–body structure is described in a $N_{\rm max}$ oscillator space, the kinetic energy is treated exactly, without truncations) and account for the non locality and l, j dependence of Eq. (2). For each partial wave and parity, the phase shifts $\delta(E)$ are obtained as function of the projectile energy, from where the differential cross section is calculated. We will show results for incident energies in the laboratory frame, except for Fig. 6 below.

3. Results

In the following, we consider the volume integrals of the real (J_V) and imaginary (J_W) parts of the self-energy (i.e., the optical potential):

$$J_V(E) = \quad 4\pi \int {\rm d}r r^2 \int {\rm d}r' r'^2 \sum_{l,j} \Re e\{\Sigma^{\star\, l,j}(r, r'; E)\} \; , \qquad (3)$$
$$J_W(E) = \quad 4\pi \int {\rm d}r r^2 \int {\rm d}r' r'^2 \sum_{l,j} \Im m\{\Sigma^{\star\, l,j}(r, r'; E)\} \; , \qquad (4)$$

since these are strongly constrained by experimental data [6].

Fig. 1 shows the volume integrals of the neutron-^{16}O potential for different model space truncations. Both the part of the self-energy below the Fermi surface (which describes the

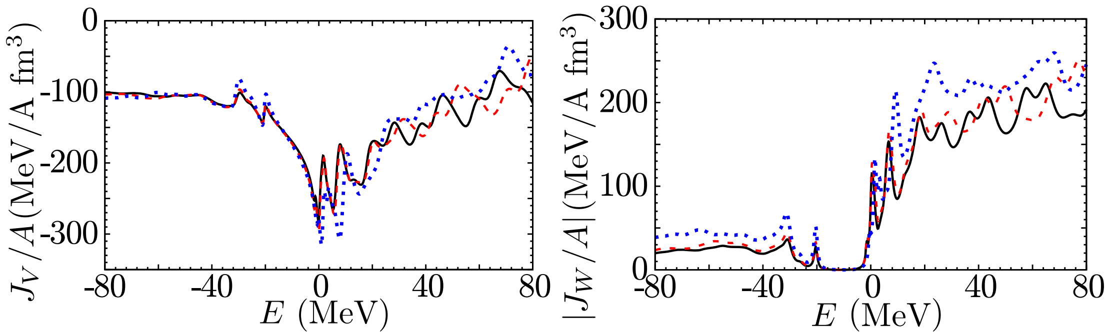

Figure 1. Volume integrals of the real (*left*) and imaginary (*right*) parts of the neutron-^{16}O optical potential calculated for different numbers oscillator shells in the model space: $N_{\rm max} = 7$ (dotted), 11 (dashed) and 13 (solid lines). Note that $\Im m\{\Sigma^\star(E{=}E_F)\}{=}0$, so $J_W(E{=}E_F){=}0$, where E_F is the Fermi energy. Thus, the potential for particle (holes) states is above (below) the gap in the J_W plot.

structure of the target) and the resonant structures for scattering at low energy are substantially converged already for $N_{\rm max}{=}11$. The oscillations seen at higher energies ($E >$10 MeV) are an artefact of using a discretized model space and keep changing with $N_{\rm max}$. They can fade away for an infinite space, or by exploiting an appropriate basis with continuum degrees of freedom.

Fig. 2 shows $|J_W|$ for neutron scattering on closed sub-shell Ca isotopes. The gap at the Fermi surface, where $\Im m\Sigma^\star(E){=}0$, shifts to higher energies and eventually crosses the continuum threshold with increasing neutron number. Compared to previous calculations using the Argonne v_{18} and N^{3}LO(500) interactions [21], the NNLO$_{\rm sat}$ predicts an increased level density in the proximity of the Fermi energy, as expected for a correct nuclear saturation.

In Fig. 3, the neutron $s_{1/2}$ and $d_{3/2}$ phase shifts for ^{16}O are shown for $N_{\rm max}{=}11$ and 13. In the $s_{1/2}$ case, the resonance at $E \approx$5 MeV changes by ≈ 0.5 MeV between the two spaces. Note that this state is dominated by 2p1h components and thus it can still be affected by many–body truncations. The wiggles computed for energies $E >$8 MeV are due to similar but very narrow resonances. Again, these are likely to be sensitive to the discretisation of the model space and drift when increasing the number of oscillator shells. On the contrary, in the $d_{3/2}$ case, the principal sharp resonance is dominated by pure single particle components, therefore it is well converged respect to the model space truncation $N_{\rm max}$. We calculate its energy to be ≈ 1.15 MeV in the c.o.m. frame, while the experimental value is 0.94 MeV.

Fig. 4 shows the phase shifts for other representative partial waves. The calculated $p_{1/2}$ and $p_{3/2}$ have both a sub-threshold bound state, although the $p_{3/2}$ is experimentally only observed in the continuum. We calculate a narrow $f_{7/2}$ resonance at 3.5 MeV close to the experimental one at 3.77 MeV (laboratory energy) [31]. Note however that there are other $f_{7/2}$ narrower resonances that are also seen experimentally lying at 1.65 and 3.01 MeV. In general, we find that NNLO$_{sat}$ predicts the location of dominant quasiparticle and holes states with a (conservative) accuracy of <2 MeV for this nucleus.

Wavefunctions can also be calculated by diagonalizing the self–energy in the continuum. Fig. 5, shows overlap wavefunctions for the addition and removal of a $p_{3/2}$ neutron to and from ^{16}O, as predicted by NNLO$_{sat}$ and SCGF.

Finally, Fig. 6 compares the differential cross section for the elastic scattering of neutrons off ^{40}Ca with the experiment at 13.56 MeV c.o.m. energy, with $N_{\rm max}{=}11$. Minima in the cross section are reproduced reasonably well, confirming the correct prediction of matter radii, but there appears to be a general lack of absorption. This may be due to either missing doorway configurations (3p2h and beyond) or to the (still crude) model space. Note that proton scattering

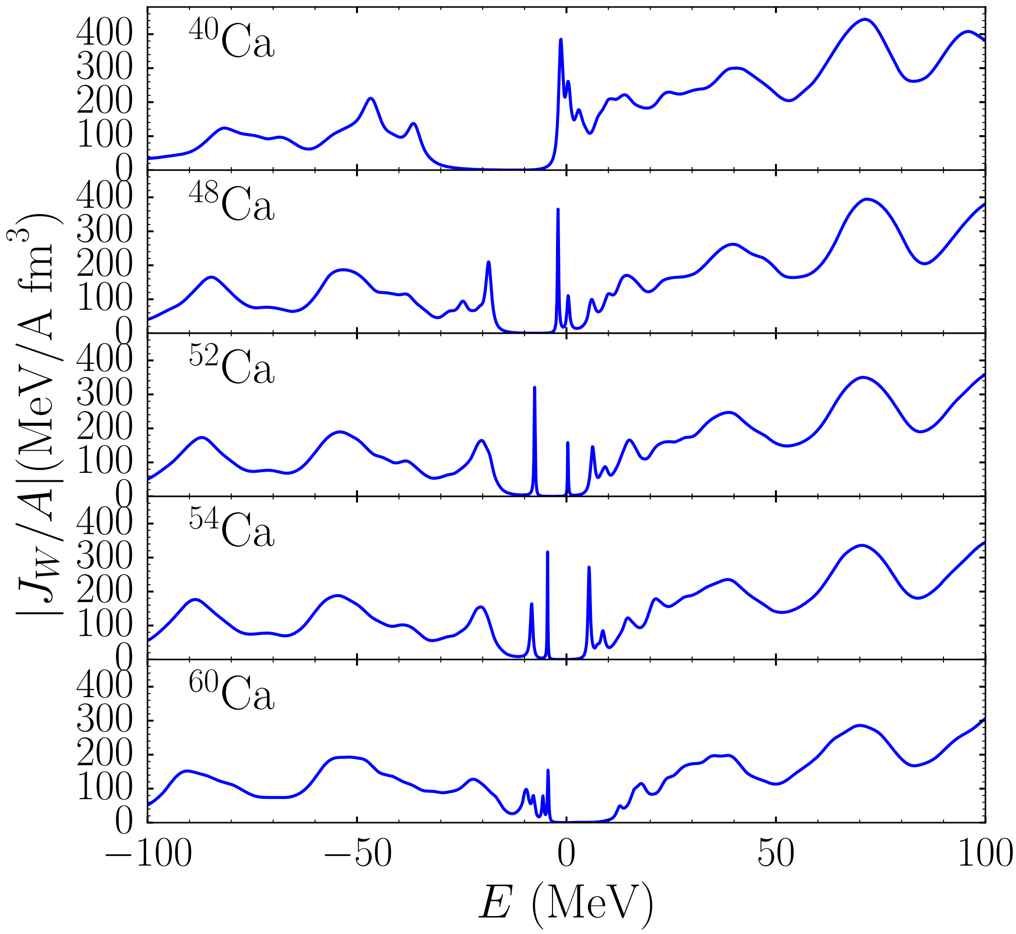

Figure 2. Volume integral of the imaginary part of the neutron optical potentials, $J_W(E)$, for targets at the subshell closure of calcium isotopes: ^{40}Ca, ^{48}Ca, ^{52}Ca, ^{54}Ca, ^{60}Ca, calculated at $N_{\max}$=11.

on ^{40}Ca was also computed in Ref. [32].

4. Conclusions

Even with the limitations of a (non optimal) oscillator basis, we found that most important features of optical potentials are well reproduced. In the long term, it will be necessary to properly account for the continuum in calculating the self-energy and to improve the realistic nuclear interactions. Nevertheless, it is clear from the present results that reliable *ab initio* calculations of optical potentials are now a goal within reach.

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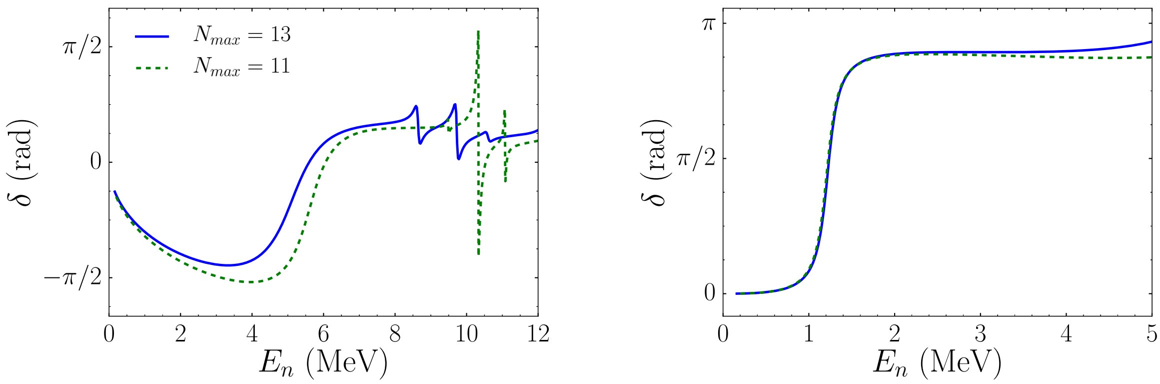

Figure 3. Nuclear phase shifts, $\delta(E)$, for neutrons scattering off ^{16}O as a function of the incident neutron energy. *Left panel*: $s_{1/2}$ partial wave phase shifts for $N_{\rm max}$=11 (dashed) and 13 (solid). All oscillations seen at energies above 8 MeV are calculated narrow resonances (originating form poles of the self-energy) and go through a full shift of π. *Right panel*: $d_{3/2}$ partial wave phase shifts for for $N_{\rm max}$=11 (dashed) and 13 (solid).

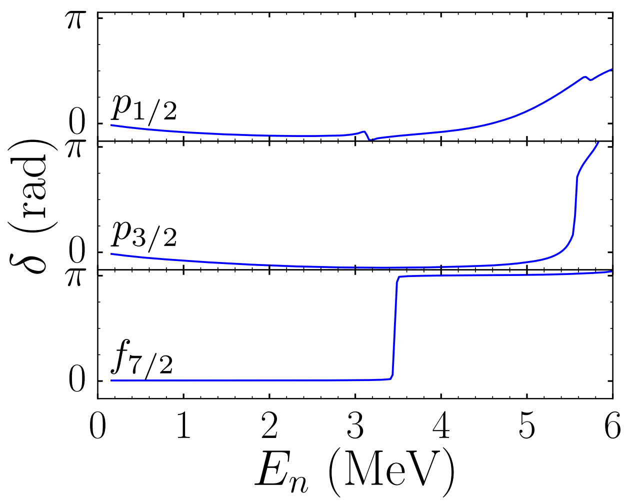

Figure 4. Nuclear phase shifts, $\delta(E)$, for scattering off ^{16}O as a function of the incident neutron energy for $p_{1/2}$, $p_{3/2}$, and $f_{7/2}$ partial waves. Experimental phase shifts from [31] (not shown on the figure) are qualitatively reproduced (e.g. the broad resonance of $p_{1/2}$) and the energy of narrow resonances is generally reproduced within 1 MeV. See also discussion the text.

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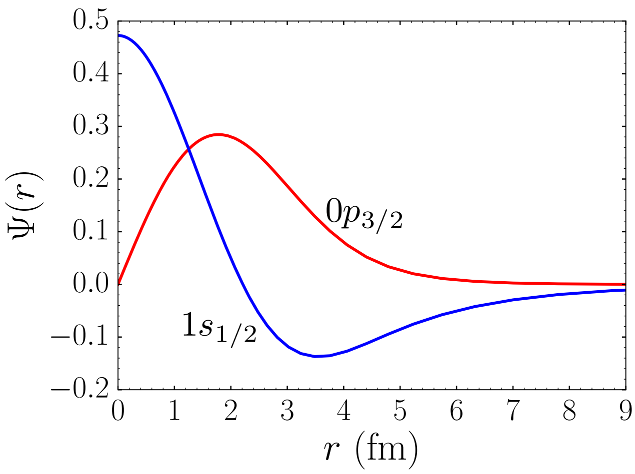

Figure 5. Radial nuclear overlap wave function for the neutron $s_{1/2}$ and $p_{3/2}$ states, obtained by diagonalizing the self energy in the exact continuum, without considering center of mass correction. The $0p_{3/2}$ hole state at -20.704 MeV (solid red line), is compared to the $1s_{1/2}$ particle state at -3.095 MeV. The spectroscopic factors are 0.80 and 0.86 respectively.

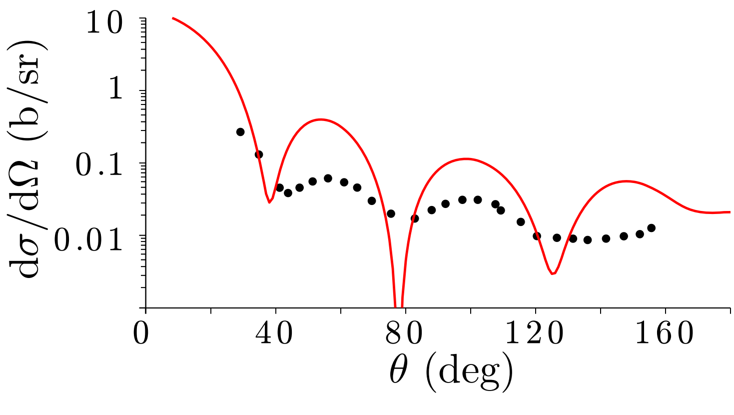

Figure 6. Plot of differential cross section for neutron elastic scattering on ^{40}Ca at 13.56 MeV of *center of mass energy* compared with experimental data from [33].

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