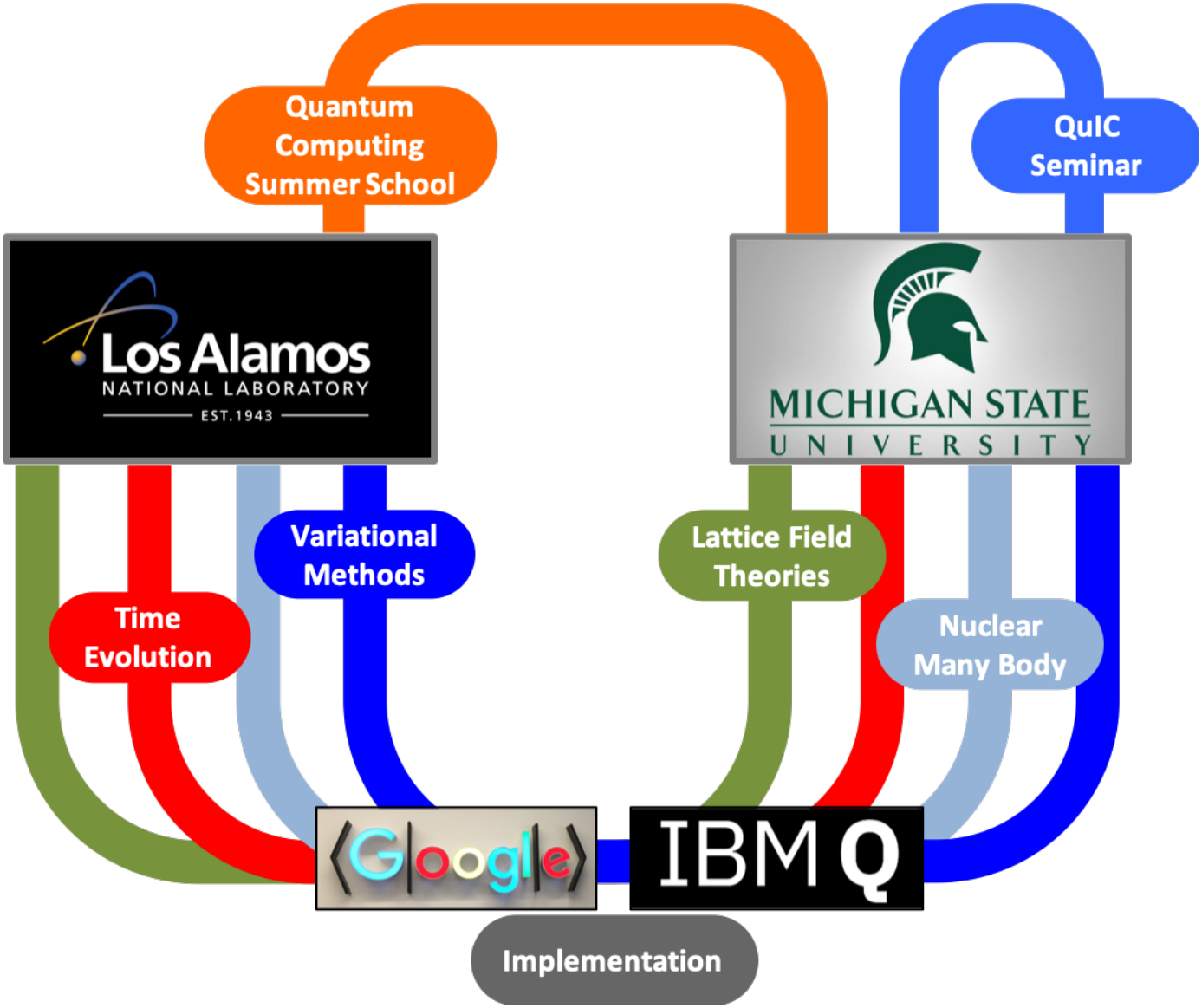
From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem [5mm]



DOE Quantum Horizons: QIS Research and Innnovation for Nuclear Science

May 26, 2019

Title: From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem

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DOE Funding Opportunity Announcement (FOA) Number: DE-FOA-0002110
FOA type: Initial
CDFA Number: 81.049
DOE/Office of Science Program Office: **Nuclear Physics**
DOE/Office of Science Program Office Technical Contact: Dr. Gulshan Rai (301-903-4702), gulshan.rai@science.doe.gov
Research Area: Theoretical Nuclear Physics; Computational Many-body Physics; Lattice Quantum Chromodynamics; Quantum Algorithms; Quantum Simulations

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Table 1: List of Team Members

Team Members			**Institution**
Last Name	First Name	Title	Institution Name
Bazavov	Alexei	Assistant Professor	Michigan State University
Bogner	Scott	Professor	Michigan State University
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Contents

1 Executive Summary

Michigan State University (MSU) and the Facility for Rare Ion Beams (FRIB) are submitting a proposal on **From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem**.

Intellectual merit: For nuclear theorists, the overarching challenge is to develop a comprehensive description of nuclei and their reactions, grounded in the fundamental interactions between the constituent nucleons with quantifiable uncertainties to maximize predictive power. As experimental frontiers have shifted to the study of rare isotopes, the predictive power of successful phenomenological approaches like the shell model and density functional theory is challenged by the scarcity of nearby experimental data to constrain model parameters. Therefore, it is expected that *ab initio* methods will play an increasingly prominent role to help improve the predictive power of such "data driven" methods as experiment moves deeper into largely unexplored regions of the nuclear chart.

To understand why nuclear matter is stable, and thereby shed light on the limits of nuclear stability, is one of the overarching aims and intellectual challenges of basic research in nuclear physics. To relate the stability of matter to the underlying fundamental forces and particles of nature as manifested in nuclear matter, is central to present and planned rare isotope facilities such as the DOE facility FRIB under construction at Michigan State University. From a theoretical standpoint, this involves understanding how the basic building blocks of Nature interact and conspire to build up atomic nuclei as we know them, with the aim to understand what makes visible matter stable. The theoretical efforts span from methods like Lattice Quantum Chromodynamics, via effective field theories to many-body theories applied to atomic nuclei and infinite nuclear matter. All these methods rely on theoretical approximations whose applicabilities are often limited by the dimensionality of the specific problem being studied. In recent years there has been considerable progress in our theoretical understanding of algorithms from quantum information applied to interacting systems, with the hope to circumvent many of the traditional dimensionality problems.

This proposals unites the efforts of nuclear many-body theorists, quantum information theorists and mathematicians, with the aim to explore and develop stable algorithms for studying nuclear systems using recent progress in quantum information theory. It involves researchers from Michigan State University (MSU) and the National Superconducting Cyclotron Laboratory (NSCL)/Facility for Rare Ion Beams (FRIB) and Los Alamos National Laboratory, with the aim to build up an interdisciplinary team of nuclear theorists and quantum information theorists in order to explore the feasibility of quantum information theory applied to the nuclear many-body problem.

Broader impacts: The training received by undergraduates, graduate students, and postdoctoral research associates in carrying out the proposed activities contributes directly to the building of a diverse scientific workforce. The present proposal has a large educational component, being part of the nuclear physics program at FRIB/MSU that was recently ranked number one in the country. The mix of analytical and numerical computations our students must employ is an excellent preparation for both academic and industrial research. The PIs are committed to diversity in science.

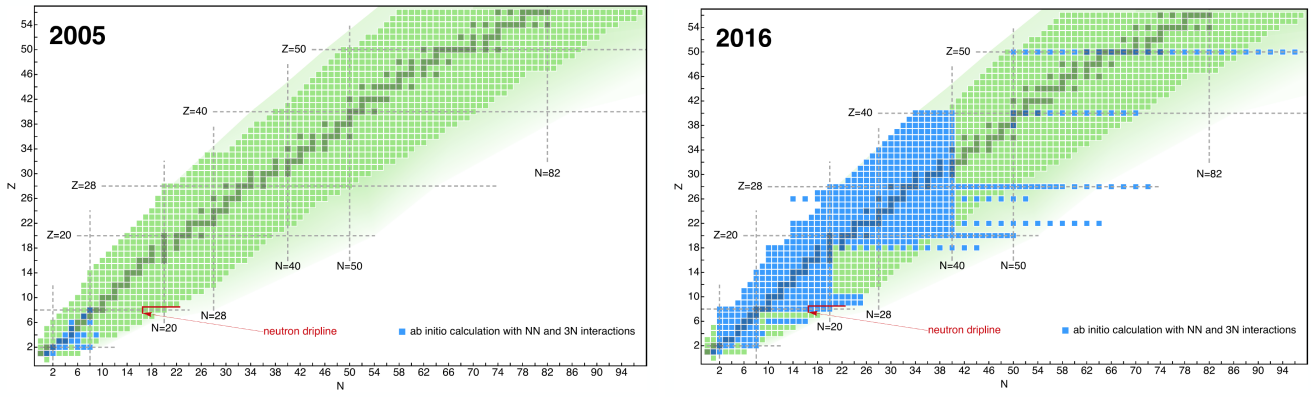
2 Introduction and Scientific Motivation

2.1 The overarching intellectual question(s)

Can we understand nuclei and nuclear matter and the limits of stability of matter in terms of the fundamental laws of motion and forces? Stated differently, can we relate what we observe experimentally to the properties of the strong force and its underlying theory quantum chromodynamics?

One of the fundamental intellectual challenges in nuclear physics is to understand why nucleonic matter is stable, how it comes into being, how it evolves and organizes itself, and what phenomena emerge. The task facing nuclear theorists is to develop the tools to help answer these questions by relating the existence and properties of nuclei to the underlying fundamental forces and degrees of freedom. As experimental efforts have shifted towards the study of rare isotopes, there has been an increased urgency to develop reliable calculations to counter the inherent limitations of "data-driven" approaches which rely on experimental data to constrain model parameters, such as the phenomenological shell model and density functional theory.

For decades progress in nuclear few- and many-body theory was slowed by the lack of a consistent theory for the strong inter-nucleon interactions, and by the computational demands required to handle the non-perturbative



(a) (b)

Figure 1: The chart of nuclides and the reach of *ab initio* calculations in (a) 2005 and (b) 2016. Nuclei for which *ab initio* calculations exist are highlighted in blue. Note that the figure is for illustrative purposes only, and is based on the authors' non-exhaustive survey of the literature.

aspects resulting from the "hard cores" and strong tensor forces found in most interaction models. For many years, the only option for controlled calculations was to use quasi-exact methods such as quantum Monte Carlo (QMC) or no-core shell model (NCSM), which limited the reach of so-called *ab initio*[1] calculations to light *p*-shell nuclei. Approximate (but systematically improvable) methods that scale favorably to larger systems, like coupled cluster (CC) theory and many-body perturbation theory (MBPT), were largely abandoned in nuclear physics, despite enjoying tremendous success in quantum chemistry.

Much has changed in recent years, as advances in chiral effective field theory (EFT), which provides a systematic framework to construct consistent two- and three-nucleon interactions, together with the development of powerful many-body methods have pushed the frontiers of *ab initio* theory well into the medium-mass region, see Fig. 1. Initial applications of these methods were limited primarily to ground-state properties of stable nuclei near shell closures with two-nucleon forces only. Substantial progress has since been made on including three-nucleon forces, targeting excited states and observables besides energy, and moving into the more challenging terrain of open-shell and unstable nuclei. The recent work of Jansen *et al* [**?**] on the structure of ^{78}Ni and nearby nuclei represents some of the progress which has been made recently in pushing the limits of first principle methods. Remarkably, progress on the many-body front has been so swift in recent years that inadequacies of the current-generation chiral two- and three-nucleon interactions, rather than the many-body calculations themselves, are the primary obstacles to systematic calculations across the medium-mass region [**?**].

The recent progress in many-body theories for nuclei are also intimately linked with the determination and our understanding of the equation of state (EoS) for nuclear matter. Bulk nucleonic matter is interesting for several reasons. The EoS of neutron matter, for instance, determines properties of supernova explosions and neutron stars and it relates the latter to neutron radii in atomic nuclei. Likewise, the compressibility of nuclear matter is probed in isoscalar giant monopole excitations, and the symmetry energy of nuclear matter is related to the difference between proton and neutron radii in atomic nuclei.

The developments of nuclear Hamiltonians from EFT, combined with improved few- and many-body theories, has prepared the ground for systematic studies of nuclear systems. The methodological and algorithmic advances seen during the last decade allow for controlled calculations (a high-resolution description) of nuclear properties. In spite of these developments there are still several unsettled aspects with nuclear Hamiltonians derived from EFT, ranging from a proper understanding of three- and many-nucleon forces to the link with the underlying theory of the strong force.

We are however now in a situation where progress in Lattice Quantum Chromodynamics (LQCD) [**?**, **?**] allows

[1]The concept *ab initio* or first principle calculations is normally reserved to calculations performed in terms of the underlying forces and elementary particles. In several few- and many-body communities this has been extended to mean exact or quasi-exact calculations with a given input Hamiltonian/Lagrangian. The latter is not necessarily the one which relates directly to the fundamental bulding blocks.

us to link theoretically EFT derived Hamiltonians with LQCD calculations. The LQCD calculations are presently performed away from the physical masses of the constituents and the future challenges involve developing the capabilities to perform calculations at both the physical point, as well as away from the physical point, using lattice spacings and volumes that can match EFT calculations. This will allow us to link properly LQCD, via EFT based Hamiltonians, with few- and many-body theories used to study nuclear systems, providing thereby a theoretical platform for understanding nuclear systems in terms of the underlying theory for the strong force, as shown schematically in the figure here.

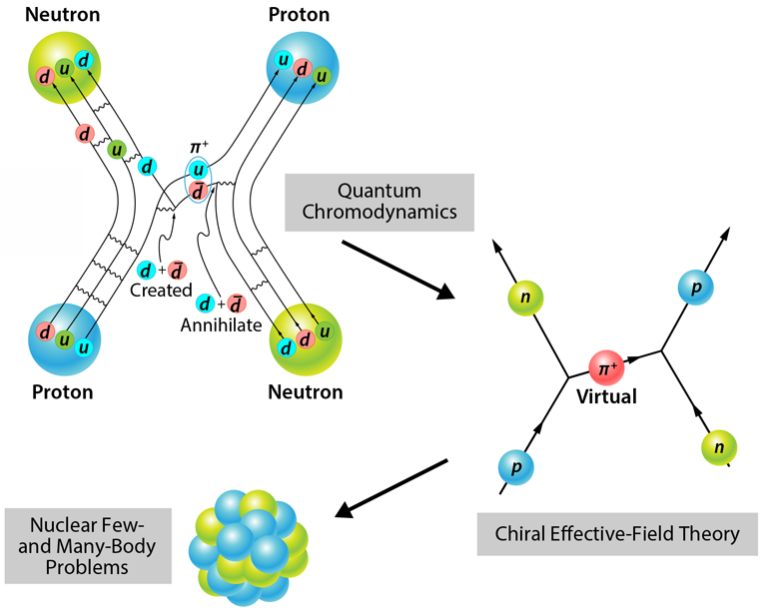


Figure 2: A first principle approach to nuclei and nuclear matter, linking QCD with few- and many-body methods.

2.2 Aims

The various few- and many-body methods mentioned above allow for controlled approximations and provide a computational scheme which accounts for successive corrections in a systematic way.

However, all these methods face in some form or the other the problem of an exponential growth in dimensionality. For a system of P fermions which can be placed into N levels, the total number of basis states are given by

$$\left(\begin{array}{c} N \\ P \end{array} \right).$$

The dimensional curse means that most quantum mechanical calculations on classical computers have exponential complexity and therefore are very hard to solve for larger systems. If we wish to study for example nuclei close to the limit of stability, the increased degrees of freedom (both in terms of possible excitations as well as the inclusion of at least two- and three-body Hamiltonians) pose severe challenges to essentially all existing classical many-body methods. On the other hand, a so-called quantum computer, a particularly dedicated computer, can improve greatly on the size of systems that can be simulated, as foreseen by Feynman [**?**, **?**]. A quantum computer does not need an exponential amount of memory to represent a quantum state. The basic unit of information for a quantum computer is the so-called qubit or quantum bit. Any suitable two-level quantum system can be a qubit, but the standard model of quantum computation is a model where two-level quantum systems are located at different points in space, and are manipulated by a small universal set of operations. These operations are called gates in the same fashion as operations on bits in classical computers are called gates.

The aim of this project/proposal is thus to explore and develop algorithms based on quantum computing in order to study nuclear systems. The first aim is to implement these algorithms on classical computers utilizing

state-of-the art technologies with both CPUs and GPUs. We will in particular focus on quantum algorithms that can be applied to

- Lattice QCD simulations of quantum field theories, with the aim to perform calculations at the physical point with relevant lattice spacings.
- Develop theory that allows for hybrid and multiscale simulations of LQCD and EFT on the lattice, linking thereby quark and gluonic degrees of freedom with nucleons and pions as effective degrees of freedom.
- The link between LQCD and lattice EFT will also explore quantum machine learning algorithms, using LQCD results and experimental data on few-nucleon systems to constrain Hamiltonians for few- and many-body methods.
- With the pertinent effective Hamiltonians, including two- and three-body forces from EFT, we aim at developing quantum algorithms for studying nuclear few- and many-body problems. The feasibility of these algorithms will be comparedto existing many-body methods like Coupled Cluster theory and in-medium Similarity Renormalization Group approaches on classical high-performance computing facilities

Strategic relevance To understand why matter is stable, and thereby shed light on the limits of nuclear stability, is one of the overarching aims and intellectual challenges of basic research in nuclear physics. To relate the stability of matter to the underlying fundamental forces and particles of nature as manifested in nuclear matter, is central to present and planned rare isotope facilities such as the DOE facility FRIB under construction at Michigan State University.

To understand the stability of nuclear matter in order to interpret the wealth of data that will come from facilities like FRIB, requires theoretical methods that span many energy and length scales[2]. To relate the theoretical interpretations with the underlying fundamental forces poses a severe challenge to first principle descriptions of nuclear systems. The theoretical modeling of nuclear matter requires thus a multiscale approach, where different degrees of freedom are present. Exploring algorithms based on quantum computing and present and future high-performance computing facilities is an essential part of our efforts to understand properly nuclear systems.

3 Proposed Research and Methods

3.1 Project Description

3.2 Quantum Simulation Algorithms

(1) Introduction The answers to many important scientific questions rely on computer simulations. Galactic evolution, weather patterns, drug discovery, and many-body physics all require high-performance computational techniques. Current computers are fundamentally limited by physical restrictions on transistor sizes—Moore's law is failing. To answer critical questions at the forefront of science, new models of computation need to be developed.

Among several promising candidates for future computing technologies (probabilistic & neuromorphic computing, tensor & graphical processing units, etc.), quantum computers (QCs) are one of the most exciting. For certain problems, algorithms for QCs (quantum algorithms/QAs) can provide exponential speedups over the best algorithms for current computers (for example, the quantum Fourier transform). With future QCs, such algorithms will enable us to compute in hours what would currently take years. However, current QCs are noisy and have not yet demonstrated clear advantage over classical computers. To do this, we must redesign existing QAs to counteract the noise of current QCs. For the long-term, we must design new QAs to expand the problem set future QCs can efficiently solve.

I propose to use machine learning (ML) to help (re)design QAs. This exciting new idea has been explored in two seminal papers [1, 2] and my own research [3]. ML can redesign existing algorithms for current/near-term QCs and design new algorithms for future QCs.

[2] A description of properties of nuclei and neutrons stars in terms of hadronic degrees of freedom spans over 19 orders of magnitude in length scale, from approximately the 10^{-15} m of the proton and neutron radii to the few kilometers which determine the radius of a neutron star.

(2) Preliminary work ML has been used to design QAs for mathematical functions, a result that provides important subroutines for other QAs [1]. ML has also been used to design a QA for computing quantum state overlap [2]. In collaboration with the authors of [2], I used this result to design a new QA for matrix diagonalization (pre-print at [4]).

Additionally, I used ML to redesign several known QAs for current QCs. This work has been published in a pre-print [3] that shows, e.g., the quantum Fourier transform (QFT) redesigned to the hardware constraints of "ibmqx4" (a current five-qubit QC). Our redesigned algorithm is more robust to noise/errors on ibmqx4 than the standard QFT algorithm.

(3) Proposed work I propose to expand on my prior work to use ML to redesign QAs for near-term QCs (see 3.1) and design new QAs for future QCs (see 3.2). A quantum algorithm $\mathcal{A}$ is defined by a set of N gates $\mathcal{A} = \{G_i(k_i, \theta_i)\}_{i=1}^{N}$ that describe a unitary matrix. Here, G_i is the ith gate that acts on qubits indexed by k_i, and θ_i denotes internal gate parameters.

(3.1) Algorithm redesign for near-term QCs I will use a "cost-driven" method to optimally redesign QAs for current/near-term QCs. Optimal algorithms need to contain as few gates as possible (due to noise), and only a limited set of gates can be implemented on current QCs. Despite this, current QCs have been used to compute the deuteron binding energy in nuclear physics, compute ground-state energies of small molecules in chemistry, and (a result of my own research [5]) learn decision boundaries for classification problems in data science. My proposed work will increase possible problem sizes (bigger nuclei/molecules/etc.) and reduce errors by redesigning QAs to have fewer gates and added "noise-adjusting" gates.

My proposed method works as follows. Let $\mathcal{U}$ be a known QA, $\mathcal{Q}$ a current/near-term QC, and $\mathcal{Q}_G$ the set of gates that can be implemented on $\mathcal{Q}$. The goal is to design a new algorithm, $\mathcal{A}$, that produces the same output as $\mathcal{U}$ but with fewer gates. We first initialize a guess for our trainable algorithm $\mathcal{A}$ with all gates G_i from $\mathcal{Q}_G$. We then evaluate the cost $C(\mathcal{A},\mathcal{U}) = ||\mathcal{A} - \mathcal{U}||$ for a given matrix norm $|| \cdot ||$. The parameters $\{G_i(\theta_i), k_i\}$ in $\mathcal{A}$ are then iteratively adjusted to minimize the cost. When the cost is exactly (approximately) zero, we learn an exact (approximate) algorithm. Using similar methods in [3], I have redesigned QAs with significantly fewer gates compared to standard *quantum compiling* methods, which only locally translate individual gates into $\mathcal{Q}_G$. Additionally, by training $\mathcal{A}$ in the presence of noise, our redesigned QAs add in gates to adjust for noise. Algorithms with fewer gates and noise-adjusting gates will enable more/larger problems to be solved on near-term QCs.

My proposed work will use this method to optimally redesign QAs for simulating fermionic systems on "ibmqx5" (a current sixteen-qubit QC). This work will enable more accurate and longer simulations of Hamiltonian evolution for many chemical systems. As QCs scale to larger sizes, my proposed method could revolutionize quantum chemistry and drug discovery.

(3.2) Algorithm design for future QCs I will use a "data-driven" method to design new QAs for future QCs. The goal is to design a new QA $\mathcal{A}$ for some function f, which could be anything from computing quantum state overlap to a mathematical operation like integration. At a low-level, however, all such functions f map bit-strings to bit-strings.

My proposed method works as follows. First, we pick a number of qubits n and evaluate f (using a classical computer) on bit-strings x_j. This provides training data $y_j = f(x_j)$, where $j = 1, ..., D$. We then train over the parameters $\{G_i(\theta_i), k_i\}$ in our algorithm $\mathcal{A}$ to minimize the cost $\sum_{j=1}^{D} ||y_j - \mathcal{A}(x_j)||^2$. Then, we repeat this process for multiple n. After, we analyze the learned algorithms to gain insight from the quantum gates that compute f on multiple problem sizes. Using pattern matching or motif recognition, we can deduce a new QA.

A similar approach was used in [2] to learn a new QA for computing state overlap. My proposed work will design new QAs for computing quantum entropies of quantum states. Such QAs, currently unknown, would be extremely useful for characterizing quantum states produced by, e.g., simulation algorithms on QCs. These functions fit well into my data-driven method because they can be computed classically & scale naturally to multiple problem sizes.

(4) Challenges In both methods, numerical optimization over the parameters $\{G_i(\theta_i), k_i)\}$ is challenging for large algorithm sizes. To overcome this, we can introduce an algorithm "ansatz," or structure, to eliminate the k_i and even G_i parameters. Additionally, for the cost-driven method, we can train over "sub-algorithms" (subsets of gates) to limit the large search space while still exploring a larger space than other quantum compiling methods.

For the data-driven method, deciding which gates to include in training is an open question. Further research is needed to identify the necessary number of training data points (i.e., the D above). Methods from active learning can significantly reduce D for large algorithm sizes.

(5) Intellectual merit The idea of ML for QA design has demonstrated initial success in seminal papers [1, 2] and my own research [3]. The cost-driven method searches a more expansive space than standard quantum compiling methods to produce more optimal and more robust QAs. This method could redesign any known QA for any given QC. Methods for designing QAs for future QCs do not exist. My proposed data-driven method could produce many new QAs with applications in many fields. The recent success of this approach in [2] necessitates further study. My knowledge of both ML and QAs is ideal for these methods.

(6) Broader impact This research will significantly increase what is possible with near-term QCs and produce new algorithms for future QCs. Both will improve our understanding of the power of QCs, which have the potential to answer some of the most important scientific questions of the 21st century. Powerful QAs could impact society outside of academia as well—e.g., efficient chemistry could discover new drugs that vastly improve human health.

3.3 Software for Quantum Simulations

3.3.1 Lattice QCD

3.3.2 Variational adiabatic evolution

In order to perform calculations of the properties of nuclear systems via quantum computing, we need to be able to prepare quantum states in an eigenstate of the nuclear Hamiltonian. The method of adiabatic evolution is one approach to quantum state preparation [**?**]. The adiabatic theorem tells us that if we start in an eigenstate of some time-dependent Hamiltonian $H(t)$, then we remain in an eigenstate of $H(t)$ so long as the time dependence is sufficiently slow and we do not pass through level crossings. Let us start with some simple Hamiltonian H_z whose ground state ϕ_z^0 can be prepared simply using single qubit gate operations. Suppose we want to produce the ground state $\phi_\odot^0$ for some nontrivial Hamiltonian $H_\odot$. We can define a time-dependent Hamiltonian $H(t)$ so that $H(0) = H_z$ and $H(\tau) = H_\odot$. If the time dependence is sufficiently slow and we do not pass through any level crossings, then we obtain an accurate representation of $\phi_\odot$ after reaching time $t = \tau$,

$$\phi_\odot^0 = T \exp\left[-i \int_0^\tau H(t) dt\right] \phi_z^0. \tag{1}$$

In practice, however, decoherence on near-term devices means that the amount of time evolution is severely limited. This problem is substantially ameliorated for an analog quantum simulator. However, there remains a general problem of dealing with the errors generated by imperfect adiabatic evolution.

The strategy of variational adiabatic evolution is to produce a subspace of states corresponding to different time-dependent Hamiltonians $H_n(t)$. We construct the time-evolved state $\psi_n = U_n \phi_z^0$, where U_n is

$$U_n = T \exp\left[-i \int_0^\tau H_n(t) dt\right]. \tag{2}$$

This unitary operation can be implemented in small time steps using the Trotter approximation. In order to compute the inner product $\psi_n|\psi_m$ and amplitude $\psi_n|H_\odot|\psi_m$ we use one auxiliary qubit. We initialize the auxiliary qubit as 0 while the main system is prepared in the state ϕ_z^0. We perform a Hadamard transform on the auxiliary qubit and implement controlled unitary gate operations to obtain

$$0\phi_z^0 \to (1/\sqrt{2}0 + 1/\sqrt{2}1)\phi_z^0 \to 1/\sqrt{2}0 U_n \phi_z^0 + 1/\sqrt{2}1 U_m \phi_z^0. \tag{3}$$

In order to compute the inner product $\psi_n|\psi_m$, we measure the expectation value of σ_x plus i times σ_y upon the auxiliary qubit. In order to compute the amplitude $\psi_n|H_\odot|\psi_m$, we measure measure the expectation value of $\sigma_x \otimes H_\odot$ plus i times $\sigma_y \otimes H_\odot$. Equipped with the inner products $\psi_n|\psi_m$ and amplitudes $\psi_n|H_\odot|\psi_m$, we can now solve for the variational ground state of $H_\odot$ in the subspace spanned by the vectors ψ_n.

We propose to test the variational adiabatic evolution method for a particle on a one-dimensional lattice of length $2L + 1$ with an attractive short-range potential at the center of the chain. We can write the pieces of the Hamiltonian as

$$H_z = \sigma_z^{(L)}, \tag{4}$$

$$H_{\rm even} = \frac{1}{2} \sum_{n=0,2,\cdots,2L-2} [\sigma_x^{(n+1)} \sigma_x^{(n)} + \sigma_y^{(n+1)} \sigma_y^{(n)}], \tag{5}$$

$$H_{\rm odd} = \frac{1}{2} \sum_{n=1,3,\cdots,2L-1} [\sigma_x^{(n+1)} \sigma_x^{(n)} + \sigma_y^{(n+1)} \sigma_y^{(n)}], \tag{6}$$

$$H_\odot = H_z + H_{\rm even} + H_{\rm odd}. \tag{7}$$

In order to describe the physics of a single particle, we consider the linear space where exactly one qubit is in the 1 state and the remaining $2L$ qubits are in the 0 state. For L_t time steps and total evolution time τ, we define the time interval $dt = \tau/L_t$. We let the unitary operator at time step n_t be

$$U(n_t, L_t, dt) = \exp(-iH_{\rm odd} n_t dt/L_t) \exp(-iH_{\rm even} n_t dt/L_t) \exp(-iH_z dt). \tag{8}$$

We will work with the evolved state,

$$\psi, \tau, L_t = U(n_t, L_t, dt) \cdots U(2, L_t, dt) U(1, L_t, dt) \phi_z^0. \tag{9}$$

We have done some preliminary work to show that this method appears viable. The exact ground state energy of $H_\odot$ in the limit $L \to \infty$ is $-\sqrt{2}$. For $L = 100$ the energy to four significant digits is -1.414. If we use the parameters $\{\tau = 1.0, L_t = 4\}$, we find that the energy expectation value of ψ, τ, L_t is -0.973. This is not an accurate estimate of the ground state energy, but as good as one might achieve with current digital quantum computing technology. If we now apply variational adiabatic evolution with two different trajectories, $\{\tau = 1.0, L_t = 4\}$ and $\{\tau = 1.5, L_t = 4\}$, we get a variational energy of -1.364. We see that there is significant improvement as the variational approach is able to remove some contamination from other low-lying energy states. If we now apply variational adiabatic evolution with three different trajectories, $\{\tau = 1.0, L_t = 4\}, \{\tau = 1.5, L_t = 4\}$, and $\{\tau = 2.0, L_t = 4\}$, we get a variational energy of -1.399. The method appears to be converging rapidly with the number of variational states.

We propose to study the convergence rate and error stabilization of variational adiabatic evolution for our quantum particle bound to a potential for various values of L. We first analyze the system using standard classical computing with simulation software such as Qiskit. We then work with our collaboration partners to implement on digital quantum computing devices at Google and IBM Q. We will compare with standard adiabatic evolution as well as the quantum approximate optimization algorithm [**?**]. We will vary the number of particles, N, and vary the width of the trapping potential in H_z. Our many-body system will correspond to N identical spinless fermions in a one-dimensional trap. For $L = 40$ and $N = 20$ the number of possible quantum states will exceed 10^{11}.

Perhaps the most important aspect of this project is error stabilization. The inner products $\psi_n|\psi_m$ and amplitudes $\psi_n|H_\odot|\psi_m$ will suffer from noise. The first step is to remove any systematic biases using known extrapolation methods [**?**]. For the remaining error we apply new tools that we have recently developed for another computational technique called eigenvector continuation [**?**]. The error stabilization algorithm involves Monte Carlo simulations of the data with estimated errors included, while throwing out trials that do not satisfy physically-motivated conditions such as norm positivity and constraints on level ordering.

If we add a complex Gaussian error with width 0.05 to each of the inner products $\psi_n|\psi_m$ and amplitudes $\psi_n|H_\odot|\psi_m$ in our previous variational calculation with three trajectories, then our error stabilization algorithm gives an estimate of $-1.51(24)$. If error size is reduced to 0.02, the estimate is $-1.46(12)$. For an error of size 0.01 the estimate is $-1.41(7)$. We propose to make further improvements to the error stabilization algorithm by studying the behavior of eigenvectors and eigenvalues under noise perturbations. We will investigate both the underlying theory and its practical implementation.

3.3.3 Spectral reconstruction and transition matrix elements

Quantum phase estimation is one approach to computing the spectrum of a Hamiltonian through real-time evolution and the inverse quantum Fourier transform [**?**]. We propose to investigate a different approach that can compute the low-lying excitation spectrum of a quantum system without the use of auxiliary qubits. The steps

are as follows. We first prepare the state ψ using imperfect adiabatic evolution, as we have discussed in the text surrounding Eq. (2). We can write ψ as a linear combination of eigenstates of $H_\odot$,

$$\psi = \sum_n c_n \phi_\odot^n. \tag{10}$$

The strategy is to prepare ψ so that the sum is dominated by only a few low-lying eigenvectors.

Let O be some Hermitian operator that does not commute with the Hamiltonian and thus induces transitions between energy eigenstates. For example, O could be an electric multipole operator for a nuclear system. We evolve the state ψ for a sequence of equally-spaced times t,

$$\psi(t) = \exp(-iH_\odot t)\psi. \tag{11}$$

We measure the expectation value of O for each t,

$$O(t) = \psi(t)|O|\psi(t). \tag{12}$$

In terms of the energy eigenstates, the expectation value is

$$O(t) = \sum_{n'} \sum_n c_{n'}^* c_n \phi_\odot^{n'} |O| \phi_\odot^n e^{-i(E_\odot^n - E_\odot^{n'})t}, \tag{13}$$

where $E_\odot^n$ is the energy corresponding to $\phi_\odot^n$. Using a classical computer, we now calculate the Fourier transform of $O(t)$. From the Fourier transform we can extract the energy differences $E_\odot^n - E_\odot^{n'}$. This gives us the excitation energies of all low-lying states with non-negligible overlap with $\psi(t)$.

We propose to develop the efficiency of this spectral reconstruction technique by exploring various transition operators O and various imperfectly-evolved states $\psi(t)$ that maximize the transition of each excited state to the ground state. We have done some preliminary work to show that this method is viable for analog quantum simulators. As an example we consider the so-called time fractal system of trapped ions as described in Ref. [**?**]. Similar to atomic nuclei, this system has a rich spectrum of bound states. The bound state energies form a geometric sequence as a consequence of discrete scale invariance.

We consider a one-dimensional chain of ions in a radio-frequency trap with qubits represented by two hyperfine "clock" states. Such systems have been pioneered by the Monroe group using $^{171}\mathrm{Yb}^+$ ions [**?**, **?**]. Off-resonant laser beams are used to drive stimulated Raman transitions for all ions in the trap. This induces effective interactions between all qubits with a power-law dependence on separation distance. We define the vacuum state as the state with $\sigma_z^{(n)} = 1$ for all sites n. We use interactions of the form $\sigma_x^{(n)}\sigma_x^{(n')} + \sigma_y^{(n)}\sigma_y^{(n')}$, to achieve the hopping of spin excitations. We then use a $\sigma_z^{(n)}\sigma_z^{(n')}$ interaction to produce a two-body potential felt by pairs of spin excitations, and we also consider an external one-body potential coupled to $\sigma_z^{(n)}$.

We can view each spin excitation with $\sigma_z^{(n)} = -1$ as a bosonic particle at site n with hardcore interactions preventing multiple occupancy. In this language, the Hamiltonian we consider has the form

$$H = \frac{1}{2}\sum_n \sum_{n' \neq n} J_{nn'}[b_n^\dagger b_{n'} + b_{n'}^\dagger b_n] + \frac{1}{2}\sum_n \sum_{n' \neq n} V_{nn'} b_n^\dagger b_n b_{n'}^\dagger b_{n'} + \sum_n U_n b_n^\dagger b_n + C, \tag{14}$$

where b_n and $b_n^\dagger$ are annihilation and creation operators for the hardcore bosons on site n. The hopping coefficients $J_{nn'}$ have the form $J_{nn} = J_0/|r_n - r_{n'}|^\alpha$, where r_n is the position of qubit n. Similarly, the two-body potential coefficients $V_{nn'}$ have the form $V_{nn'} = V_0/|r_n - r_{n'}|^\beta$.

We now add to U_n a deep attractive potential at some chosen site n_0 that traps and immobilizes one boson at that site. Without loss of generality, we take the position of that site to be the origin and add a constant to the Hamiltonian so that the energy of the trapped boson is zero. We then consider the dynamics of a second boson that feels the interactions with this fixed boson at the origin. In order to produce a quantum system with a geometric spectrum and discrete scale invariance, we choose $\beta = \alpha - 1$. As an example, we consider a system with $\alpha = 2$,

Figure 3: Plot of the normalized wave functions for the first twelve even-parity bound states for the case $\alpha = 2$, $\beta = 1$, $J_0 = -1$, and $V_0 = -30$. We plot the region $r > 0$, where r is measured in lattice units.

Figure 4: Plot of the real-time dynamics of a single particle released from the left edge of an $L = 30$ trap. We are plotting the particle density for several time snapshots, with later times linearly displaced in the vertical direction.

$\beta = 1$, $J_0 = -1$, and $V_0 = -30$. The wave functions for the first twelve even-parity bound states are shown in Fig. 3. We plot the normalized wave function for $r > 0$, where r is measured in lattice units.

We propose to reconstruct the excitation spectrum of the time fractal system using transition operators of the form $b_n^\dagger b_n$ for some particular value of n. This is analogous to the single-nucleon charge density operator. In addition to the energy differences $E_\odot^n - E_\odot^{n'}$, we can also extract $c_{n'}^* c_n \phi_\odot^{n'} |O| \phi_\odot^n$. Given the fact that $\sum_n |c_n|^2 = 1$, this provides a lower bound on the magnitude of the transition matrix element, $|\phi_\odot^{n'}|O|\phi_\odot^n|$. We propose to study different imperfectly-evolved states $\psi(t)$ to generate many different coefficients c_n and thus estimate the magnitude of the transition matrix elements $|\phi_\odot^{n'}|O|\phi_\odot^n|$.

3.3.4 Scattering, reactions, and few-body dynamics

We propose to study the real-time dynamics of colliding particles and bound states. The goal is to provide data from analog quantum simulators that can be used to benchmark state-of-the-art tools used for nuclear scattering and reactions such as the adiabatic projection method [**?**]. For this purpose we use again the time fractal system with Hamiltonian described in Eq. (14). In this case, however, we do not include any trapping potential at the center. Instead we have keep the system uniform except for the open boundary conditions at the ends of the trap.

We have performed preliminary work showing that we can study the real-time dynamics of colliding particles and bound states in this manner. As discussed above, we define the vacuum state as the state with $\sigma_z^{(n)} = 1$ for all sites n. We can view each spin excitation with $\sigma_z^{(n)} = -1$ as a bosonic particle at site n with hardcore interactions preventing multiple occupancy. If we initialize the system with one particle at the left edge of the ion trap, we can produce a wave packet that moves to the right and bounces elastically off the trap boundaries. In Fig. 4 we plot the real-time dynamics of a single particle released from the left edge of an $L = 30$ trap. We are plotting the particle density for several time snapshots, with later times linearly displaced in the vertical direction.

In a similar fashion we can initialize a dimer (two-particle) wave packet by putting two particles on adjacent sites at the edge of the ion trap. In Fig. 5 we plot the real-time dynamics of a dimer and particle released from the left and right edges respectively of an $L = 30$ trap. We are plotting the particle density for several time snapshots, with later times linearly displaced in the vertical direction.

The collisions between any N_1-body state and N_2-body state can be realized in this trapped ion system. We propose to study how to extract scattering observables from real-time processes on analog quantum simulators. For elastic scattering we propose to determine reflection and transmission coefficients. For inelastic scattering we would also like to determine transfer and breakup probabilities for both inclusive and exclusive process. We propose to produce high-quality scattering and reaction data that can be used to benchmark the adiabatic projection method currently being used for nuclear scattering and reactions in lattice effective field theory.

3.4 Nuclear structure, Finite Nuclei and Infinite Nuclear Matter

Simulation of Many-Body Hamiltonians Given a Hamiltonian in second-quantized form

$$H = \sum_{pq} h_{pq} a_p a_q + \sum_{pqrs} h_{pqrs} a_p a_q a_s a_r$$

Figure 5: Plot of the real-time dynamics of a dimer and a single particle released from the left and right edges respectively of an $L = 30$ trap. We are plotting the particle density for several time snapshots, with later times linearly displaced in the vertical direction.

for example, one can use a quantum computer to estimate the energy eigenvalues of the Hamiltonian E_n where $H\psi_n = E_n\psi_n$. First, one maps the Hamiltonian to quantum gates via a mapping such as the Jordan-Wigner transformation

$$a_i = \sigma_z^{\otimes i-1} \otimes \sigma_+ \otimes \mathbb{I}^{\otimes n-i}$$
$$a_i = \sigma_z^{\otimes i-1} \otimes \sigma_- \otimes \mathbb{I}^{\otimes n-i}$$

The most efficient mapping is still unknown. Then, one must approximate the time-evolution operator

$$U = e^{-iHt/\hbar} = e^{-i\sum_k H_k t/\hbar}$$

using an approximation such as Suzuki-Trotter

$$e^{A+B} = \lim_{n\to\infty} \left(e^{A/n} e^{B/n}\right)^n$$

Which approximation to use for a given problem is an active area of research. Next, one maps the time-evolution operator into quantum circuits consisting of 2-qubit gates. The mapping that results in the shortest depth quantum circuit is an open question. Finally, one plugs the quantum circuit for U into the phase estimation algorithm.

This process can be used to simulating nuclear systems such as infinite matter (jellium) or be used to estimate binding energies. The theoretical expertise hear at the NSCL/FRIB is extremely helpful in setting up the problems in such a way that they can be most efficiently solved by a quantum computer.

In the near-term, the variational quantum eigensolver algorithm is best suited to solve problems. It is a hybrid quantum-classical algorithm that is based on the variational principle of quantum mechanics

$$\psi(\theta) H \psi\theta \geq E_0$$

where E_0 is the ground state. The quantum computer is used to prepare an initial state that one guesses and measure the expectation value of the Hamiltonian in that state. The initial state is then slightly varied by a small change in the parameters θ and the expectation value is measured again. The classical computer computes some norm of the difference between the iterations of the expectation values and stops when this norm is sufficiently small. The algorithm will converge to the ground state energy of the Hamiltonian. The excited energies can be calculated by shifting the Hamiltonian and repeating the algorithm.

3.4.1 Broader Impacts

The academic environment at MSU provides numerous opportunities for the PIs to attract bright young people to high-level research in nuclear physics. For example, the theory group at the NSCL is very active in mentoring undergraduate students in the NSF sponsored Research Experience for Undergraduates (REU) program in the summer months, with the PIs successfully supervising two REU students over the past three years. Many of the projects in this proposal can be tested in prototype toy-model problems that manage to simultaneously i) illustrate cutting-edge concepts to the student at a technical level appropriate for an undergraduate physics major, and ii) benefit the overall progress of the PIs' research program.

One of the primary *broader impacts* of our previous NSF award, which we will continue in the current award, is the development of an open source library that can be used by other theorists and serve as a educational resource for graduate students and postdocs learning about advanced many-body methods like CC and IMSRG. In our recent Lecture Notes in Physics book [**?**], we have together with our graduate students and other colleagues, written two long chapters on the application of the above many-methods to neutron star studies. These chapters contain links to our codes, which are fully open source and contain benchmark calculations as well, making thereby our science reproducible. They can be accessed via the GitHub link `https://github.com/ManyBodyPhysics/LectureNotesPhysics/tree/master/doc/src`. As we implement the infinite matter projects described in the current proposal (e.g., inclusion of NNN forces and approximate triples excitations, calculation of spin-isospin response functions, etc.), the codes in the repository will be updated accordingly.

The PIs are requesting support for three graduate students plus one postdoc to work on the projects outlined above. The methods at the center of this proposal are at the forefront of basic research in many-body physics and

low-energy nuclear physics.The many collaborations of the PIs with academic institutions world wide provides an excellent platform for developing the communication skills of the supported students. Global collaboration, and collaboration within the local group, requires skills in project management in order to adequately communicate the progress of the project and to meet deadlines. Participation in international conferences and visits at research centers can be expected within the time period the proposed project. This will equip the involved participants with skills in presentation techniques. Proper documentation, both internally and in peer-reviewed international journals, in writing is expected. The project is grounded in nuclear physics but there is a very large overlap with computational science and numerical analysis. These two complementary aspects will form a natural part of the everyday work and therefore add to the total competence of the participants. Naturally, this will add to the number of possible career paths.

3.5 Tasks

4 Workforce Development

4.1 Mentoring Plan

The mentoring of the graduate students postdoc located at the FRIB/NSCL facility will be fully incorporated in the existing mentoring program of FRIB/NSCL. At any time there are about 15 experimental and theoretical postdocs and approximately 100 graduate students at the FRIB/NSCL. It is an ideal research environment which will enable the graduate students and postdoc to work and interact with students, postdocs and more senior researches with diverse backgrounds on a daily basis. A few years ago FRIB/NSCL strengthened and improved the mentoring of graduate students and postdocs at the FRIB/NSCL with the appointment of an Associate Director for Education. A formal half-year review of all postdocs was initiated. It begins with an entry interview where the postdoc and supervisor discuss expectations and future career plans of the postdoc guided by a form containing standard topics and questions related to the research activities. This initial discussion is then followed but by similar meetings every 6 months. These reviews occur in April and October of each year and are required and monitored by the Associate Director for Education. The Associate Director for Education meets with all FRIB/NSCL postdocs on a monthly basis to keep them informed about FRIB/NSCL related news and activities. During these meetings the representative of the various committees also report back to the group. Postdocs also maintain their own website, where they share experiences, hints and collect and list job openings. Postdocs are also encouraged to participate in activities and programs offered by the University and the professional societies. For example, recent postdocs have been participating in an MSU sponsored Work/Life balance workshop and the APS professional development workshops. The FRIB/NSCL especially focuses on career planning. Every semester two seminar speakers are especially chosen to present a broad view of career opportunities outside the traditional academic track. Yearly alumni events offer additional interaction of current students and postdocs with successful NSCL alumni in a variety of careers. The FRIB/NSCL alumni contact list currently contains the names of 250 alumni who offered to be contacted by students and postdocs for career advice (`http://www.nscl.msu.edu/ourlab/alumni`). The list can be filtered by profession and geographic distribution. Finally, the postdocs are an integral part of all laboratory social activities at the NSCL which include the Tuesdays coffee and bagel, Thursdays ice cream social, as well as summer BBQs and welcome receptions. These activities further foster the interaction between all laboratory employees.

5 Timetable of Activities

6 Project Management plan

7 Project Objectives

8 Budget Justification

8.1 Senior Personnel

This grant proposal covers the research of XXX

8.2 Graduate Students and Post-Graduates

We are requesting full support for three graduate students at MSU, plus one postdoc who will work on XXX

There is an excellent pool of graduate students from the Department of Physics and Astronomy at MSU, many of whom come specifically to work in a highly ranked graduate nuclear physics program at the National Superconducting Cyclotron Laboratory. More text to come

8.3 Equipment

The Institute for Cyber Enabled Research (iCER) at MSU is offering xxx

8.4 Travel

The PIs and the graduate students are expected to attend the spring APS or fall DNP annual meetings, in addition to relevant domestic conferences such as topical programs at the Institute for Nuclear Theory. Funding is also requested for

In general, the theory group at the NSCL recognizes the importance of travel to the success and professional development of a young physicist's career, and we strongly encourage our graduate students and postdoctoral research associates to attend important workshops and conferences. Therefore, $XXXX in travel funds is requested in the first year of the grant (split 50/50 between domestic and international travel, and adjusted in subsequent years assuming a 3% inflation rate).

8.5 Materials and Supplies

8.6 Other

This covers graduate student tuition plus fees.

8.7 Indirect Costs

Indirect costs are not charged on graduate student tuition and fees.

A Biographical Sketches

B Current and Pending Support

C Bibliography and References Cited

D Facilities and other Resources

E Data Management plan

Data Management Plan

The primary data collected or created during this project include: source codes, intermediate output from large runs and final results to be used in publications. All this data will be stored in digital form at the Facility of Rare Ion Beams(FRIB)/National Superconducting Cyclotron Laboratory(NSCL) by each member of the group. A shared group directory will be created by the NSCL computer department for our group. When a milestone in a project is reached, or a member leaves the group (e.g. after graduation), the person directly involved will prepare a clean directory with all relevant information (source codes, results, figures, etc) and copied it over to the shared group directory.

The FRIB/NSCL computer department has a multi-level backup system, with daily logs and off-site copies ensuring a safe long-term archive. If requested, data can be made available to other researchers in our field. Codes that are produced for the projects included in this proposal will be made available upon request, after publication of our results.

F Additional perspectives

F.1 Relevance and benefit to society

F.2 Environmental impact

This project and its realization has no significant environmental impacts.

F.3 Ethical perspectives

Ethical aspects concerning XXX

F.4 Gender issues

The project will consist of both male and female researchers, and we will actively recruit female students and researchers for the various activities.