Forging new pathways to improved nuclear-reaction predictions

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Introduction - How do neutrons and protons arrange themselves to produce an atomic nucleus? This fundamental question has been the underlying motivation in the advancement of nuclear physics for over half a century now. After all this time, even with all the discoveries and advancements in the field, we still don't have the answer to this simple question. Much progress has been made toward an answer by investigating the nature of atomic nuclei through nuclear scattering experiments. By observing (and quantifying) the collision of nuclei, the mechanisms that dictate the subsequent motion of nucleons (protons or neutrons) can be unravelled. To reach a fundamental understanding of nuclei, a suitable reaction theory is vital in order to interperet experimental data. Experimental techniques, instruments, and facilities are advancing at a rapid rate, so nuclear reaction theory must progress in tandem. A looming challenge in nuclear reaction theory is to provide state-of-the-art predictions for the wealth of experimental data now being produced at DOE's flagship facility for nuclear science, the Facility for Rare Isotope Beams (FRIB), which started user operations in May 2022. FRIB is a facility that generates high-energy rare (unstable, exotic) isotope beams which allows for the study of these short-lived nuclei which otherwise could not be studied (since they are too short lived to act as targets). This exploration of nuclei approaching the limits of stability will provide new insights into the fundamental nuclear force as well as reveal emergent phenomena in the structure of these exotic systems. Indeed, the evolution of nuclear structure as we approach the limits of stability is an overarching theme of the recent DOE Town Hall Meeting which will determine the 2023 Nuclear Long Range Plan. Indeed, from the 2012 Decadal study of Nuclear Physics by the National Academies of Sience, "Nuclear Physics: Exploring the Heart of Matter", it was said that, "Many of today's most important advancements in medicine, materials, energy, security, climatology, and dozens of other sciences emanate from the wellspring of basic research and development in nuclear physics. Answers to some of the most important questions facing our planet will come from nuclear science, interdisciplinary efforts in energy and climate, and marketplace innovations". It is these observations that motivate our proposal to develop more complete reaction descriptions that will help to propel our understanding of nuclear physics to the limits of stability.

The first big step toward understanding the structure of atomic nuclei (that is, the way in which neutrons and protons arrange themselves inside the nucleus) was the advent of the nuclear shell model by Maria Goeppert Mayer in 1948 [CITE]. While this elegant model does a remarkable job describing stable nuclei, it diverges from reality when considering nuclei away from stability (nuclei with excess neutrons or excess protons). Indeed, a rich set of interesting features start to appear for these exotic nuclei (such as halo clustering, shape coexistence, deformations) that the independent shell model has no way of describing. Thus, more complicated nuclear structure models have been developed to try and account for these features, but it is still quite difficult to correctly describe these nuclei near the limits of stability. Naturally, these exotic phenomena can be investigated through the scattering of rare isotopes (of which many systems were not possible to study before FRIB). However, connecting this rich nuclear structure to the experimental data is no easy task. In order to bridge the gap between scattering data and nuclear structure, nuclear reaction theories have been developed. Thus, the path toward understanding nuclei at the limits of stability is the unified, simultaneous development and communication between three areas: improved experimental techniques and facilities to measure unstable nuclei (i.e. FRIB), the development of more precise nuclear structure models, and the development of better reaction theories.

Our approach to improving nuclear-reaction calculations is to develop an effective nucleon-nucleon interaction. The need for an effective interaction is most clearly demonstrated in so-called knockout reactions where a projectile is used to knockout one or more protons (or neutrons) from a nucleus. Employing a dispersive optical model (DOM), developed recently in the PI's PhD, the PI previously performed reaction calculations of both electron-induced knockout $(e, e'p)$ and proton-induced knockout $(p, 2p)$ from the same nucleus ^{40}Ca. The theoretical calculations of these two knockout reactions combine the same structure and continuum information from ^{40}Ca, all of which is consistently provided by the same model - the DOM. The only difference between the two calculations is the interaction between the probe (electron or proton) and ^{40}Ca (see the bottom two schematics in Fig.). Even though most of the ingredients are the same in these two calculations, there is a clear difference in the results when confronted with experimental data (see the top left and right panels in Fig.). Until now, there was not a model like the DOM that could provide the same, consistent ingredients to these reaction calculations. With only one difference between the two calculations, it is clear that the deficiency in the proton-induced calculation is rooted in the interaction between the probing proton and ^{40}Ca. Indeed, the interaction of electrons with nucleons is well-understood so it is not surprising that the proton-induced reaction is more difficult. This lack of consistency poses a problem, since while both reactions probe the same nuclear structure, any structure information extracted from the proton-induced experiment will be off by roughly 20%. To rectify the deficiency in the proton-induced reaction calculation, we will improve the proton-proton interaction causing the issue. Fortunately, we are in a great position to accomplish this by combinine many-body theory and the DOM to generate a more realistic proton-proton interaction that is encoded with ^{40}Ca - see Fig.

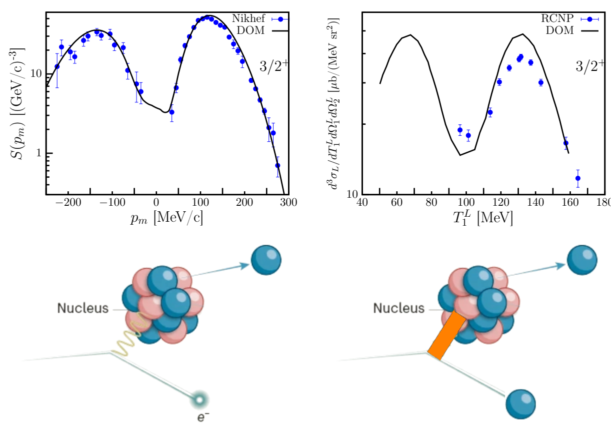


Figure 1: The left figure shows the results of a DWIA calculation of ^{40}Ca$(e, e'p)^{39}$K using DOM ingredients. The right figure shows a similar DWIA calculation, except the probe is now a proton rather than an electron, ^{40}Ca$(p, 2p)^{39}$K. While the same DOM ingredients are used in both cases, the electron-induced knockout reaction [left] reproduces the experimental data much more accurately than the proton-induced knockout reaction [right]. Below each curve is a schematic of each process.

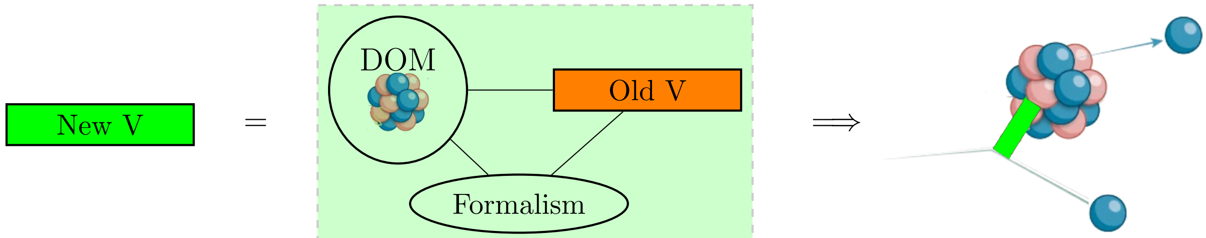


Figure 2: Schematic of the how the effective interaction is generated and how it is used to improve the proton-induced knockout reaction

Until the DOM was developed, previous calculations of (p,2p) were always scaled to match the experimental data - meaning that there was no way to tell if there were a discrepancy in the structure description. Because of this, the proton-proton interaction used in the (p,2p) reaction has not seen development for over two decades. The most recent development was in 2000[CITE] where a group from Melbourne used infinite nuclear matter (an idealized nuclear system) in order to include some kind of nuclear-medium effects. Our implementation will be the first to actually include effects from finite nuclei in the effective interaction implemented in the proton-induced reaction. It may seem that a simpler solution to the difficulties of proton-induced reactions is to focus on electron-induced reactions since they pose less issues. The problem with electron-induced reactions it they require a stable target, and we (as a scientific community) are interested in the structure of nuclei near the limits of stability. As we mentioned earlier, unstable nuclei can only be studied with rare isotope beams like those generated at FRIB. Thus, we are working toward improving proton-induced (and more generally nucleon-induced) nuclear reactions through the development of an effective nucleon-nucleon interaction - an improvement that could account for discrepancies of roughly 20%.

Project Plan - To develop a finite-nucleus-informed effective interaction for nuclear reactions we consider the many ways in which a nucleon interacts as it propagates through a nucleus. A natural language to discuss this is the through Green's functions (or single-particle propagators) and perturbation theory [1]. Indeed, knowing the single-particle propagator of a nucleus is a powerful lever-arm in perturbation theory. We already have an accurate single-particle propagator from the DOM. With this, we have the basic building-block to construct the effective interaction. By combining a bare nucleon-nucleon interaction and the DOM single-particle propagator, the effective interaction can be calculated using already-derived many-body formalism. The approximation that we can implement will be valid at energies approximately greater than 70 MeV/u, which also corresponds to the region of validity for the DWIA reaction description of (p,2p).

While the many-body formalism of this approximation to an effective interaction has been known for some time now, it has only been possible to implement in the fictional system of infinite nuclear matter [CITE]. The limitation, until now, has been obtaining an accurate single-particle propagator for finite nuclei. Now that the DOM provides the single-particle propagator in finite nuclei, we can apply this formalism in a realistic system. Implementing the many-body formalism in a finite system is still nontrivial however, even starting from an already-known propagator. The largest bottle neck in the computation of this interaction will be a large matrix inversion. Not only will the matrix inversion be computationally costly, but the generation of the matrix involves multi-dimensional integrals which will be computationally demanding. The limitation of computational power has also been a contribution to the inability to implement this formalism in the past. While this many-body formalism will be implemented in a general way, we will specifically be calculating the effective interaction in ^{40}Ca as it is a doubly-magic nucleus and the DOM describes it well. Generally, our objectives are to generate this effective interaction then demonstrate how it enhances reaction theory through some specific cases:

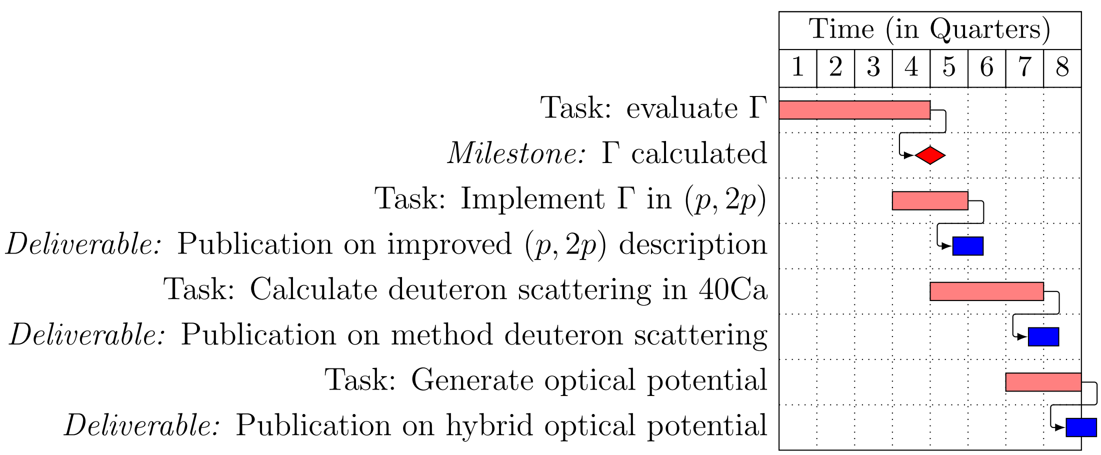
Objective I: Calculate the effective interaction in ^{40}Ca I will combine a chiral NN interaction (the ones typically used in *ab initio* calculations [CITE]) with the DOM proton propagator of ^{40}Ca to generate an effective proton-proton interaction in ^{40}Ca. This objective will involve heavy code development as the many-body formalism has not been implemented for finite nuclei. I plan to utilize parallel programming so that the multi-dimensional integrals needed in the many-body calculation will be tractable. The PI will be developing the code for this objective with general guidance from Co-Is Sofia Quaglioni and Gregory Potel. The expertise of Wim Dickhoff will be invaluable when implementing this many-body formalism. I can test my code by using it to calculate free NN scattering, since the formalism will exactly correspond to free-nucleon scattering if I use free propagators in the calculation rather than the DOM ^{40}Ca propagators.

Objective II: Calculate ^{40}Ca$(p,2p)^{39}$K using the ^{40}Ca effective interaction Once the effective proton-proton interaction is generated in ^{40}Ca, it will be straightforward to calculate the ^{40}Ca$(p,2p)^{39}$K cross section in the same way that Fig. was generated. The pipeline with outside collaborator Yoshida is already in place to use the DOM ingredients in the reaction calculation. The only difference in the calculation will be that now I can also provide the proton-proton interaction that will be used in the calculation. We don't foresee any complications arising in linking our new effective interaction with the existing $(p,2p)$ reaction code. This will result in an improved calculation which will ideally address the discrepancy see in Fig. , confirming that the effective interaction is indeed incorporating in-medium effects in a realistic way.

Objective III: From the effective interaction, calculate deuteron scattering in ^{40}Ca After demonstrating the usefulness of the effective interaction in proton-induced knockout, we can also use it to improve deutron-based reactions. The deuteron is a nucleus consisting of one proton and one neutron bound together. Thus, the relevant interaction involving deuterons is a proton-neutron interaction. Instead of calculating the proton-proton effective interaction, it is no extra work to calculate the proton-neutron effective interaction. Using this proton-neutron effective interaction, we can calculate the proton-neutron propagation through a nucleus (in this specific case it will be ^{40}Ca). Using this proton-neutron propagator, we can describe deuteron elastic scattering with ^{40}Ca. Once this is established and verified by comparing with elastic scattering data, the deuteron propagator can then be used to improve more complicated reactions such as (d,p) and (p,d). These reactions can act as surrogates to neutron-induced reactions (neutron capture, for example). This objective will demonstrate another class of reactions that will benefit from the calculation of this effective interaction. The PI will work closely with co-I Potel when implementing the deuteron propagator.

Objective IV: From the effective interaction, calculate an optical potential in ^{40}Ca Another immediate application our effective interaction is the ability to generate an proton (or neutron) optical potential. An optical potential describes the scattering of protons (or neutrons) with nuclei (in this case it will be ^{40}Ca). Almost any theoretical description of a reaction involving medium-to-heavy mass nuclei requires an optical potential. Building an optical potential from our effective interaction is a way of explicitly including the NN interaction into the DOM which is purely phenomenological. We see two motivations for generating this optical potential. The first is that it provides an improvement (in the form of microscopic elements) to the DOM, marking the advent of a new class of hybrid optical potentials which could lead to better extrapolations of nuclei off stabilty. The second is that it paves the way toward a truly *ab initio* optical potential.

Deliverables and Milestones The timeline of the project is outlined in the Gantt chart below. Deliverables consist of publishing three papers in high-profiles papers, one for each implementation of the developed interaction.



Project Impact - This project builds a pathway toward better reaction predictions which will help to launch LLNL further into the forefront of probing new physics in exotic nuclei. In addition to providing a deeper understanding nuclear structure, this project also supports LLNL's Stockpile Stewardship mission through better reaction calculations. Improved reaction descriptions will greatly enhance the scientific community's ability to extract structure information from the wealth of reaction data coming from FRIB. This will help to strengthen the already-healthy relationship between LLNL and FRIB. Additionally, cultivating new collaborations with Washington Univeristy in St. Louis and the Japanese Atomic Energy Agency will expand LLNL's scientific network.

Risks and Mitigations - Even with the reaction description improved dramatically (and made more consistent), it is possible that implementing the effective interaction won't fully account for the discrepancy in the (p,2p) results in Fig. . If this turns out to be the case, the work is still important because it will inform us that something in the reaction description itself is now the problem. With a full treatment of the boundstates, scattering states, and effective proton-proton interaction consistently derived from the same DOM potential, this calculation would show without ambiguity that the reaction description needs more development.
Project Team - The team consists of postdoctoral researcher Mack Atkinson (PI), staff scientist Gregory Potel (co-I), staff scientist Cole Pruitt (co-I), and NACS group leader Sofia Quaglioni (co-I), outside collaborator Willem Dickhoff (full professor at Washington University in St. Louis), and outside collaborator Yoshida Kazuki (staff scientist at the Japan Atomic Energy Agency (JAEA)). Atkinson is an expert in many-body theory and reaction theory. He will be developing the code to calculate the effective interaction. Potel is an expert in reaction theory, particularly those involving deuterons. He will be involved with Objective III when implementing the effective interaction to calculate deuteron scattering. Pruitt is an expert in optical potentials and the DOM. He will assist in integrating the effective-interaction-derived optical potential (Objective IV) into the DOM. Quaglioni is a world-recognized expert in *ab initio* reaction theory who will provide guidance throughout the life of the project. Dickhoff is an expert in many-body theory; he will lend support for Objective I when calculating the effective interaction in 40Ca. Yoshida is an expert in (p,2p) reactions and will be heavily involved in objective II when the effective interaction is applied in the $^{40}\mathrm{Ca}(p,2p)^{39}\mathrm{K}$ reaction.
Budget - We request funding in the amount of \$221k for Year 1 and \$230k for Year 2 to support: the PI at 50%, Potel at 10%, Pruitt at 10%, and Quaglioni at 5%. The funding will also include travel for the PI to disseminate the results of the project at conferences/workshops.
Exit Plan - This project will enhance LLNL's capability to predict a variety of high-energy nuclear reactions important for nuclear astrophysics and National Security applications which will help to grow LLNL's DOE Office of Science (DOE/SC) base funding for nuclear physics. This project will boost the visibility of the PI and set the stage for pursuing a DOE Early Career Award. Upon completion of the effective interaction, the applications to other nuclear reactions are many. While this project focuses on ^{40}Ca the code to generate the effective interaction will be agnostic to the particular nucleus, so this method can then be applied to any nucleus. Thus, we can continue to utilize the machinery for generating the effective interactions relevant to many other reactions. Furthermore, the particular reactions that we choose to demonstrate during the project are just a subset of what is possible with this formalism. The consistent description of the (p,2p) reaction can lead to an analysis of many other (p,2p) data and could even help to address the polarization puzzle to which there is no current solution. With the endorsement of FRIB400 (a higher energy beam at FRIB) in the Nuclear Structure and Reactions Town Hall Meeting in 2022, there will certainly be many new (p,2p) experiments being performed at the limits of stability whose analysis will benefit from this effective interaction machinery. The deuteron studies will be highly relevant for

many deuteron-based experiments at FRIB. Finally, the beginnings of a hybrid optical potential that is both phenomenological while also containing microscopic elements could help to control the extrapolation of these potentials away from stability.

Summary - We will develop a method to generate an effective nucleon-nucleon interaction in nuclei improve nuclear-reaction calculations. The need for this effective interaction is most clearly demonstrated in the knockout reactions presented in Fig. , revealing a 20% discrepancy in what boundstate information can be extracted from this reaction. Employing our proposed effective interaction in this calculation will remedy this situation, thus enabling the community to reliably extract nuclear structure properties from these complex nuclear reactions. This will be the first time a nucleon-nucleon interaction is dressed specifically with finite-nucleus information. The effective interaction can improve many other reaction calculations beyond just $(p, 2p)$, two of which we will explicity demonstrate during our project (deuteron scattering and optical potentials). Without accurate nuclear-reaction predictions, very little could be learned from nuclear scattering experiments. Thus, our improvements to nuclear-reaction descriptions help to harness the wealth of experimental data coming from the DOE-funded facility FRIB to investigate nuclei approaching the limits of stablity. Our improvements to nuclear-reaction predictions are vital to further unravelling the mystery of how protons and neutrons arrange themselves in nuclei.

References

[1] W. H. Dickhoff, D. Van Neck, Many-Body Theory Exposed!, 2nd edition, World Scientific, New Jersey, 2008.