Microscopic optical potential from chiral nuclear forces

J. W. Holt\textsuperscript{1}, N. Kaiser\textsuperscript{2}, G. A. Miller\textsuperscript{1} and W. Weise\textsuperscript{2,3}

\textsuperscript{1}Physics Department, University of Washington, Seattle, Washington 98195, USA
\textsuperscript{2}Physik Department, Technische Universität München, D-85747 Garching, Germany
\textsuperscript{3}ECT\textsuperscript{*}, Villa Tambosi, I-38123 Villazzano (TN), Italy

The energy- and density-dependent single-particle potential for nucleons is constructed in a medium of infinite isospin-symmetric nuclear matter starting from realistic nuclear interactions derived within the framework of chiral effective field theory. The leading-order terms from both two- and three-nucleon forces give rise to real, energy-independent contributions to the nucleon self-energy. The Hartree-Fock contribution from the two-nucleon force is attractive and strongly momentum dependent, in contrast to the contribution from the three-nucleon force which provides a nearly constant repulsive mean field that grows approximately linearly with the nuclear density. Together, the leading-order perturbative contributions yield an attractive single-particle potential that is however too weak compared to phenomenology. Second-order contributions from two- and three-body forces then provide the additional attraction required to reach the phenomenological depth. The imaginary part of the optical potential, which is positive (negative) for momenta below (above) the Fermi momentum, arises at second-order and is nearly inversion-symmetric about the Fermi surface when two-nucleon interactions alone are present. The imaginary part is strongly absorptive and requires the inclusion of an effective mass correction as well as self-consistent single-particle energies to attain qualitative agreement with phenomenology.

I. INTRODUCTION

Nuclear optical model potentials provide a highly successful framework for describing nucleon-nucleus scattering across extended regions of the nuclear chart. While local and global phenomenological optical potentials \cite{1-3} have been used to describe total cross sections, elastic scattering angular distributions, and analyzing powers for reactions on target nuclei close to the valley of stability, microscopic optical potentials have no adjustable parameters and may therefore provide the best means for extrapolating to rare isotope reactions that will be studied at the next generation of radioactive beam facilities. Neutron-capture cross sections on exotic, neutron-rich isotopes are particularly relevant for a detailed understanding of heavy-element formation in \( \beta \)-process nucleosynthesis. Although such reactions are experimentally unfeasible in the near future, neutron capture on rare isotopes can be probed indirectly in current and future rare isotope experiments through the \((d, p)\) stripping reaction, a process that is most easily modeled as a three-body problem requiring the nucleon-nucleon potential as well as the nucleon-nucleus optical potential \cite{4} as input.

Phenomenological optical potentials possess several adjustable parameters that characterize the shape of the nuclear density distribution of the target nucleus and that vary smoothly with the energy of the projectile and mass number of the target. Microscopic optical potentials, on the other hand, are derived from an underlying model of the nucleon interaction fit to elastic nucleon-nucleon scattering data as well as properties of the lightest nuclei. Within such a microscopic treatment, the optical potential is identified with the nucleon self-energy, a density-dependent complex-valued function given in terms of the nucleon energy and momentum. The nucleon self-energy has been constructed within numerous theoretical frameworks, including Brueckner-Hartree-Fock (BHF) theory \cite{12-11}, Dirac-Brueckner-Hartree-Fock (DBHF) theory \cite{12-16}, the Green’s function formalism \cite{17-18}, and chiral perturbation theory \cite{19-20}. The inclusion of three-nucleon forces, while often neglected in microscopic calculations of the optical potential, would seem highly relevant given their importance in achieving nuclear matter saturation at the correct density and binding energy per particle. Nevertheless, recent BHF calculations \cite{21} included effects of the Urbana IX three-nucleon force \cite{22} in a simplified manner \cite{23} and found only a modest improvement in the comparison to elastic scattering data for intermediate-energy scattering of protons from \( ^{40}\text{C} \) and \( ^{208}\text{Pb} \), despite a sizeable reduction of the central potential in the dense interior. A more accurate investigation of three-body forces is, however, desirable.

In the present work we make use of the progress that has been achieved in the last decade in constructing high-precision nuclear interactions within the framework of chiral effective field theory. As a first step in the development of microscopic optical potentials capable of describing reactions on rare isotopes, we compute the first- and second-order perturbative contributions to the nucleon self-energy in a medium of isospin-symmetric nuclear matter employing realistic chiral two- and three-nucleon interactions. Extensions to finite nuclei and isospin asymmetric systems relevant for reactions on nuclei far from the valley of stability will be presented in future work. The resulting optical potentials for infinite nuclear matter can be benchmarked against properties of well-established phenomenological potentials, such as their depth and energy dependence.
We will show that at nuclear matter saturation density \( \rho_0 \simeq 0.16 \text{fm}^{-3} \), the leading-order Hartree-Fock contributions from two- and three-nucleon forces are strongly competitive, with the two-body component significantly attractive and the three-body component mildly repulsive. Alone they would give rise to a mean field whose depth for a nucleon at vanishing energy (with respect to the Fermi energy) would be \( U \simeq -26 \text{MeV} \), much smaller than the empirical value of \( U \simeq -52 \text{MeV} \) determined from phenomenological optical model fits to reactions on heavy stable nuclei \([3]\). Second-order perturbative contributions from two- and three-nucleon forces yield considerable additional attraction of approximately 30 MeV, leading to overall reasonable agreement with phenomenology. The imaginary part, however, turns out to be nearly twice as strong as phenomenological optical potentials at intermediate scattering energies when single-particle energies are not treated self-consistently.

The paper is organized as follows. In Section II, we introduce the relevant formalism and make a connection between the in-medium nucleon self-energy and the nucleon-nucleus optical potential. Explicit formulas are given without any simplifying approximations for the first and second-order perturbative contributions in terms of a partial-wave decomposition of the nucleon-nucleon interaction. We present as well the formulas for the Hartree-Fock contribution to the single-particle potential constructed by summing one nucleon over the filled Fermi sea. Our results for the real and imaginary potential depths as well as their energy dependence is compared to those of phenomenological optical potentials fit to reactions on stable nuclei. We end with a summary and conclusions.

II. MICROSCOPIC OPTICAL MODEL POTENTIALS

A. First- and second-order contributions from two-body forces

In the nuclear optical model, the complicated many-body problem associated with the elastic scattering of a nucleon off a target nucleus is replaced by the more practicable problem of a single nucleon scattering from an equivalent complex mean-field potential:

\[
V(\vec{r}, \vec{r}'; E) = U(\vec{r}, \vec{r}'; E) + iW(\vec{r}, \vec{r}'; E),
\]

which in general is both non-local and energy-dependent. The imaginary part in Eq. (1) accounts for the presence of inelastic scattering, which reduces the total reaction flux in the elastic scattering channel. The simplest phenomenological optical potentials are taken to be local and of Woods-Saxon form in both the real and complex components:

\[
U(r; E) = \frac{-U_0(E)}{1 + e^{(r-R)/a_r}},
\]

\[
W(r; E) = \frac{-W_0(E)}{1 + e^{(r-R)/a_i}},
\]

where the parameters \( U_0(E), W_0(E), R_{r,i} \) and \( a_{r,i} \) vary smoothly with the mass number \( A \) of the nucleus and, in the case of the well-depth parameters \( U_0 \) and \( W_0 \), also the projectile energy \( E \).

Beyond energies of \( E \sim 200 \text{MeV} \), this Woods-Saxon form is no longer sufficient, and the real part of the central potential develops a “wine-bottle” shape \([3]\). Although not relevant for the present calculations with isospin-symmetric nuclear matter, phenomenological optical potentials possess real and imaginary spin-orbit terms as well as an imaginary surface term, all of which are proportional to the gradient of the Woods-Saxon distribution. Extensive analysis of the available experimental scattering data yields a real potential well depth \( U_0 \simeq 50 - 52 \text{MeV} \) for projectile nucleons with very low energies incident on heavy target nuclei. The depth of the imaginary potential vanishes at the Fermi energy and grows to typical values of \( W_0 \simeq 10 - 12 \text{MeV} \) for projectile energies close to 100 MeV.

Microscopically the optical model potential can be identified with the nucleon self-energy \( \Sigma(\vec{r}, \vec{r}'; E) \) in a nucleus \([24]\). For scattering states with \( E > 0 \), \( \Sigma(\vec{r}, \vec{r'}; E) \) is the nuclear optical potential, while for bound states with \( E < 0 \), the real part of \( \Sigma(\vec{r}, \vec{r'}; E) \) represents the shell model potential. In the present work we consider isospin-symmetric nuclear matter at uniform density \( \rho = 2k_f/3\pi^2 \), in which case it is more appropriate to compute the resulting spin- and isospin-independent self-energy in momentum-space \( \Sigma(q, \omega; k_f) \). A local optical model potential for nucleon-nucleus scattering can then be obtained by solving the self-consistent equation for the on-shell energy in terms of the momentum and then folding the resulting density-dependent mean field with a realistic point-nucleon density distribution of the target nucleus. The off-shell dependence of the self-energy \( \Sigma(q, \omega; k_f) \) on both \( q \) and \( \omega \) is necessary to describe the nucleon spectral function and nucleon momentum distribution. A complementary work studying the off-shell self-energy, including the effects of three-nucleon forces, is given in Ref. \([22]\).

The first-order Hartree-Fock contribution \( \Sigma^{(1)}(q, \omega; k_f) \) to the self-energy from two-body forces is shown diagrammatically in Fig. 1 for states above (1a) and below (1b) the Fermi surface. The Hartree-Fock
respectively. The second-order contributions to the particle self-energy are labeled (2a) and (2b), while the two contributions to the hole self-energy are labeled (2c) and (2d). The wavy line represents the antisymmetrized two-nucleon interaction $V_{2N}$, including direct and exchange terms.

\[
\Sigma_{2N}^{(1)}(q, \omega; k_f) = \sum_{n_1} \langle \vec{q} \vec{n}_1 s_1 t_1 t_2 | V_{2N} | \vec{q} \vec{n}_1 s_1 t_1 t_2 \rangle n_1, \tag{3}
\]

is real, $\omega$-independent, and changes smoothly as the external momentum $q$ crosses the Fermi surface. In Eq. (3), $V_{2N}$ denotes the antisymmetrized potential, $n_1 = \theta(k_f - |\vec{n}_1|)$ is the zero-temperature occupation probability, and the sum is taken over the momentum, spin, and isospin of the intermediate hole state $|\vec{n}_1, s_1, t_1\rangle$. The decomposition of the Hartree-Fock contribution in terms of partial-wave matrix elements of the interaction can be simplified by noting that $\Sigma(q, \omega; k_f)$ is spin and isospin independent when computed for a background medium of isospin-symmetric nuclear matter. Averaging over $s$ and $t$ in Eq. (3) then yields the single-particle potential

\[
U(q, k_f) = \frac{1}{2\pi^2} \sum_{lSJT} (2T + 1)(2J + 1)
\times \int_{\max\{0,(q-k_f)/2\}}^{(q+k_f)/2} dp \, p^2 \min\{2, (k_f^2 - (q - 2p)^2)/4pq\}
\times \langle lSJT|V_{2N}|lSJT\rangle, \tag{4}
\]

where $\vec{p} = (\vec{q} - \vec{n}_1)/2$ is the relative momentum of the interacting particles.

At second-order in perturbation theory, $\Sigma(q, \omega; k_f)$ develops both a real and imaginary part. For particle states above the Fermi surface, there are two distinct contributions labeled (2a) and (2b) in Fig. 1. The contribution (2a) arises from the external particle coupling to a hole state inside the Fermi sea and reads:

\[
\Sigma_{2N}^{(2a)}(q, \omega; k_f) = \frac{1}{2} \sum_{123} \langle \vec{p}_1 \vec{p}_3 s_1 t_1 t_3 | V_{2N} | \vec{q} \vec{n}_2 s_2 t_2 \rangle^2
\times (2\pi)^3 \delta(\vec{p}_1 + \vec{p}_3 - \vec{q} - \vec{n}_2), \tag{5}
\]

where $\vec{n}_k = 1 - n_k$ denotes a particle state lying above the Fermi momentum. We construct the momentum-dependent mean field by setting $\omega = q^2/(2M_N)$. Fixing $\vec{p}_3$ by momentum conservation, aligning the total momentum $\vec{p}' = \vec{p}_1 + \vec{p}_3 = \vec{q} + \vec{n}_2$ in the $\vec{e}_z$ direction, and averaging over the external particle spin, isospin and momentum direction then yields the partial-wave decomposition:

\[
U(q, k_f) + iW(q, k_f) = \frac{8M_N}{(4\pi)^3} \sum_{l_{123}l_{123}l_{123}l_{123}} (2T + 1) \int_{p'_a}^{p_b} dp' \int_{q_{1a}}^{q_{1b}} dq_{1a} \int_0^{x_0} d\cos \theta_1 \bar{P}_{l_{1a}}(\cos \theta_1) \bar{P}_{l_{1a}}(\cos \theta_1)
\times \int_{q_{2a}}^{q_{2b}} dq_2 \bar{P}_{l_{2a}}(\cos \theta_2) \bar{P}_{l_{2a}}(\cos \theta_2)
\times \frac{p'_aq'_b}{(q_2 - q_1 + i\eta)(q_2 + q_1)} \int_{l_2 + l_3 - l_1 - l_4} \bar{C}_{l_{1a}l_{2a}l_{3a}l_{4a}} \bar{C}_{l_{1a}l_{2a}l_{3a}l_{4a}}(q_1 l_{1a} S J T | V_{2N} | q_2 l_{2a} S J T)(q_1 l_{2a} S J T | V_{2N} | q_2 l_{3a} S J T), \tag{6}
\]

where $\vec{q}_1 = (\vec{p}_1 - \vec{p}_3)/2$, $\vec{q}_2 = (\vec{q} - \vec{n}_2)/2$, $\bar{P}_{l_{1a}}$ is the associated Legendre function $P_{l_{1a}}$ multiplied by the factor $\sqrt{(2l + 1)(l - m)!/(l + m)!}$, $\cos \theta_2 = (\vec{q}^2 - \vec{q}_2^2 - p'^2/4)/(\vec{p}' q_2)$, $x_0 = \min\{1, (q_1^2 - k_f^2 + p'^2/4)/\vec{p}' q_1\}$, and
the limits of integration are
\[ p'_{ia} = \max\{0, q - k_j\}, \quad p'_b = q + k_f, \]
\[ q_{1a} = \sqrt{\max\{0, k_j^2 - p'^2/4\}}, \quad q_{1b} = \infty \]
\[ q_{2a} = |q - p'/2|, \]
\[ q_{2b} = \min\left\{ \sqrt{(k_j^2 + q^2)/2} - p'^2/4, q + p'/2 \right\}. \]

The expression in Eq. (6) holds also for the hole contribution labeled (2c) in Fig. 1 except that since \( q < k_f \) the contribution is purely real and one can drop the \(+i\eta\) in the energy denominator.

The diagrams labeled (2b) and (2d) in Fig. 1 are both given by the following expression
\[
\Sigma^{(2b)}_{2N}(q, \omega; k_f) = \frac{1}{2} \sum_{a123} |(\vec{h}_1 \vec{h}_3 s_3 t_1 t_2 | V_{2N} | \vec{p}_2 s_2 t_2 t_1 \rangle|^2 n_1 n_2 n_3
\]
\[ \times (2\pi)^3 \delta(\vec{r}_1 + \vec{r}_3 - \vec{q} - \vec{p}_2). \]

In contrast to Eq. (5), here the contribution picks up an imaginary part for hole states below the Fermi surface and is purely real for particle states above the Fermi surface. The partial-wave decomposition is very similar to that for \( \Sigma^{(2a)}_{2N}(q, \omega; k_f) \), except that \( q_1 = (\vec{h}_1 - \vec{h}_3)/2 \), \( q_2 = (\vec{q} - \vec{p}_2)/2 \), and one must make the following replacements:
\[ +i\eta \rightarrow -i\eta, \quad x_0 \rightarrow \min\{1, (k_j^2 - q_1^2 - p'^2/4)/(p'q_1)\}, \]
\[ p'_a \rightarrow \max\{0, k_f - q\}, \quad p'_b - 2k_f, \]
\[ q_{1a} \rightarrow 0, \quad q_{1b} \rightarrow \sqrt{k_j^2 - p'^2/4}, \]
\[ q_{2a} \rightarrow \max\left\{ \left| q - p'/2 \right|, \sqrt{(k_j^2 + q^2)/2} - p'^2/4 \right\}, \]
\[ q_{2b} \rightarrow q + p'/2. \]

The numerical accuracy of the above formulas for the second-order contributions to the nucleon self energy in nuclear matter has been checked against semi-analytic expressions obtained for a simple scalar-isoscalar exchange model of the nuclear force (see the Appendix for details). Although the contributions labeled (2a) and (2c) in Fig. 1 may potentially be divergent, for the scalar-isoscalar exchange interaction all integrals converge. Across a range of momenta and densities we find the agreement between our numerical calculations and the semi-analytical results to be within 1%. The formulas for iterated one-pion exchange given in Refs. [19, 20] have been used as well for checking the partial-wave representation of the second-order contribution.

### B. Leading-order contribution from three-body forces

The methods described above for two-body forces can be extended to nuclear many-body forces. For a general three-nucleon force, the first-order Hartree-Fock contribution to the nucleon self-energy is real and energy independent. Summing two of the nucleons over the fully-antisymmetrized three-body interaction.

In the present work we consider only the leading-order N³LO chiral three-nucleon force, which has three terms proportional to the low-energy constants \( c_1, c_3, c_4, c_D \), and \( c_E \). The two-pion exchange component has the momentum-space representation:
\[
V^{(2\pi)}_{3N}(q, \omega; k_f) = \sum_{i\neq j\neq k} \frac{g_A^2}{8f_A^2} \frac{\vec{\sigma}_i \cdot \vec{q}_i}{m_n^2} \frac{\vec{\sigma}_j \cdot \vec{q}_j}{m_n^2} \frac{\vec{\sigma}_k \cdot \vec{q}_k}{m_n^2} F_{ijk}^\alpha F_{ijk}^\beta. \]
In Fig. 2 we show the diagrammatic contributions to the nucleon self-energy arising from the leading-order chiral three-nucleon force. The direct Hartree diagrams, labeled as (a) and (b) in Fig. 2, of the chiral two-pion exchange three-nucleon force are non-vanishing only for the terms proportional to the low-energy constants $c_1$ and $c_3$. The sum of these two diagrams gives

$$U(q, k_f) = \frac{g_3^2 m_\pi^6}{(2\pi f_\pi)^4} \left\{ 14(c_3 - c_1)u^4 + (3c_1 - 2c_3)u^2 - 4c_3u^6 + (12c_1 - 10c_3)u^3 \right\} \arctan 2u + \arctan(u + x) + \arctan(u - x) + \left[ \frac{c_3}{2} (1 + 9u^2) - \frac{3c_1}{4} (1 + 8u^2) \right] \ln(1 + 4u^2) + \frac{u^3}{x} \left[ 3c_1 - 3c_2 - 2c_1 + 2(c_1 - c_3)(x^2 - u^2) \right] \ln \left( \frac{1 + (u + x)^2}{1 + (u - x)^2} \right),$$

where $u = k_f/m_\pi$ and $x = q/m_\pi$

The Fock diagrams, labeled as (c) and (d) in Fig. 2, are non-vanishing for all terms in the two-pion exchange three-nucleon force:

$$U(q, k_f) = \frac{g_3^2 m_\pi^6}{(2\pi f_\pi)^4} \left\{ 3c_1 H^2(x, u) + \left( \frac{c_3}{2} - c_4 \right) G_S^2(x, u) + (c_3 + c_4) G_T^2(x, u) + \int_0^u d\xi \left[ 6c_1 H(\xi, u) \frac{\partial H(\xi, x)}{\partial x} + (c_3 - 2c_4) G_S(\xi, u) \frac{\partial G_S(\xi, x)}{\partial x} + 2(c_3 + c_4) G_T(\xi, u) \frac{\partial G_T(\xi, x)}{\partial x} \right] \right\},$$

with the auxiliary functions:

$$H(x, u) = u(1 + x^2 + u^2) - \frac{1}{4x} \left[ 1 + (u + x)^2 \right] \ln \left( \frac{1 + (u + x)^2}{1 + (u - x)^2} \right),$$

$$G_S(x, u) = \frac{4ux}{3} (2u^2 - 3) + 4x \left[ \arctan(u + x) + \arctan(u - x) \right] + (x^2 - u^2 - 1) \ln \left( \frac{1 + (u + x)^2}{1 + (u - x)^2} \right),$$

$$G_T(x, u) = \frac{ux}{6} (8u^2 + 3x^2) - \frac{u}{2x} (1 + u^2)^2 + \frac{1}{8} \left( \frac{1 + u^2}{x^2} \right)^2 \left[ -x^4 + (1 - 3u^2)(1 + u^2 - x^2) \right] \ln \left( \frac{1 + (u + x)^2}{1 + (u - x)^2} \right).$$

As shown in Section III the sum of the Hartree and Fock contributions from the two-pion exchange three-nucleon force gives rise to a significantly repulsive mean field. The Hartree term is approximately 75% larger in magnitude and of opposite sign as the attractive Fock term.

The contribution to the single-particle potential arising from the one-pion exchange three-nucleon force, proportional to $c_D$, is given by

$$U(q, k_f) = \frac{g_A c_D m_\pi^6}{(2\pi f_\pi)^4} \left\{ u^6 - \frac{7u^4}{4} + \frac{u^2}{8} + \frac{1 + 12u^2}{32} \ln(1 + 4u^2) + u^3 \left[ \arctan 2u + \arctan(u + x) + \arctan(u - x) \right] + \frac{u^3}{4x} (x^2 - u^2 - 1) \ln \left( \frac{1 + (u + x)^2}{1 + (u - x)^2} \right) \right\},$$

which depends very weakly on the momentum $q$ and is attractive for $c_D < 0$. The first-order contribution from the N$^2$LO contact interaction is independent of the external momentum and has the form

$$U(q, k_f) = -\frac{c_E k_0^2}{4\pi^2 f_\pi^4} \chi, \quad \text{with} \quad \chi = \frac{1}{4x} \left[ 1 + (u + x)^2 \right] \ln \left( \frac{1 + (u + x)^2}{1 + (u - x)^2} \right),$$

which is of course repulsive for $c_E < 0$. As we will find in Section III, together $V_{1N}^{\chi}$ and $V_{3N}^{\chi}$ provide a nearly constant repulsive mean field.

The above analytical expressions result from an exact calculation of the Hartree-Fock contribution to the
In the present section we employ the N³LO chiral two-body interaction of Ref. [26] together with the N²LO chiral three-body interaction with low-energy constants given in Section III to compute the contributions to the nuclear optical potential up to second order in perturbation theory. In addition we perform calculations of the nuclear mean field also for hole states with $q < k_f$. We are particularly interested in comparisons of our microscopic optical potential to local phenomenological potentials and in the effects from three-nucleon forces, which until now have been treated only approximately in several complementary studies [21, 22].

In Fig. 3 we plot the real part of the on-shell self-energy contribution to the momentum- and density-dependent optical potential. The solid and dashed-dotted lines are the first- and second-order contributions, respectively from the N³LO chiral two-body potential, while the dashed line is the first-order contribution from the N²LO chiral three-nucleon force. The vertical dotted line denotes the Fermi momentum, and the dashed-double-dotted line denotes the second-order contribution without three-body forces. The results are shown for the case $\omega = q^2/(2M_N)$.

In Fig. 4 we plot the real part of the Hartree-Fock contributions to the nuclear optical potential from chiral three nucleon forces. The two-pion exchange, one-pion exchange, and contact three-nucleon force contributions are evaluated from Eqs. (15)-(21) and plotted separately as a function of the momentum.
energy \( \omega = q^2/(2M_N) \) as a function of momentum and density. The thick solid line denotes the Hartree-Fock contribution from two-body forces, and the vertical dotted lines show the Fermi momentum corresponding to the densities \( \rho = \{0.2\rho_0, 0.4\rho_0, 0.6\rho_0, 0.8\rho_0, 0.9\rho_0, \rho_0\} \) from the upper left corner to the bottom right, where \( \rho_0 \approx 0.16 \text{ fm}^{-3} \). The Hartree-Fock term has a nearly parabolic form, and when summed with the free-particle kinetic energy \( q^2/(2M_N) \) it can be well approximated as [31]:

\[
\epsilon_q = \frac{q^2}{2M^*} + \Delta, \tag{22}
\]

where \( M^* \) is the effective mass and the energy shift \( \Delta \) is independent of momentum. In Fig. 3 the momenta are taken up to \( q = 2.5 \text{ fm}^{-1} \), which, for all the densities considered here, corresponds to possible two-particle relative momenta well below the cutoff of \( \Lambda \approx 2.5 \text{ fm}^{-1} \).

The Hartree-Fock three-body force contribution exhibits a very weak density dependence that would give rise to only a small decrease in the effective mass at the Fermi surface [32]. The strength of the mean field from chiral three-nucleon forces increases nearly linearly with the density of the medium. At saturation density it gives a repulsive contribution of approximately 20 MeV. In Fig. 4 we plot separately the mean fields associated with the different contributions \( V_{3N}^{2\pi} \), \( V_{3N}^{1\pi} \), and \( V_{3N}^{\text{CT}} \) at nuclear matter saturation density, corresponding to \( k_f = 1.33 \text{ fm}^{-1} \). The 2\( \pi \)-exchange chiral three-nucleon force provides much of the observed repulsion from three-body forces and accounts also for most of the momentum dependence, which arises primarily for momenta above the Fermi surface. The 1\( \pi \) and contact interactions together give rise to a small net repulsive mean field that is nearly momentum independent. For nucleon-nucleus scattering, it therefore appears that the low-energy constants \( c_D \) and \( c_E \) are strongly correlated, with variations along the line

\[
c_E = \alpha \cdot c_D + \text{const} \tag{23}
\]

giving nearly equivalent descriptions of the mean field, where the constant of proportionality \( \alpha \approx 0.21 \pm 0.02 \) is weakly dependent on momentum and density. Inspection of Eq. (21) reveals that in the chiral limit only the leading \( k_0^6 \) term survives, and the correlation coefficient would be \( \alpha = g_A/4 \approx 0.3 \).

The second-order contributions to the nuclear mean field are shown as the dashed-dotted lines in Fig. 3. Below the Fermi surface, they have a momentum dependence that is nearly opposite to that of the Hartree-Fock contribution, giving rise to a quasiparticle effective mass at the Fermi surface that is close to the mass in vacuum [31]. In Fig. 3 we plot also the second-order contribution without three-nucleon forces, denoted by the dashed-double-dotted line. Despite the fact that the three-nucleon force gives rise to substantial repulsion at the Hartree-Fock approximation, it appears that second-order effects are quite small and produce additional attraction at both low and high momenta.

It is common in the literature to include self-consistent single-particle energies in the denominators of the second-order contributions. Then the on-shell condition reads:

\[
\epsilon_p = \frac{p^2}{2M_N} + \text{Re} \Sigma(p, \epsilon_p; k_f). \tag{24}
\]

Such a prescription reduces the second-order contributions due to the larger energy difference between particle and hole states. The value in using the free-particle spectrum is that various thermodynamic identities, such as the Hugenholtz–Van-Hove [33] and Luttinger [34] theorems

\[
\frac{k_f^2}{2M_N} + U(k_f, k_f) = \bar{E}(k_f) + \frac{k_f}{3} \frac{\partial \bar{E}(k_f)}{\partial k_f}
\]

\[
W(q, k_f) = C |k_f - q(k_f - q) + \cdots \tag{25}
\]

are automatically fulfilled when the relevant quantities are computed to a particular order in perturbation theory. Nevertheless, to achieve a better description of phenomenology may require using the self-consistent energies Eq. (24).

The combined real part of the nucleon self-energy is shown in Fig. 5 as a function of density and momentum. We note that for low to moderate densities, the mean field for states with momenta \( q < k_f \) is nearly constant, but in the vicinity of the saturation density, three-nucleon forces at second-order introduce additional attraction for low values of \( q \). The well depth for a scattering state at zero incident energy is approximately \( -57 \text{ MeV} \), which is
within 10% of the depth, −52 MeV, of phenomenological optical potentials. The well depth at q = 0 as a function of density is shown in Fig. 6 for two-nucleon forces alone as well as for combined two- and three-body forces. Three nucleon forces become relevant at about 40% of nuclear matter saturation density and result in a mean field that is significantly nonlinear in the density.

Finally, we plot in Fig. 7 the imaginary part of the nucleon self-energy arising from the second-order perturbative contributions (both with and without three-nucleon forces) as a function of momentum and density. In agreement with Luttinger's theorem [34], the imaginary part vanishes quadratically in the vicinity of the Fermi surface above and below k_f for both two- and three-nucleon force contributions. Omitting the chiral three-body force, we find that the imaginary part is approximately inversion-symmetric about the Fermi momentum, W(q, k_f) ≃ −W(2k_f − q, k_f), a property which is often assumed in the dispersion optical model formalism [35]. This feature is, however, modified with the inclusion of three-nucleon forces, which provide an attractive contribution at both very low and very high momenta.

The overall strength of the imaginary potential at nuclear matter saturation density for an intermediate scattering energy of E ≃ 100 MeV is approximately 30 MeV, which would seem too large compared to the empirical value, |W| ≃ 10 MeV [3]. This large magnitude of the imaginary part of the optical potential is a feature shared by many microscopic calculations. Already second-order one-pion exchange gives rise to quantitatively similar results (see Fig. 6 in Ref. [20]). However, as noted in Refs. [36, 37], the imaginary part of the self-energy should not be compared with the imaginary part of phenomenological optical potentials. Rather, the precise relationship between the microscopic and phenomenological potential is given by

\[ W_{ph}(q, E) = \left( 1 + \frac{M_N}{q} \frac{\partial U}{\partial q} \right)^{-1} W_{mc}(q, E). \]  

With the so-called k-mass factor \( \left( 1 + \frac{M_N}{q} \frac{\partial U}{\partial q} \right)^{-1} \approx 0.75 \), the value of the imaginary part of the optical potential derived from our microscopic calculation is W(q = 100 MeV) = −22.5 MeV. Since this value is still rather large compared to the empirical optical potential, it appears that the inclusion of self-consistent energies in the denominators of Eqs. (5) and (8) may be necessary in order to achieve a quantitatively successful imaginary microscopic potential. In addition one should recall that the phenomenological absorptive strength |W| is deduced for finite nuclei which have a characteristic gap in the single-particle energy spectrum around the Fermi energy. The nuclear matter calculation does not feature such a gap at the Fermi surface so that there is an increased phase space open for absorptive processes, leading to an overestimate of |W|.

IV. CONCLUSIONS

We have performed a microscopic calculation of the on-shell self-energy of a nucleon in a medium of isospin-symmetric nuclear matter at uniform density p up to second order in many-body perturbation theory. The starting point is a realistic N^3LO chiral two-nucleon potential supplemented with the N^2LO chiral three-nucleon force. The first- and second-order contributions from two-body forces are attractive, but below the Fermi momentum they have an opposite dependence on the momentum. The N^2LO chiral three-body force is found to provide substantial repulsion that grows slowly with momentum and nearly linearly with the density. Summing up all of these contributions, the resulting microscopic nuclear mean field agrees qualitatively with the depth of phenomenological optical potentials. The absorptive strength of the imaginary part of the potential calculated in nuclear matter is considerably larger than the empirical one deduced for finite nuclei. This suggests that a self-consistent treatment of single-particle energies (including the energy gap at the Fermi surface) may be necessary in order to achieve a successful description of nucleon-nucleus scattering at low to intermediate energies. In the future we plan to extend our calculations to finite nuclei and isospin asymmetric nuclear matter that will be important to describe neutron-capture cross sections on neutron-rich isotopes.

Work supported in part by BMBF, the DFG cluster of excellence Origin and Structure of the Universe, by
the DFG, NSFC (CRC110) and US DOE Grant No. DE-FG02-97ER-41014.

V. APPENDIX: NUCLEAR OPTICAL POTENTIAL FROM SECOND-ORDER SCALAR-ISOSCALAR BOSON EXCHANGE

As a benchmark for our involved numerical calculations of the nuclear mean field at second order in perturbation theory, we derive exact semi-analytical expressions for the on-shell self-energy arising from scalar-isoscalar boson exchange. The attractive central NN-potential in momentum space is given by:

$$V_C(Q) = -\frac{g^2}{m^2 + Q^2},$$  \hspace{1cm} (27)

with $g$ the coupling constant, $m$ the boson mass, and $Q$ the momentum transfer between the two nucleons.

The first-order contribution to the real part of the optical potential for states both above $(q > k_f)$ and below $(q < k_f)$ the Fermi surface reads:

$$U(q, k_f) = g^2 m \frac{\pi}{4} \left\{ -\arctan(u + x) - \arctan(u - x) + u - \frac{8u^3}{3} + \frac{1 + u^2 - x^2}{4x} \ln \frac{1 + (u + x)^2}{1 + (u - x)^2} \right\},$$  \hspace{1cm} (28)

with abbreviations $u = k_f/m$ and $x = q/m$.

Due to the presence of poles in Fermi sphere integrals, the analytic expression of the second-order contributions cannot be continued directly from below to above the Fermi surface. We therefore distinguish the contributions to the optical potential for momenta $q < k_f$ and $q > k_f$. Setting $\omega = q^2/(2M_N)$, the complex-valued mean field $U(q, k_f) + iW(q, k_f)$ inside the Fermi sphere $q < k_f$ is given by the sum of the following contributions (in these expressions the superscript "$H$" and "$F$" refer to Hartree and Fock diagrams, and the subscript denotes the number of medium insertions [19]):

$$U_2(q, k_f)^{(H)} = g^4 M_N \frac{8\pi^3}{9} \left\{ \arctan(u + x) + \arctan(u - x) - u + \frac{x^2 - u^2 - 1}{4x} \ln \frac{1 + (u + x)^2}{1 + (u - x)^2} \right\},$$  \hspace{1cm} (29)

FIG. 7: The imaginary part of the momentum- and density-dependent optical potential arising from chiral two- and three-nucleon forces iterated to second order. The vertical dotted line denotes the Fermi momentum.
\[ U_2(q, k_f) = \frac{g^4 M_N}{16 \pi^3} \left\{ \int_0^{(u-x)/2} d\xi \frac{8 \xi}{1 + 2 \xi^2} - \int_{(u-x)/2}^{(u+x)/2} d\xi \frac{8 \xi}{1 + 2 \xi^2} \right\} \arctan \frac{2 \xi - \arctan \xi}{1 + 2 \xi^2}, \] (30)

\[ U_3(q, k_f) = \frac{g^4 M_N}{8 \pi^4} \int_0^1 dy \left\{ \ln(1 + \sigma^2) \right\} \times \ln(1 + t^2) \frac{\theta(1 - y^2 - z^2)}{4 \pi \sqrt{1 - y^2 - z^2}} \]

\[ U_3(q, k_f) = \frac{g^4 M_N}{8 \pi^4} \int_0^1 dy \left\{ \int_0^u d\xi \frac{\xi^2 \sigma^2}{x R} \theta(x - |y|) \ln(1 + \sigma^2) \right\}, \] (36)

with auxiliary functions \( s = xy + \sqrt{u^2 - x^2 + y^2} \) and \( \sigma = \xi y + \sqrt{u^2 - \xi^2 + \xi^2 y^2} \).

\[ U_3(q, k_f) = \frac{g^4 M_N}{16 \pi^3} \left\{ \int_0^u d\xi \frac{\xi^2}{x R} \ln(1 + \sigma^2) \right\} \times \arctan \frac{2 \xi - \arctan \xi}{1 + 2 \xi^2}, \] (32)

with auxiliary functions \( t = xz + \sqrt{u^2 - x^2 + z^2} \) and \( R = \sqrt{1 + x^2 - \xi^2 + \xi^2 y^2} \).

\[ W_2(q, k_f) = \frac{g^4 M_N}{16 \pi^3} \left\{ \ln(1 + (u + x)^2) \right\} \times \ln(1 + (u - x)^2) - \frac{2 x^2}{3} \]

\[ + \ln(1 + (u - x)^2) - 2(1 + u^2) + \frac{2 x^2}{3} \]

\[ + \frac{1 + u^2 - x^2}{x} \left[ \arctan(u + x) - \arctan(u - x) \right] \}, \] (33)

\[ W_2(q, k_f) = \frac{g^4 M_N}{16 \pi^3} \left\{ \int_0^{(u-x)/2} d\xi \frac{8 \xi}{1 + 2 \xi^2} + \int_{(u-x)/2}^{(u+x)/2} d\xi \frac{8 \xi}{1 + 2 \xi^2} \right\} \ln(1 + 4 \xi^2), \] (34)

\[ W_3(q, k_f) = \frac{g^4 M_N}{16 \pi^3} \int_1^1 dy \left\{ (1 + u^2 - 2 x^2 y^2) \frac{s^2}{1 + s^2} \right\} \times \arctan \frac{2 \xi - \arctan \xi}{1 + 2 \xi^2}, \] (35)
\[ U_3(q, k_f)(F) = \frac{g^4 M_N}{16\pi^4} \left\{ - \int_{y_{\text{min}}}^{1} dy \int_{y_{\text{min}}}^{1} dz A_y \ln(1 + s^2) \right\} \]

\[ \times A_z \ln(1 + t^2) \left[ \frac{\theta(y^2 + z^2 - 1)}{4\sqrt{y^2 + z^2 - 1}} + \int_{-1}^{1} dy \int_{0}^{u} d\xi \frac{\xi^2}{x R} \right] \]

\[ \times \ln(1 + s^2) \ln\left( \frac{x R + (x^2 - t^2 - 1) y \xi}{x R + (1 + t^2 - x^2) y \xi} \right) \right\}, \quad (42) \]

\[ W_2(q, k_f)(H) = \frac{g^4 M_N}{16\pi^3} \left\{ \ln \frac{1 + (u + x)^2}{1 + (u - x)^2} - \frac{2u}{3x} (3 + 2u^2) \right. \]

\[ + \frac{1 + u^2 - x^2}{x} \left[ \arctan(u + x) - \arctan(x - u) \right] \right\}, \quad (43) \]

\[ W_2(q, k_f)(F) = \frac{g^4 M_N}{32\pi^3} \int_{(x-u)/2}^{(u+x)/2} d\xi \left[ u^2 - (2\xi - x)^2 \right] \]

\[ \times \ln\left( 1 + 4\xi^2 \right) \frac{1}{1 + 2\xi^2} \right\}, \quad (44) \]

\[ W_{34}(q, k_f)(H) = \frac{g^4 M_N}{16\pi^3} \left\{ \frac{1}{x} \left[ \frac{u}{2} + \frac{4u^3}{3} - \frac{1}{4} (1 + 4u^2) \right] \right. \]

\[ \times \arctan 2u + \theta(\sqrt{2}u - x) \int_{y_{\text{min}}}^{u/x} dy (x^2 y^2 - u^2) \]

\[ \left. \times A_y \left[ \frac{s^2}{1 + s^2} \right] + \int_{y_{\text{min}}}^{1} dy A_y \left[ - \ln(1 + s^2) + \frac{s^2}{1 + s^2} \right] \right\} \]

\[ \times (1 + u^2 - x^2 y^2) + 2xy \left( \arctan s - \frac{s}{1 + s^2} \right) \right\}, \quad (45) \]

\[ W_{34}(q, k_f)(F) = \frac{g^4 M_N}{16\pi^3} \left\{ \frac{\theta(\sqrt{2}u - x)}{4\pi} \int_{y_{\text{min}}}^{1} dy \right. \]

\[ \int_{y_{\text{min}}}^{1} dz \frac{\theta(1 - y^2 - z^2)}{\sqrt{1 - y^2 - z^2}} A_y \ln(1 + s^2), A_z \ln(1 + t^2) \]

\[ - \int_{-1}^{1} dy \int_{0}^{u} d\xi \frac{\xi^2}{x R} \ln(1 + s^2) \right\}, \quad (46) \]

Finally, we note that the total imaginary part \( W(0, k_f) \) evaluated at zero nucleon-momentum (\( q = 0 \)) can even be written in closed analytical form:

\[ W(0, k_f) = \frac{g^4 M_N}{16\pi^3} \left\{ \frac{\pi^2}{12} + \text{Li}_2(-1 - u^2) - \frac{2u^2}{1 + u^2} \right. \]

\[ + \left[ 2 + \ln(2 + u^2) - \frac{1}{2} \ln(1 + u^2) \right] \ln(1 + u^2) \right\}, \quad (47) \]

where \( \text{Li}_2(\ldots) \) denotes the conventional dilogarithmic function. The behavior of \( W(0, k_f) \) at small densities is \( k_f^4 \).