Ab initio optical potentials and nucleon scattering on medium mass nuclei

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We derive *ab initio* optical potentials from self-consistent Green's function (SCGF) theory and compute the elastic scattering of neutrons off oxygen and calcium isotopes. The comparison with scattering data is satisfactory at low scattering energies. The method is benchmarked against no-core shell model with continuum (NCSMC) calculations, showing that virtual excitations of the target are crucial to predict proper fragmentation and absorption at higher energies. This is a significant step toward deriving optical potentials for medium mass nuclei and complex many-body systems in general.

Introduction. Reactions are a fundamental aspect of nuclear physics since they are used experimentally to determine many properties of atomic nuclei. They are also a key component to significant scientific questions, such as the reaction networks that control nucleosynthesis. Unfortunately, first principles theoretical descriptions for scattering on medium-mass nuclei are still lacking. Even tough ground state properties and excited states can be calculated *ab initio*, the complexity of many-body dynamics forces us to model the reaction mechanisms in terms of phenomenological optical potentials. This lack of consistency among the structure and reaction theories has been a major issue for nuclear physics for decades.

Optical models are an effective way to decouple the scattering wave function of the projectile from the internal structure of the target. Thus, microscopic (non-phenomenological) formalisms have also been proposed to compute them [1, 2], although working implementations are still scarce. In this Letter, we discuss an *ab initio* calculation of optical potentials that starts from saturating nuclear forces and compares favourably with low-energy scattering data. In doing so, we also identify key ingredients needed to improve the predicability at higher energies. This represent a successful step toward gaining insight into the reaction dynamics and to perform reliable predictions of scattering with exotic nuclei.

Many-body Green's function methods are particularly suited to pursue this goal for medium and heavy nuclei since their central quantity, the self-energy, is naturally linked to the Feshbach theory of optical potentials [1, 3]. While the particle part of the self-energy is equivalent to the original formulation of Feshbach, its hole part also describes the structure of the target [4]. Hence, it facilitates a consistent treatment of scattering and structure, based on the same microscopic Hamiltonian.

Some related (semi–)phenomenological attempts to exploit Green's function methods include the nuclear field theory [5, 6] and its extension to nuclear transfer reactions [7, 8]. Another incarnation of Green's function related theories is the dispersive optical model (DOM) [9], which is a data driven formulation of global (local and non local) potentials constructed as the best possible parameterization of a microscopic self-energy [10, 11]. The nuclear structure method (NSM) was applied recently obtaining good reproduction of ^{40}Ca scattering based on the Gogny D1S interaction [12]. Other approaches, based on the nucleon-nucleon T-matrix and folding with the nuclear density have proven to be effective [13–16].

Ab initio methods have been successful in direct calculations of scattering when only few nucleons are at play. Green function Monte Carlo (GFMC) has been historically used for light nuclei [17, 18] and was recently applied to alpha–nucleon scattering exploiting chiral three–nucleon (3N) forces [19]. The no-core shell model with resonating group method (NCSM/RGM) or with continuum (NCSMC) have been successful in calculating scattering and transfer reactions for light targets [20–22]. Coupled cluster theory has also been employed with a Gamow basis for proton–^{40}Ca [23] and combined with a Green's function approach to compute phase shifts for ^{16}O [24, 25]. On the other hand, the self-consistent Green's function (SCGF) formalism [26, 27] can calculate the microscopic optical potential directly even for heavier nuclei. This approach has been used to compute phase shifts [28] and to investigate analytical properties of DOMs [29]. However, these early studies were limited to two-nucleon (NN) forces and a comparison to the experiment has been hindered by the lack of realistic Hamiltonians capable to reproduce the radius of the target.

Three-body interactions have been recently formulated and implemented for SCGF theory in [30–32]. Moreover, the introduction of saturating nuclear interactions [33] has allowed a good reproduction of radii and binding energies across the oxygen [34] and calcium chains [35]. Hence, we are now in the position to meaningfully compare first principle approaches to scattering data in medium-mass nuclei. In the following, we perform state of the art SCGF calculations to test the quality of current *ab initio* methods by comparing to NCSM/RGM and NCSMC results with NN interactions. We will then use

a saturating chiral Hamiltonian with full NN+3N forces to study elastic scattering of neutrons on ^{16}O and ^{40}Ca.

Formalism. The Hamiltonian used to compute the self-energy is

$$H(A) = \hat{T} - \hat{T}_{c.m.}(A+1) + \hat{V} + \hat{W} \tag{1}$$

where $\hat{T}_{c.m.}(A+1)$ is the center of mass kinetic energy for the A-nucleon target plus the projectile and $\hat{V}$ and $\hat{W}$ are the NN and 3N interactions. $\hat{W}$ is included as an equivalent effective two–body interaction, averaged on the correlated propagator as discussed in Refs. [31, 36]. The SCGF calculation proceeds by solving the Dyson equation $g(\omega) = g^0(\omega) + g^0(\omega)\Sigma^\star(\omega)g(\omega)$ in an harmonic oscillator (HO) basis of $N_{\max}$+1 shells, where $g^0(\omega)$ is the free particle propagator and the irreducible self-energy $\Sigma^\star(\omega)$ has the following general spectral representation:

$$\Sigma^\star_{\alpha\beta}(E,\Gamma) = \Sigma^{(\infty)}_{\alpha\beta} + \sum_{i,j} \mathbf{M}^\dagger_{\alpha,i} \left[\frac{1}{E - (\mathbf{K}^> + \mathbf{C}) + i\Gamma} \right]_{i,j} \mathbf{M}_{j,\beta} + \sum_{r,s} \mathbf{N}_{\alpha,r} \left[\frac{1}{E - (\mathbf{K}^< + \mathbf{D}) - i\Gamma} \right]_{r,s} \mathbf{N}^\dagger_{s,\beta} \,. \tag{2}$$

In Eq. (2), α and β label the single particle quantum numbers of the HO basis and $\Sigma^{(\infty)}$ is the correlated and energy independent mean field. We performed 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 [37, 38]. All intermediate 2p1h and 2h1p states (respectively labelled by indices i, j and r, s) were included in our calculations. For $N_{\max} = 13$, this corresponds configurations up to about 400 MeV of excitation energy and partial waves of the projectile up to angular momentum $j = 27/2$ for both parities.

The resulting dressed single particle propagator can be written in the Lehmann representation as

$$g_{\alpha,\beta}(E,\Gamma) = \sum_n \frac{\langle \Psi^A_0 | c_\alpha | \Psi^{A+1}_n \rangle \langle \Psi^{A+1}_n | c^\dagger_\beta | \Psi^A_0 \rangle}{E - E^{A+1}_n + E^A_0 + i\Gamma} + \sum_k \frac{\langle \psi^A_0 | c^\dagger_\alpha | \Psi^{A-1}_k \rangle \langle \Psi^{A-1}_k | c_\beta | \Psi^A_0 \rangle}{E - E^A_0 + E^{A-1}_k - i\Gamma} \,. \tag{3}$$

The poles of the forward-in-time propagator, $E^{A+1}_n - E^A_0$, indicate then the energy of the nth exited state of the $(A+1)$-nucleon system with respect to the ground state of the target A. Hence, they are directly identified with the scattering energy. For each many-body state $|\Psi^{A+1}_n\rangle$ in the continuum, the corresponding overlaps $\psi_n(\alpha) \equiv \langle \Psi^{A+1}_n | c^\dagger_\alpha | \Psi^A_0 \rangle$ are associated with the elastic scattering wave function through Feshbach theory [1, 2].

Although the scattering waves are unbound and they cannot be efficiently expanded in oscillator basis, the self-energy $\Sigma^\star(\omega)$ is associated with the optical potential and it is localized. Thus, we proceed by calculating Eq. (2) in HO basis and transform it to momentum space before solving the scattering problem. This will ensure that the proper asymptotic behaviours of both bound and scattering states are obtained. The optical potential for a given partial wave (l, j) is then expressed as

$$\Sigma^{\star\, l,j}(k,k';E,\Gamma) = \sum_{n,n'} R_{n,l}(k)\, \Sigma^{\star\, l,j}_{n,n'}(E,\Gamma)\, R_{n',l}(k') \,, \tag{4}$$

which is non local and energy-dependent and where $R_{n,l}(k)$ are the radial HO wavefunctions in momentum space. Through Eqs. (2) and (4), the SCGF approach provides a parametrized, separable and analytical form of the optical potential.

The parameter Γ sets the time ordering boundary conditions, but it does not affect the solution of the many-body problem that comes from the diagonalization of the equation of motion [6, 28, 38]. However, we retain it in Eq. (4) to introduce a small finite width for the 2p1h/2h1p configurations, which would otherwise be discretised in the present approach. We checked that this does not affect our conclusions below.

We use the intrinsic Hamiltonian of Eq. (1) and large enough HO spaces so that the intrinsic ground state decouples from the center of mass motion [39]. Even if decoupled, the latter is not fully suppressed and the self-energy (4) is still computed in laboratory frame. We correct for this by rescaling the scattering momentum appropriately, which naturally leads to the correct center of mass energy $E_{c.m.}$ and reduced mass $\mu = \gamma m$, with $\gamma \equiv A/(A+1)$. The Dyson equation eventually reduces to the following one-body eigenvalue problem [26, 38]:

$$\left[E_{c.m.} - k^2/(2\mu)\right] \psi_{l,j}(k) = \int \mathrm{d}k' k'^2 \gamma^3 \, \Sigma^{\star\, l,j}(\gamma k, \gamma k'; \gamma E_{c.m.}, \Gamma)\, \psi_{l,j}(k'), \tag{5}$$

We diagonalize this Schrödinger–like equation in momentum space so that the kinetic energy is treated exactly–without truncations in HO space–and we account for the non locality and l, j dependence of Eq. (4). 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 can be calculated. The bound states solutions of Eq. (5) yields overlap wave functions between $|\Psi^A\rangle$ and $|\Psi^{A+1}\rangle$ [40]. Hence, they provide spectroscopic factors and asymptotic normalization coefficients that can be employed for the consistent computation of nucleon absorption and knockout processes.

Results. We first compare to the NCSM/RGM results from Ref. [20], where neutron scattering off ^{16}O was computed with a NN-only interaction derived from the chiral N^{3}LO force of Ref. [41] (EM500) and evolved with free space similarity renormalization group (SRG) [42] to a cutoff $\lambda = 2.66$ fm^{-1}. These early NCSM/RGM computations did not include virtual excitations of the

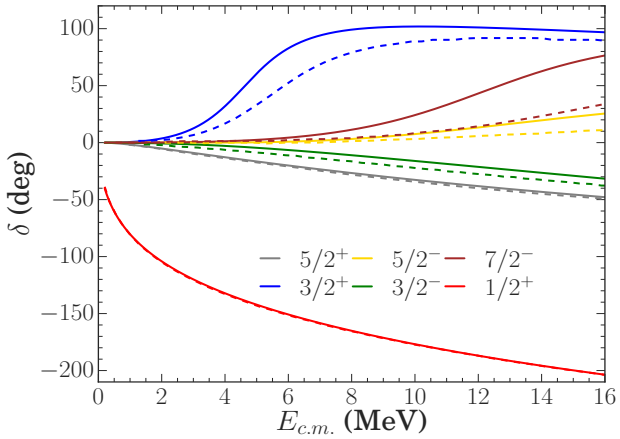

FIG. 1. (Color online) Real part of nuclear phase shifts, $\delta(E_{c.m.})$, for neutrons scattering off ^{16}O as a function of energy obtained from the EM500-SRG interaction in a model space of HO frequency $\hbar\Omega = 24$ MeV. The calculation using only the static part of the self energy $\Sigma^{(\infty)}$ (solid lines) are compared with the NCSM/RGM of Ref. [20] (dashed lines), which included only the ground state of ^{16}O and used a no-core model space up to $N_{\rm NCSM} = 18\hbar\omega$.

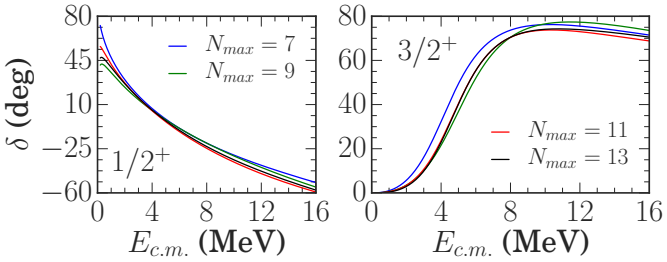

FIG. 2. (Color online) Phase shifts, $\delta(E_{c.m.})$, for neutron scattering off ^{16}O in the $s_{1/2}$ (left panel) and $d_{3/2}$ (right panel) partial waves. The sole static self-energy, $\Sigma^{(\infty)}$, was used with the NNLO$_{\rm sat}$ interaction. Different model spaces with frequency $\hbar\Omega$= 20 MeV and sizes $N_{\rm max} = 7$ to 13 are shown.

target nucleus. Consistently, we performed our SCGF calculations with the same Hamiltonian but evaluated the phase shifts using only the static self-energy, $\Sigma^{(\infty)}$. The comparison is shown in Fig. 1 and it is very satisfactory for the $j^\pi = 1/2^+$ and $5/2^+$ partial waves. For this light nucleus, the discrepancy of about 1 MeV for the energy of the $3/2^+$ resonance is also consistent with the uncertainty in the transformation to the center of mass system done in Eq. (5). As we discuss below, doorway excitations of the target ground state have a strong impact on the energies of single particle resonances. To account for this, we performed new NCSMC calculations that can also include low-lying excitations of ^{16}O. Extrapolating from model spaces of $N_{\rm max} = 6 - 10$ we find quasiparticle energies of -3.4, -2.7, and 3.2 MeV for the $5/2^+, 1/2^+$ bound states and the $3/2^+$ resonance, respectively. The corresponding results from SCGF, including the full $\Sigma^\star(\omega)$ self-energy, are -6.3, -5.5, and 0.5 MeV. These should be expected to be more bound since SCGF introduces a larger number of 2p1h doorway configurations. At the same, time the excitation energies relative to the ^{17}O ground state agree to within 200 keV, which is a satisfactory agreement given the different many-body truncations of the two approaches.

We now turn to the chiral NNLO$_{\rm sat}$ NN+3N interaction from Ref. [33], wich was constructed to reproduce correct nuclear saturation properties of medium mass nuclei, including binding energies and radii. The constraint on radii is crucial to predict elastic scattering observables that can be reasonably compared to the experiment. Fig. 2 demonstrates phase shifts for the $s_{1/2}$ and $d_{3/2}$ partial waves using the sole static self-energy $\Sigma^{(\infty)}$. These converge well with respect to the truncation in the number of oscillator shells $N_{\rm max}$ up to 15 MeV, akin to what was found for the SRG-EM500 case in Ref. [20].

Virtual excitations of the target have the double effect of increasing the attraction of the real part of the optical potential (hence, lowering the single particle spectrum) and of generating a large number of narrow resonances. This is clearly seen in Figs. 3 that displays the phase shifts for neutron elastic scattering predicted by the whole self-energy of Eq. (2). Most of the virtual excitations responsible for this, especially at low energy, are accessed by coupling to hundreds of 2p1h configurations for ^{17}O. The SCGF-ADC(3) approach has the advantage of including these states naturally, even to large energies energies, so it describes efficiently the relevant physics.

Table I compares the energies of some representative bound and scattering states to the experiment. The $d_{3/2}$ single particle resonance is computed at 0.91 MeV in the c.o.m. frame, very close the experimental value. The first $p_{1/2}$ and $p_{3/2}$ are both predicted as bound states, although experimentally they are found inverted with the $p_{3/2}$ in the continuum. We calculate a narrow width for a $f_{5/2}$ and a $f_{7/2}$ resonances, corresponding to excited states, close to the ones observed at 3.02 and 3.54 MeV [44]. However, there are other very narrow f-wave resonances, measured between 1.55-2.82 MeV, that our SCGF calculations do not resolve. In general, we find that NNLO$_{\rm sat}$ predicts the location of dominant quasi-

ε (MeV)	$5/2^+$	$1/2^+$	$1/2^-$	$5/2^-$	$3/2^-$	$3/2^+$	$5/2^+_*$	$5/2^-_*$	$7/2^-_*$
exp.	-4.14	-3.27	-1.09	-0.30	0.41	0.94	3.23	3.02	3.54
NNLO$_{\rm sat}$	-5.06	-3.58	-0.15	-1.23	-2.24	0.91	4.57	3.36	3.37

TABLE I. Excitation spectrum of ^{17}O with respect to the ^{16}O+n threshold, as obtained from Eq. (5) and the NNLO$_{\rm sat}$ interaction and compared to the experiment [43]. Broad resonances in the continuum (most notably, the $5/2^+$) are evaluated at midpoint. The asterisks ($_*$) indicate higher excited states, above the lowest one, for each partial wave.

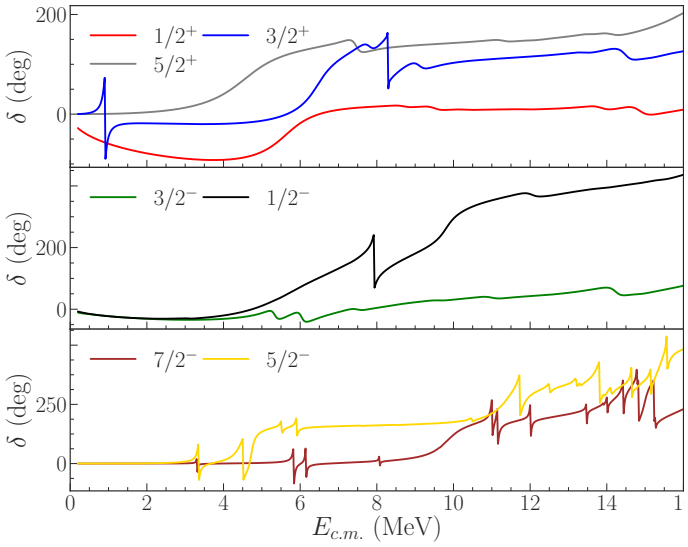

FIG. 3. (Color online) Real phase shifts, $\delta(E_{c.m.})$, for neutrons scattering off ^{16}O using the complete self-energy, $\Sigma^{(\infty)} + \widetilde{\Sigma}(\omega)$, and NNLO$_{\rm sat}$. Positive parity (upper panel), p (central panel) and f partial waves (lower panel) are shown.

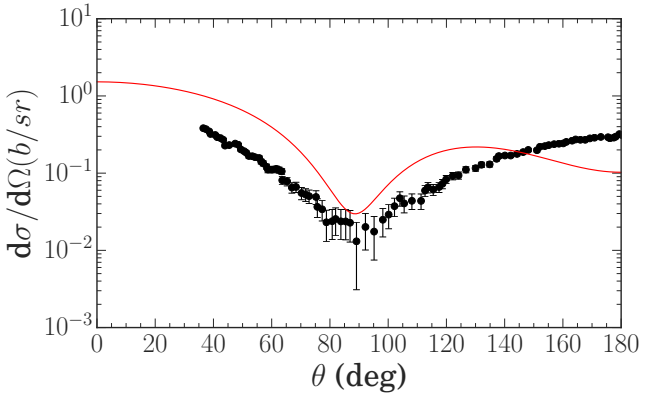

FIG. 4. (Color online) Differential cross section for neutron elastic scattering on ^{16}O at 3.286 MeV of neutron energy, with NNLO$_{\rm sat}$ and compared with experimental data from [44].

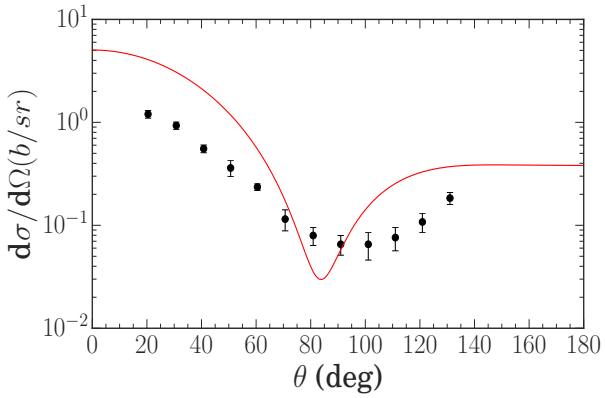

FIG. 5. (Color online) Differential cross section for neutron elastic scattering on ^{40}Ca at 3.2 MeV of neutron energy, with NNLO$_{\rm sat}$ and compared with experimental data from [47].

particle and holes states with an accuracy of $\lesssim 1$ MeV for this nucleus.

We also computed the differential cross sections for neutron scattering using Eq. (5). These are compared to the data for n+^{16}O at 3.258 MeV and n+^{40}Ca at 3.2 MeV in Figs. 4 and 5, respectively. The minima in the cross sections are well reproduced, confirming the correct prediction of the density distribution from NNLO$_{\rm sat}$ [33, 35, 45]. However, there appears to be some lack of absorption that is related to missing doorway configurations (3p2h and beyond) and it is bound to increase with scattering energy. Note that there are more than 200 experimentally observed excitations between the ground state and the neutron separation threshold in ^{41}Ca [46], while the SCGF-ADC(3) predicts only about 40 of them. Since dominant low-lying quasiparticle energies are already predicted close to the empirical value at the ADC(3) level, many of these many of the missing doorway states will have weak coupling with the one-neutron elastic scattering channel near the Fermi surface. However, they rapidly increase in number at larger energies and it must be expected that more realistic density of states will be required correctly predict absorption.

To conclude, we have benchmarked optical potentials generated through SCGF theory to analogous full scale NCSMC simulations and to data for neutron elastic scattering at low energy. For both theory approaches, the correct asymptotic behaviour of the scattering wave are reproduced even if the target wave function and the optical potentials and expanded in a HO basis. The theory benchmark, with freezing of virtual excitation of the target, is very encouraging. The SCGF approach has the capability of accounting for a large number of such doorway states up to very large energies, and it achieves a promising description of complex resonance states from first principles. The use of saturating chiral interaction allows us to make a meaningful comparison to the experiment, which was not possible in previous investigation of this approach. Overall, we found that the most important features of optical potentials at low energy are well reproduced, together with key observables related to elastic scattering.

The present study also puts in evidence how the lack of absorption normally observed in *ab initio* generated optical potentials is directly linked to the neglect of doorway configurations beyond 2p1h ones. Thus, addressing this challenge will be the next fundamental step toward predictive theories at medium scattering energies. It remains clear from the present results that reliable *ab initio* calculations of optical potentials directly from the self-energy are becoming a goal within reach. The present findings open a path to establish consistent theories of structure

and reactions for medium–mass nuclei.

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