Systematic Matter and Binding-Energy Distributions from a Dispersive Optical Model Analysis

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(Dated: May 29, 2020)

We present the first systematic nonlocal dispersive optical model analysis using both bound-state and scattering data of \(^{16,18}\)O, \(^{40,48}\)Ca, \(^{58,64}\)Ni, \(^{112,124}\)Sn, and \(^{208}\)Pb. In all systems, roughly half the total nuclear binding energy is associated with the most-bound 10% of the total nucleon density. The extracted neutron skins reveal a complex interplay of asymmetry, Coulomb, and shell effects on the skin thickness. Our results indicate that simultaneous optical-model fits of inelastic scattering and structural data on isotopic pairs is effective for constraining asymmetry-dependent nuclear structural quantities otherwise difficult to observe experimentally.

Introduction.– Despite much investigation, the detailed behavior of individual nucleons in the nuclear ground state remains poorly understood. While many models can reproduce nuclear masses and charge radii across the nuclear chart, none can fully account for the distribution of nucleons in the nuclear ground state. While many models have examined only a single Ca isotope each, while in contrast, the DOM defines the complex, nucleon self-energy, \(\Sigma(\alpha, \beta; E)\), above and below the Fermi energy. This potential-like object encodes the correlations experienced by a nucleon as it moves from state \(\alpha\) to \(\beta\) in the nuclear medium at energy \(E\). As in past DOM treatments, the self-energy domain was restricted to \(-300\) MeV to \(200\) MeV with respect to the Fermi energy, a first-order relativistic correction was included, and only two-body forces were considered. The self-energy is comprised of three subcomponents:

\[ \Sigma^*(\alpha, \beta; E) = \Sigma_s(\alpha, \beta) + \Sigma_{im}(\alpha, \beta; E) + \Sigma_d(\alpha, \beta; E) \]  

(1)

The “static” part of the self-energy \(\Sigma_s(\alpha, \beta)\) includes all real energy-independent contributions, taken here as a Hartree-Fock term evaluated at the Fermi energy, \(\epsilon_F\), plus a spin-orbit term. Each of these subterms is parameterized with a Woods-Saxon form coupled to a Gaussian nonlocality. The energy-dependent imaginary component \(\Sigma_{im}(\alpha, \beta; E)\) consists of energy-dependent surface- and volume-associated terms at both positive and negative energies, again with nonlocal Woods-Saxon terms included. The existence of “neutron skins”, \(\Delta\), is one that has received immense theoretical and experimental interest in recent years (thoroughly reviewed in [1]). The existence of “neutron skins”, \(\Delta\), on the surface of these and other stable nuclei is expected to correlate strongly with the density dependence of the nuclear symmetry energy, a major uncertainty in the neutron-star equation-of-state [2–4]. Before presenting these results, we review a few salient elements of the DOM formalism and the MCMC implementation in the following sections.

Relevant DOM Formalism.– Classical optical models describe nucleon-nucleon scattering with various forms of local phenomenological potentials defined only at positive energies [5, 6, 7]. In constrast, the DOM defines the complex, nucleon self-energy, \(\Sigma(\alpha, \beta; E)\), both above and below the Fermi energy. This potential-like object encodes the correlations experienced by a nucleon as it moves from state \(\alpha\) to \(\beta\) in the nuclear medium at energy \(E\). As in past DOM treatments, the self-energy domain was restricted to \(-300\) MeV to \(200\) MeV with respect to the Fermi energy, a first-order relativistic correction was included, and only two-body forces were considered. The self-energy is comprised of three subcomponents:

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Saxons, or their derivatives, for radial dependence. Physically, these terms account for inelastic processes and short- and long-range correlations (SRCs and LRCs) and are the most challenging terms to calculate fully in ab initio and shell-model treatments. To constrain these terms, the DOM instead relies on fitting experimental data. The “dynamic” (energy-dependent) real term \( \Sigma_d(\alpha, \beta; E) \) is completely determined by integrating the imaginary term over the entire energy domain. It ensures that the full self-energy obeys the required subtracted dispersion relation. The parameterization used here is available in the companion article [21] and additional detail can be found in [22].

Following [24], the single-nucleon propagator is generated from the self-energy via the Dyson Equation and the hole spectral function extracted from the propagator:

\[
S^h_{\ell j}(\alpha; E) = \frac{1}{\pi} \text{Im}(G_{\ell j}(\alpha, \alpha; E)) \quad \text{for } E \leq \epsilon_F.
\]  

Here we explicitly label \( G \) and \( S \) with the (conserved) angular momentum \( \ell \) and total angular momentum \( j \). Intuitively, the hole spectral function is the probability for removal of a particle with quantum numbers \( \alpha \) from the ground state and leaving the residual nucleus with the energy \( E_0^N - E \). If an \( r \)-space basis is chosen, the nucleon point density is simply:

\[
\rho(r) = \frac{1}{4\pi r^2} \int_{-\infty}^{\epsilon_F} \left( 2j + 1 \right) S^h_{\ell j}(r; r; E) dE.
\]  

Finally, the total binding energy can be calculated per the Migdal-Galitsky rule, which is exact when only two-body interactions are included:

\[
E_0^N = \frac{1}{2} \left[ \sum_{\alpha\beta} (\alpha|\hat{T}|\beta) n_{\alpha,\beta} + \sum_\alpha \int_{-\infty}^{\epsilon_F} dE \ E \ S^h_{\ell j}(\alpha; E) \right],
\]  

where \( \hat{T} \) is the kinetic energy operator appropriate for the single-particle basis. Three-body terms do not induce important corrections when energy densities are considered, supporting the use of Eq. (4) in DOM applications [23].

To constrain the self-energy, we applied nine sectors of experimental data for each nucleus: differential elastic-scattering cross sections, analyzing powers, reaction cross sections, total cross sections, the binding energy, rms charge radius, charge-density distribution, single-nucleon separation energies, and particle numbers. For fits on \(^{16,18}\text{O}, ^{40,48}\text{Ca}, ^{58,64}\text{Ni}, \text{and} ^{112,124}\text{Sn}, \) all available data for each isotope pair were simultaneously fit using the same asymmetry-dependent potential; for \(^{208}\text{Pb}, \) only the \(^{208}\text{Pb} \) data were used. To calculate scattering cross sections from the self-energy, an R-matrix approach was used (detailed in [22, 25]). The new experimental isotopically-resolved neutron total cross sections that motivated this work are reported in the companion experimental paper [21]. The companion paper also includes a detailed comparison of DOM calculations to all experimental data.

**Potential Optimization with MCMC.**—Several aspects of the DOM potential make optimization challenging. Even with the reduced number of potential parameters used in this work (42 for \(^{208}\text{Pb} \) and 43 for all other pairwise fits) compared to past DOM studies (60 or more), we found that classical gradient-descent methods were inappropriate for reliably searching the parameter space. A recent study [26] systematically compared Bayesian optical model optimization techniques to frequentist methods, the type almost universally used in previous analyses, and found that traditional algorithms may be overconfident in their parameter estimation, jeopardizing predictive power. To avoid these problems, we used the affine-invariant MCMC library, emcee [27], for optimization and uncertainty characterization. Several hundred “walkers” were initialized uniformly in the parameter space for each fit and allowed to traverse the space. The details of the likelihood function and prior distributions, convergence tests, and parameter estimates with uncertainties are included in the companion paper [21]. Importantly, we found that the inclusion of a reasonable model discrepancy term in our utility function improved the visual fit to experimental data while broadening parameter uncertainties, in keeping with the methodological findings of [28].

**Binding Energies.**—Figure 1 shows the breakdown of particle density and binding energy for optimized fits of \(^{16,18}\text{O} \) and \(^{40,48}\text{Ca} \). As in an independent-particle model, the vast majority of both proton and neutron density rests in the shells below the Fermi level. However, due to significant imaginary strength, a small but significant fraction, around 10%, appears in higher shells that would be fully unoccupied in a naïve mean-field picture.

For both protons and neutrons, an outsized fraction of the binding energies comes from the most-bound levels. For example, the \( s_{1/2} \) states in \(^{16}\text{O} \) possess roughly 20% of the nucleon density but almost 60% of the binding energy. In both systems, the protons’ fraction of the total binding energy is slightly reduced compared to that from the neutrons, a consequence of the Coulomb interaction. Overall, the substantial depletion of mean-field occupancies even in light systems (and associated broadening of the bound-nucleon spectral functions, visualized in [15]) is critical for achieving an average binding energy per nucleon of 8 MeV/nucleon. We note that the binding energy distribution we recover for \(^{16}\text{O} \) agrees with that from the Brueckner-Hartree-Fock (BHF) treatment of [15].

Finally we turn to the binding energy distributions for asymmetric \(^{18}\text{O} \) and \(^{48}\text{Ca} \) in Fig. 1. In these systems, the minority species (protons) experiences a deeper mean-field potential and enhanced correlations, increasing each proton’s relative share of the binding energy. For the majority species (neutrons), the effect is reversed: binding
FIG. 1. DOM calculations of nucleon occupation and binding energy contributions as a function of angular momenta $\ell j$ in $^{16,18}\text{O}$ and $^{40,48}\text{Ca}$. The results shown are using the median posterior parameter values from MCMC sampling.

is reduced for each shell compared to the symmetric system. For the valence $d_{5/2}$ neutrons in $^{18}\text{O}$ (in blue) and $f_{7/2}$ neutrons in $^{48}\text{Ca}$ (in orange), the contribution to the total binding is negative — that is, unbinding — because the bulk of their spectral density resides in quasiholes at or near the Fermi surface. This effect is more than compensated by the extra binding energy these valence neutrons induce in the protons compared to the symmetric case, such that the net effect is increased overall binding. Such an asymmetry-stimulated enhancement of SRCs for the minority species echoes the findings of [29] in their investigation of enhanced minority-nucleon momenta.

Figure 2 gives an $\ell j$-independent illustration of how binding energy is distributed. For each system, the fraction of the total binding energy possessed by the most-bound 10% of the nucleon density ($BF_{10\%}$), regardless of quantum number, is plotted. For all the systems we analyzed, this fraction exceeds 40%. A linear modeling of the data,

$$BF_{10\%} = x_0 + A x_A + \frac{N - Z}{A} x_\alpha,$$

with $N$, $Z$, and $A$ the neutron, proton, and total nucleon numbers, respectively, yields $x_0 = 36^{31}_{30}$, $x_A = 4.1^{1.1}_{1.5}$, and $x_\alpha = 3^{31}_{26}$, where the 16th, 50th, and 84th percentiles from the parameter posteriors are reported as 50$^{46}_{44}$. Thus the $BF_{10\%}$ depends only weakly on the size of the system and is independent of asymmetry, an indication that even in light nuclei, the bulk of the total binding comes from the few most-bound nucleons.

Neutron skins. – The neutron skin:

$$\Delta r_{np} \equiv r_{rms}(n) - r_{rms}(p),$$

was first identified as an important observable by Wilkinson over fifty years ago [30]. Neutron skins on neutron-rich nuclei are connected to other nuclear structural quantities, including the electric dipole polarizability, the location of the pygmy and giant dipole resonances, the density dependence of the symmetry energy, and the size of neutron stars [2, 4, 31–33]. The neutron skins extracted from the present work are depicted in Fig. 3, revealing delicate interplay between several factors (median values and uncertainties are available in Table I). We find that the degree of asymmetry,
$\alpha \equiv \frac{N-Z}{A}$, correlates strongly ($r = 0.89$) with the median skin thicknesses. If a simple linear dependence in $\alpha$ is assumed, extrapolation from the $^{58,64}\text{Ni}$ skins gives a $^{56}\text{Ni}$ skin thickness of $-0.04 \pm 0.03$ fm. A similar calculation with $^{112,124}\text{Sn}$ yields a $^{100}\text{Sn}$ skin thickness of $-0.07 \pm 0.06$ fm. In the symmetric systems $^{16,18}\text{O}$ and $^{40,48}\text{Ca}$, Coulomb repulsion nudges proton density outward from the core, resulting in a small negative neutron skin (that is, a proton skin). Again assuming simple linear dependence of this Coulomb effect, extrapolation from $^{16,18}\text{O}$ and $^{40}\text{Ca}$ gives neutron skins of $-0.07\pm0.02$ fm for $^{56}\text{Ni}$ and $-0.12\pm0.04$ fm for $^{100}\text{Sn}$, each slightly more negative than, but in keeping with, the linear extrapolation from $^{58,64}\text{Ni}$ and $^{112,124}\text{Sn}$. Besides Coulomb and asymmetry-dependent effects, the large $^{48}\text{Ca}$ median skin of 0.22 fm and near-zero median $^{64}\text{Ni}$ skin of -0.01 fm show the importance of shell effects for certain systems (cf. with $^{208}\text{Pb}$ results of [15]). To wit, most of the excess neutrons in $^{48}\text{Ca}$ and $^{64}\text{Ni}$ enter the $^{1}p_{7/2}$ and $^{1}p_{3/2}$ shells, respectively, as seen in Fig. 1 for $^{48}\text{Ca}$. The mean radius of the $^{1}p_{7/2}$ shell is larger than that of all deeper shells; thus, when neutron density is added, the size grows rapidly. In $^{64}\text{Ni}$, the $^{1}p_{3/2}$ rms radius is closer to the overall $r_{rms}(n)$ of $^{58}\text{Ni}$, so the additional neutrons of $^{64}\text{Ni}$ do little to grow the skin thickness.

For $^{18}\text{O}$, the mirror-nuclei logic of [34] can be applied to cross-check our skin value. Assuming isospin symmetry and minimal deformation, the difference between the $^{18}\text{Ne}$ and $^{18}\text{O}$ charge radii should be a good proxy for the $^{18}\text{O}$ neutron skin thickness, up to a small Coulomb correction. Per [35], the raw charge radius difference between $^{18}\text{Ne}$ and $^{18}\text{O}$ is 0.199±0.009 fm. Given our $^{16}\text{O}$ skin value of -0.025 fm, the Coulomb correction for $^{18}\text{Ne}$ can be estimated as -0.031 fm, or 25% larger than that of $^{16}\text{O}$. This results in a Coulomb-corrected $^{18}\text{Ne}$-$^{18}\text{O}$ charge radius difference of 0.168±0.013 fm. Because $^{18}\text{Ne}$ is more deformed ($\beta_2 = 0.68$) than $^{18}\text{O}$ ($\beta_2 = 0.37$) [39], any additional deformation correction will further reduce the difference in radii, so the corrected difference can only be taken as an upper limit on the $^{18}\text{O}$ neutron skin. Our skin prediction for $^{18}\text{O}$ of 0.06±0.02 fm is compatible with this upper limit of 0.168 fm.

Our median results for $^{48}\text{Ca}$ (0.22 fm) and $^{208}\text{Pb}$ (0.18 fm) are somewhat smaller than those from the previously-mentioned DOM case studies but with significant uncertainty-range overlap [14, 15]. We attribute the variation to differences in the potential parameterization, our joint fitting of isotope pairs, and our Bayesian optimization approach. Because $^{208}\text{Pb}$ was fit by itself (not as part of an isotopic pair), the skin uncertainty we report is larger than from any other system studied. The values reported here for $^{48}\text{Ca}$, $^{208}\text{Pb}$ are quite close both to those from recent experimental studies [37, 39] and to those from the relativistic density functional

![Figure 3](image-url)

**FIG. 3.** Neutron-skin probabilities via MCMC sampling for $^{16,18}\text{O}$, $^{40,48}\text{Ca}$, $^{58,64}\text{Ni}$, $^{112,124}\text{Sn}$, and $^{208}\text{Pb}$. Each axis shows a single element. For elements with two isotopes histogrammed, the lighter isotope is shown using light bars, and the heavier isotope is shown with dark bars. The heights of each distribution have been arbitrarily rescaled to facilitate comparison.

| $^A\text{X}$ | $^A\text{O}$ | $^{40}\text{Ca}$ | $^{48}\text{Ca}$ |
|-------------|-------------|-----------------|-----------------|
| $-0.025\pm0.023$ | $-0.06\pm0.02$ | $-0.051\pm0.04$ | $0.22\pm0.19$ |
| $-0.03\pm0.02$ | $-0.01\pm0.03$ | $0.05\pm0.02$ | $0.17\pm0.12$ | $0.18\pm0.12$ |

**TABLE I.** Neutron skins ($\Delta r_{np}$), in fm, from this work.
model FSUGold as reported in [1]. However, our predicted skin range for \(^{48}\text{Ca}\) differs significantly from the recent coupled-cluster-based prediction of 0.12-0.15 fm from [40], a discrepancy we hope the proposed CREX experiment will resolve. Lastly, the median skins we recover for \(^{112,124}\text{Sn}\) (0.05 and 0.17 fm, respectively) are almost identical to those extracted by [41] (0.06 and 0.18 fm, respectively) from analysis of 295-MeV proton elastic scattering on Sn isotopes.

Conclusions. – Using a newly-generalized version of the DOM, we performed the first systematic DOM analysis across nine isotopes from \(A=16\) to \(A=208\) to extract matter and binding-energy density distributions. By using MCMC with model discrepancy terms and joint fitting of multiple isotopes, we generated realistic uncertainties for all potential parameters and extracted quantities. Our results quantitatively indicate how asymmetry, Coulomb, and shell effects contribute to neutron skin generation and drive a disproportionate share of the total binding energy to the deepest nucleons. Using simple trends in \(^{16}\text{O}, \ ^{40}\text{Ca}, \ ^{58,64}\text{Ni}, \ ^{112,124}\text{Sn}\), we estimate the \(^{56}\text{Ni}\) neutron skin as between -0.04 and -0.07 fm and between -0.07 and -0.12 fm for \(^{100}\text{Sn}\). Our skin thickness for \(^{18}\text{O}\) agrees with the mirror-nucleus upper bound expectation, and the agreement of our \(^{48}\text{Ca}, \ ^{112,124}\text{Sn}, \ ^{208}\text{Pb}\) skin thicknesses with recent external predictions augers well for a future truly global DOM treatment.

Acknowledgments. – This work is supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under awards numbers DE-FG02-87ER40316, by the U.S. National Science Foundation under grant PHY-1613362 and PHY-1912643, and was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. C.D.P. acknowledges support from the Department of Energy, National Nuclear Security Administration, under Award Number de-na000383i, the Center for Excellence in Nuclear Training And University-based Research (CENTAUR).

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