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QIS Research and Innovation for Nuclear Science

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

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1 Executive Summary

Collaboration Team: This proposal assembles a team of leading experts in nuclear theory, quantum computing, machine learning, and mathematics, with the goal of designing new applications of quantum computing and information theory to the most challenging problems in nuclear physics. The team members are distinguished researchers from Los Alamos National Laboratory; IBM; and the Departments of Physics and Astronomy, Computational Mathematics, Science and Engineering (CMSE), and Facility for Rare Isotope Beams (FRIB) / National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University (MSU).

Scientific Goals, Opportunities, and Challenges: How do we connect fundamental physics to forefront experiments? With new science waiting to be discovered at experimental facilities such as FRIB, this question is a profound challenge and opportunity for nuclear theory. We would like to know how nuclear forces emerge from the interactions of quarks and gluons in quantum chromodynamics, what is the internal partonic structure of nucleons, what are the signatures of physics beyond the Standard Model in atomic nuclei, how do we predict nuclear structure and reactions from the microscopic interactions of nucleons, and what are the properties of strongly-interacting matter under extreme conditions. There have been many important and profound advances in recent years, with some of the most creative and impactful developments led by investigators on this proposal. But there are limits to what can be done even with the most powerful supercomputers in this soon-to-be era of exascale computing. Unfortunately, some of the most interesting scientific questions remain unexplored such as the real-time dynamics of hadronic and nuclear reactions and the properties of dense nuclear and neutron matter. For computational methods that construct quantum wave functions, the problem is the curse of large dimensionality and the impossibility of storing exponentially large vectors as classical bits. For computational methods that rely on Monte Carlo simulations, the obstacle is the Monte Carlo sign problem, where positive and negative contributions cancel to produce exponentially small signals.

Quantum computing has emerged as a new computational paradigm that offers the hope of evading both of these fundamental problems. By allowing for arbitrary quantum superpositions of tensor products of qubits, one can store exponentially more information than classical bits. Furthermore, qubits naturally evolve with unitary real-time dynamics. Clearly there are tremendous opportunities in this new paradigm for solving the most profound problems in nuclear physics. But with these great opportunities, there are enormous challenges to realizing their promise. All of the currently available digital quantum computing devices suffer from short decoherence times and significant readout errors. Meanwhile all of the currently available analog quantum simulators have inherent quantum characteristics that are not directly applicable to address systems of relevance to nuclear physics.

In order to meet these formidable challenges, we have proposed a series of new projects that bridge the gap between quantum computing as it exists today and the targeted territory of unsolved nuclear physics problems. Some of the projects focus on variational methods and developing new algorithms for optimizing quantum wave functions. We also explore new applications of error stabilization techniques, machine learning, and quantum compiling to make efficient short-depth quantum circuits. Other proposed projects focus on real-time evolution, the calculation of observables using new algorithms, and creative adaptations of quantum simulators to nuclear physics. We are confident that the scientific output of this collaboration will have a significant and lasting impact on the landscape of quantum computing applied to nuclear physics. While the focus is on applications to nuclear physics, all of the work products are new algorithms and methods of general applicability, and so they should have an equally important impact on quantum computing and quantum information science.

Benefit to Society: Sustaining future progress in nuclear physics and quantum computing depends on training the next generation of thinkers and innovators. Towards this purpose, our proposal has a very significant educational component involving the Quantum Computing Summer School at Los Alamos

National Laboratory, the student-run Quantum Information and Computing (QuIC) seminar series at Michigan State University, a proposed Training in Advanced Low Energy Nuclear Theory (TALENT) summer school, as well as student and postdoctoral travel funds for collaborative work between Los Alamos and Michigan State. The students also benefit from being a part of the nuclear physics program at FRIB and Michigan State, which is currently ranked the number one graduate program in the country according US News and World Report. The mix of analytical and computational skills that the students learn and implement provides excellent preparation for both academic and industrial research. All of the investigators on this proposal are committed to diversity in science and will seek to build a diverse scientific workforce and an inclusive environment for learning and research.

2 Introduction and Scientific Motivation

2.1 Grand Challenges in Nuclear Physics and Quantum Computing

How do we understand nuclei, strongly-interacting matter, and the limits of stable matter in terms of the fundamental laws of motion and forces? How do we explain what we observe in experiments from first principles, starting from quantum chromodynamics and the fundamental interactions of the quarks and gluons? One of the key 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.

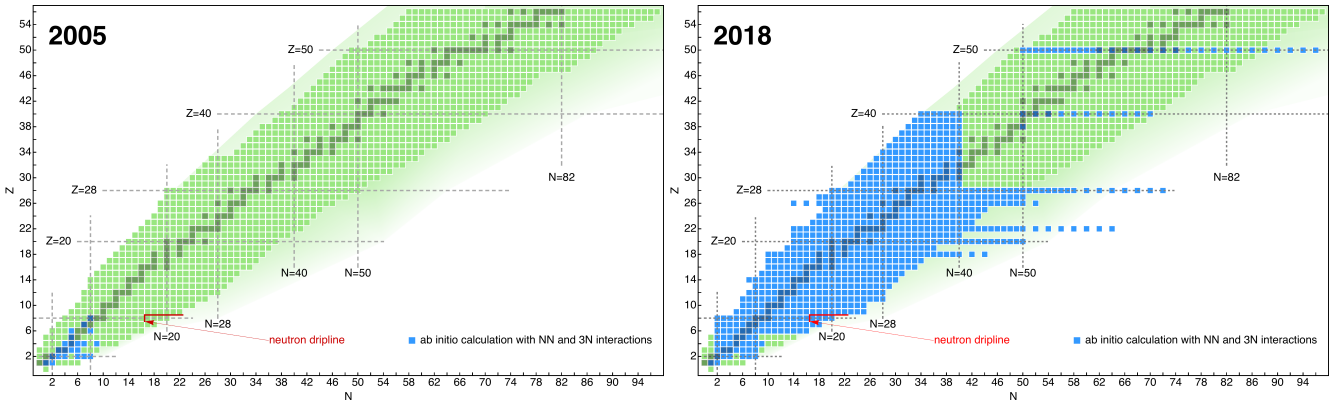
For decades progress in nuclear few- and many-body theory was slowed by the lack of a consistent theory for the strong inter-nucleon interactions, and by the computational demands required to handle the non-perturbative aspects resulting from the "hard cores" and strong tensor forces found in most interaction 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 Morris *et al.* [1] 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 [2].

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 de-

[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 building blocks.



(a) (b)

Figure 1: The chart of nuclides and the reach of *ab initio* calculations in (a) 2005 and (b) 2018. 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.

scription) 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 us to link 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 Fig. 2.

In spite of the rapid developments and profound progress in nuclear theory over the past few years, there are some problems in nuclear physics which remain out of reach of even the most advanced computational methods running on the most powerful supercomputers. Some examples include first principles calculations of the real-time dynamics of non-equilibrium processes such as hadronic and nuclear reactions and electroweak response functions. Some other extremely challenging problems include the calculation of atomic nuclei directly from lattice QCD and the properties of dense nuclear and neutron matter.

In classical computing there are two main approaches to computing interacting quantum systems. Some computational methods explicitly construct quantum wave functions, either exactly or by approximate methods. For very large systems the problem with this approach is the practical limit of computer memory when storing vectors with dimensions that grow exponentially with the number of degrees of freedom. On the other hand, some other computational methods rely on Monte Carlo simulations, which is the use of random numbers to sample over quantum amplitudes. In this case the main challenge is the Monte Carlo sign problem, where positive and negative contributions cancel to produce signals that become exponentially small with increasing system size.

Recently, quantum computers have emerged as a promising new paradigm that can evade both of these problems, thereby offering the potential to address the most challenging problems of large-scale quantum systems with reduced computational complexity. But as we await the dawning of the age of "quantum supremacy", we must learn to face the reality of the current era of noisy devices with short decoherence times and non-negligible readout errors.

Originally proposed by Feynman [3], the efficient simulation of quantum systems by other, more con-

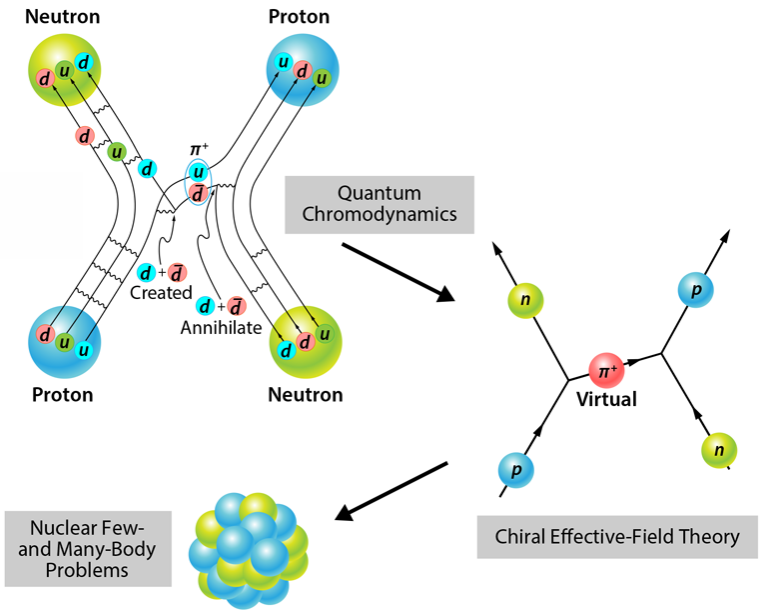


Figure 2: A first principles approach to nuclei and nuclear matter, linking QCD with few- and many-body methods. (Image by APS/Alan Stonebraker.)

trollable quantum systems formed the basis for modern constructions of quantum computation. This early insight has since been refined to encompass more universal and versatile constructions of simulation [4, 5]. By combining quantum phase estimation [6] with these techniques, Aspuru-Guzik et al. showed the first efficient quantum algorithm for solving quantum chemistry problems [7]. This initial algorithm was based on adiabatic state preparation combined with Trotter-Suzuki decomposition of the unitary time-evolution operator [8, 9] in second quantization.

Many algorithmic and theoretical advances have followed since the initial work in this area. The quantum simulation of electronic structure has been proposed via an adiabatic algorithm [10], via Taylor series time-evolution [11], in second quantization, in real space [12, 13], in the configuration interaction representation [14, 15], and using a quantum variational algorithm [16, 17]. Starting with [18], researchers have sought to map these algorithms to practical circuits and reduce the overhead required for implementation by both algorithmic enhancements [19, 20, 21, 22] as well as physical considerations [23, 24]. As a second quantized formulation is generally regarded as most practical for near-term devices, many works have also tried to find more efficient ways of mapping fermionic operators to qubits [25, 26, 27, 28, 29].

With recent developments in quantum computing hardware [30, 31, 32, 33, 34], there is an additional drive to identify early practical problems on which these devices might demonstrate an advantage [35]. The challenge of using such devices in the near-term is that limited coherence requirements necessitates algorithms with extremely low circuit depth. Toy demonstrations of quantum chemistry algorithms have been performed on architectures ranging from quantum photonics and ion traps to superconducting qubits [36, 37, 38, 16, 39, 40, 41]. In particular, the variational quantum algorithm [16, 17] has been shown experimentally to be inherently robust to certain errors [40], and is considered to be a promising candidate for performing practical quantum computations in the near-term [42, 43].

2.2 Project Goals

We have proposed a series of new projects that bridge the gap between the current state of quantum computing on noisy devices and the grand challenge nuclear physics problems we endeavor to address in the future. Several of the projects we propose use variational methods where we develop novel algorithms for optimizing quantum wave functions. In some other projects we explore new applications of error stabilization techniques, machine learning, and quantum compiling to make efficient short-depth quantum circuits. In the other remaining proposed projects we study real-time evolution, the calculation of observables using new algorithms, and creative adaptations of quantum simulators to nuclear physics.

While our scientific focus is on applications to nuclear physics, all of the projects we propose involve new algorithms and methods of general applicability, with an equally important impact on nuclear physics and on quantum computing and quantum information science. The following is a list of our main project objectives.

- Make the grand scientific challenges of nuclear physics known and visible to the quantum computing and quantum information communities.
- Develop and optimize quantum computing algorithms to address unsolved problems in nuclear physics, especially in the areas of lattice QCD and nuclear many-body physics.
- Explore new synergies and hybrid approaches connecting quantum and classical computing paradigms while benchmarking new methods against existing techniques.
- Develop new fundamental tools designed for nuclear physics but of general character and importance that can impact the fields of quantum computing and information science.
- Build an interdisciplinary team that brings together innovators from different communities, and which recruits and develops new talent in quantum computing and nuclear physics.
- Play a formative role in the development of quantum computing in nuclear physics by contributing to the identification of key missing elements in the architecture of future quantum computing platforms and strategies.
- Share discoveries, results, and resources with the nuclear physics and quantum computing communities through comprehensive outreach activities including summer schools, publications, research talks, public lectures, and open code access.

3 Proposed Research and Methods

In order to achieve our scientific goals, our application is divided into five work packages, four of these deal with our scientific goals while work package 5 details our plans for workforce developments. In Fig. 3 we show the connectivity and links between institutions involved in this proposal through the proposed research projects and the training initiatives.

3.1 Work Package 1 (WP1): Quantum Simulation Algorithms

Lead Scientists: Patrick Coles (LANL), Matthew Hirn (MSU), and Ryan LaRose (MSU Ph.D. Student)

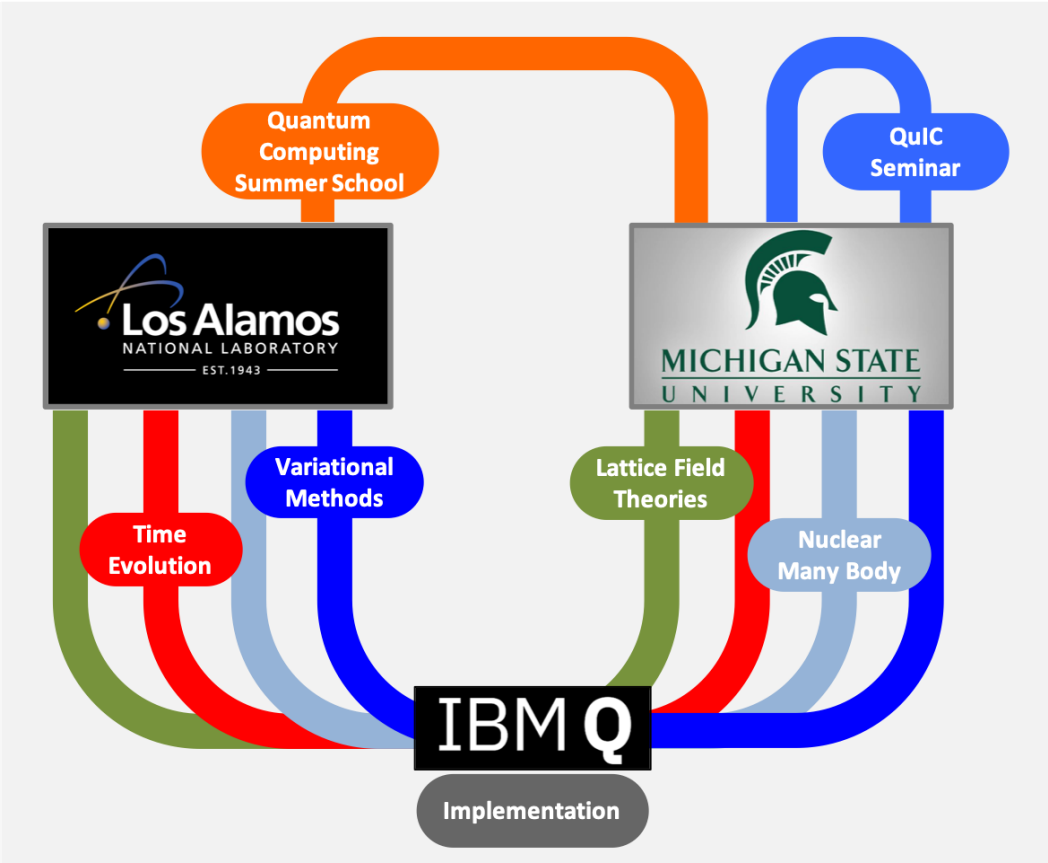


Figure 3: This figure shows the links between each of the institutions involved in the proposal. We show the connectivity involving the proposed research projects and as well as training initiatives.

3.1.1 Introduction

As proposed by Feynman, the holy grail for quantum computers (QCs) is to provide an exponential speedup in simulating quantum systems. Since 2015, small QCs of limited coherence time have become available in the cloud. Additionally, DOE testbed QCs are being constructed for dedicated use by researchers. With recent developments in quantum computing hardware [30, 31, 32, 33, 34], there is an additional drive to identify early practical problems on which these devices might demonstrate an advantage [44, 35].

These machines are not fault-tolerant and, due to their noise, require short-depth algorithms to perform computations. There exist quantum simulation methods [45] tailored for fault-tolerant QCs; however, their gate depth grows with simulation time. This issue makes them infeasible for near-term QCs. This motivates the need for quantum simulation methods that employ short-depth quantum circuits and hence can be implemented in the near-term.

Machine learning (ML) provide a strategy towards this end. ML can redesign and optimize existing quantum algorithms (QAs) for noisy QCs, and it can also discover new QAs. For example, ML has been used to design an improved QA for computing quantum state overlap [46]. ML has also been used to design QAs for mathematical functions, a result that provides important subroutines for other QAs [47].

To address the scaling issue of applying ML to quantum systems, one can consider quantum machine learning (QML) methods. QML involves evaluating the cost function (efficiently) on a quantum computer, and then feeding the result to a classical optimizer, which then adjusts the parameters of the quantum algorithm. Such QML methods are typically called variational hybrid quantum-classical

algorithms (VHQCAs). VHQCAs have demonstrated utility for other applications like ground state preparation [16] and factoring [48], and our group has developed such algorithms for quantum compiling [49], quantum state diagonalization [50], and characterizing quantum stochastic processes [51]. VHQCAs have been shown experimentally to be inherently robust to certain errors [40], and are considered to be a promising candidates for performing practical quantum computations in the near term [42, 43].

3.1.2 Preliminary Work

We have applied the (classical) ML methods from [46] to the problem of quantum simulation. Here, the goal is produce a short-depth quantum circuit that approximately implements the propagator e^{-iHt} for some Hamiltonian H. As a simple example, we applied this ML approach to the Ising model for a small number of spins, and it resulted in gate sequences of much shorter depth than what we obtained from the standard Trotterization approach (for the same simulation error). While these results were encouraging, future work is needed to make this classical ML approach more scalable to larger problem sizes. One approach is to develop automated methods for motif recognition that we discuss in the next subsesction, and the other approach is to use VHQCAs.

Along the lines of the latter strategy, we recently published [49] a VHQCA called quantum-assisted quantum compiling (QAQC), where the goal was to take a long gate sequence U and compile it to a much shorter gate sequence V. We proved that evaluating our cost function in QAQC is inefficient on a classical computer but efficient on a quantum computer. Hence QAQC may be useful for reducing the circuit depth of large-scale QAs, i.e., QAs that could not be optimally compiled with classical methods. We implemented QAQC on cloud quantum computers and on classical simulators to redesign several known QAs for current QCs. For example, the quantum Fourier transform (QFT) was 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.

In preliminary work, we have investigated the possibility of using our QAQC algorithm for the purpose of quantum simulation. Our idea is to use QAQC to compile the propagator $U = e^{-iH\Delta t}$, where Δt is a very short time, into a form V that can be easily extended to longer times t. This easily extendable form is based on diagonalization. This approach is inspired by the following fact. For some Hamiltonians (e.g., the Ising model) that can be exactly diagonalized, QAs exist for performing quantum simulations that require only a constant number of gates, irrespective of whether the time to be simulated is short or long [45]. Inspired by this, we have investigated using QAQC to approximately diagonalize more general Hamiltonians. This would allow us to simulate long time evolutions using quantum circuits with a constant number of gates. Hence, unlike standard quantum simulation methods, our method would not be limited to simulation times shorter than the decoherence time of the quantum computer. We remark that some Hamiltonians are known to be fast-forwardable while the general question is an open problem [52].

3.1.3 Proposed Work

We propose to expand on our prior work to use classical and quantum ML to design and optimize QAs for quantum simulation.

Classical machine learning. The ML approach that we have developed [46] discovers algorithm instances, i.e., optimal gate sequences for achieving a specific computation with a fixed number of qubits. The resulting algorithms will necessarily be for small problem sizes, due to both the computational complexity of training for large problem sizes. Our ultimate aim, however, is to find algorithms for arbitrary problem size. That is, we will additionally need to generalize learned algorithm instances for small problem sizes to arbitrary size to discover how they scale. To help with generalization, we propose

to develop automated tools for motif recognition in quantum gate sequences. For this purpose, we will construct a library from discovered algorithm instances, as follows.

In our approach to finding automated tools to help understand algorithm scaling, we will iteratively construct a motif library. Initially, the library will consist of standard one- and two-qubit gates with the addition of standard motifs, such as Toffoli, controlled-Swap, quantum Fourier transform, and other known algorithmic structures. Then, as we learn new algorithm instances, all previously learned motifs, including all previous algorithm instances learned on fewer qubits will be incorporated into the library, recursively. In this way, motifs will be used as building blocks for successively larger algorithm discovery. This approach will allow us to explore motif structure as a function of the number of qubits, and learn whether and how specific algorithms generalize as the number of qubits increases.

Ultimately this will allow us to uncompile our gate sequences into a form that can be generalized. Aided by the aforementioned automated motif recognition, we will study how specific quantum simulation algorithms scale as a function of the number of qubits. Namely, we will use our uncompiled algorithms for generalization to arbitrary problem size.

Quantum machine learning. Our second approach focuses on VHQCAs for quantum simulation. This approach consists of finding VHQCAs for operator diagonalization. Diagonalization simplifies the exponentiation of an operator, and theoretically would allow us to simulate quantum systems at arbitrary times using a fixed number of gates. In practice, only approximate diagonalization is achieved, and hence arbitrary times are not realistic. Nevertheless, longer times than standard methods may be achievable. We emphasize that the best classical algorithms for diagonalization scale polynomially in the matrix dimension, while our proposed VHQCAs scale logarithmically on the matrix dimension.

Operator diagonalization can come in different flavors depending on the structure of the operator to be diagonalized. Because QCs inherently implement unitary operators, these are the most straightforward to diagonalize with a VHQCA. Our approach for unitary diagonalization is to use a VHQCA to find operators, W and D, that diagonalize a Trotterized unitary operator, $U(\Delta t) \approx e^{-iH\Delta t}$, implementing a single timestep, Δt, of a quantum simulation, i.e., $U(t) = WD(\Delta t)W^\dagger$. Here, W is a product of unitary gates that represents the eigenvectors of U, and $D(\Delta t)$ is a product of commuting unitary gates. With this approach, we have full knowledge of how to construct the operators making up the diagonalization using the parameters learned with our VHQCA. Thus, we can construct a quantum circuit with fixed structure, where by simply changing the internal parameters of the gates in D, we implement the quantum simulation represented by $U(p\Delta t) \approx WD(p\Delta t)W^\dagger = e^{-iHp\Delta t}$, where p is an arbitrary scalar. We have shown that this method works for small quantum simulations.

Diagonalizing a Hamiltonian is more complicated than diagonalizing a unitary operator because it must be expressed as a weighted sum of unitary operators, and the cost function for the optimization becomes more complicated. However, the advantages of diagonalizing the Hamiltonian (as opposed to the simulation unitary) are 1) there is no Trotterization error and 2) the cost-evaluation circuit will use fewer gates. Therefore, our longer term goal will be to develop a VHQCA for Hamiltonian diagonalization, while in the short term, we will make use of our VHQCA for unitary diagonalization.

In both the unitary and Hamiltonian cases, the most challenging technical issue is to train the parameters of W to achieve diagonalization. We have extensive experience with optimization of quantum gate sequences of this sort [49, 50]. In particular, local minima and barren plateaus in the cost landscape are two major issues. We have developed methods to simultaneously address both of these issues, by proper initialization of the circuit parameters (which initializes away from barren plateaus) and by enlarging the parameter space (which helps to escape out of local minima) [50].

3.1.4 Challenges and Outlook

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.

The idea of ML for QA design has demonstrated initial success in Ref. [47, 46] and our own research [49]. 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. Our proposed data-driven method could produce many new QAs with applications in many fields. The recent success of this approach in Ref. [46] necessitates further study. Our knowledge of both ML and QAs is ideal for these methods.

The time line for WP1 is summarized in the table here:

Milestones	2020				2021				2022			
Cost-driven redesign for current QCs	•	•	•	•	•	•	•	•				
Data-driven design for future QCs					•	•	•	•	•	•	•	•

3.2 Work package 2 (WP2): Quantum State Preparation and Dynamics

Lead Scientists: Dean Lee (MSU) and Jacob Watkins (MSU Ph.D. Student)

The research activity of the Lee group focuses on developing new algorithms for quantum state preparation and time evolution that are sufficiently robust to operate on noisy near-term devices. These include both digital quantum computers and analog quantum simulators. The problems we address are designed to probe correlations in nuclear structure, the spectrum of nuclear energy levels, transition matrix elements, and the dynamics of nuclear scattering and reactions. Graduate student Jacob Watkins has worked on the topics presented in this proposal and funds would be used to support his continuing research in quantum computing applied to nuclear physics.

3.2.1 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 [53]. 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 $|\phi_z^0\rangle$ can be prepared simply using single qubit gate operations. Suppose we want to produce the ground state $|\phi_\odot^0\rangle$ 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 $|\phi_\odot\rangle$ after reaching time $t = \tau$,

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

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 $|\psi_n\rangle = U_n |\phi_z^0\rangle$, 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 $\langle\psi_n|\psi_m\rangle$ and amplitude $\langle\psi_n|H_\odot|\psi_m\rangle$ we use one auxiliary qubit. We initialize the auxiliary qubit as $|0\rangle$ while the main system is prepared in the state $|\phi_z^0\rangle$. We perform a Hadamard transform on the auxiliary qubit and implement controlled unitary gate operations to obtain

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

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

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

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

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

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

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

We note that all of the terms in H_{even} commute with each other and all of the terms in H_{odd} commute with each other. This simplifies the unitary time evolution. In order to describe the physics of a single particle, we consider the linear space where exactly one qubit is in the $|1\rangle$ state and the remaining $2L$ qubits are in the $|0\rangle$ 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

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

We will work with the evolved state,

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

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 $|\psi, \tau, L_t\rangle$ 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 IBM Q. We will compare with standard adiabatic evolution as well as the quantum approximate optimization algorithm [54]. 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 $\langle\psi_n|\psi_m\rangle$ and amplitudes $\langle\psi_n|H_\odot|\psi_m\rangle$ will suffer from noise. The first step is to remove any systematic biases using known extrapolation methods [55]. For the remaining error we apply new tools that we have recently developed for another computational technique called eigenvector continuation [56]. 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 $\langle\psi_n|\psi_m\rangle$ and amplitudes $\langle\psi_n|H_\odot|\psi_m\rangle$ 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.

3.2.2 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 [57]. 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 $|\psi\rangle$ using imperfect adiabatic evolution, as we have discussed in the text surrounding Eq. (2). We can write $|\psi\rangle$ as a linear combination of eigenstates of $H_\odot$,

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

The strategy is to prepare $|\psi\rangle$ 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 $|\psi\rangle$ for a sequence of equally-spaced times t,

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

We measure the expectation value of O for each t,

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

In terms of the energy eigenstates, the expectation value is

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

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

We propose to develop the efficiency of this spectral reconstruction technique by exploring various transition operators O and various imperfectly-evolved states $|\psi(t)\rangle$ 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. [58]. 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 [59, 60]. 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 $\alpha = 2$, $\beta = 1$, $J_0 = -1$, and $V_0 = -30$. The wave functions for the first twelve even-parity bound states are shown in Fig. 4. 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 $E^n_\odot - E^{n'}_\odot$, we can also extract $c^*_{n'}c_n \langle\phi^{n'}_\odot|O|\phi^n_\odot\rangle$. This is enough information to calculate the ratio of transition matrix elements $\langle\phi^{n'}_\odot|O|\phi^n_\odot\rangle \,/\, \langle\phi^{n'}_\odot|O'|\phi^n_\odot\rangle$ for any pair of observables O and O'. Given the fact that $\sum_n |c_n|^2 = 1$, we can also determine a lower bound on the magnitude of $|\langle\phi^{n'}_\odot|O|\phi^n_\odot\rangle|$. We propose to study different imperfectly-evolved states $|\psi(t)\rangle$ to generate many different coefficients c_n and thus estimate the magnitude of the transition matrix elements $|\langle\phi^{n'}_\odot|O|\phi^n_\odot\rangle|$.

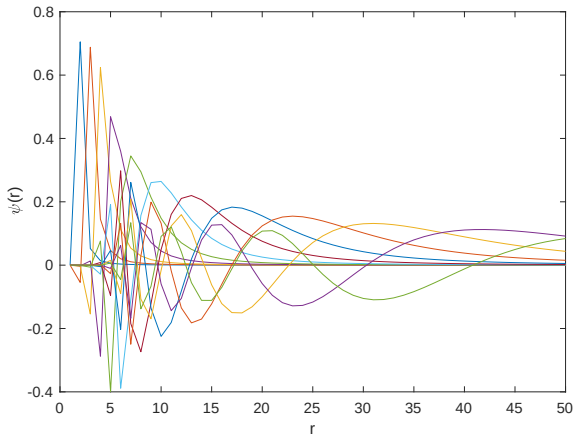


Figure 4: Plot of the normalized wave functions for the first twelve even-parity bound states for the case $\alpha = 2$, $\beta = 1$, $J_0 = -1$, and $V_0 = -30$. We plot the region $r > 0$, where r is measured in lattice units.

3.2.3 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 [61]. 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 the left panel of Fig. 5 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 the right panel of 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.

The time line for the development of the various elements of WP2 is

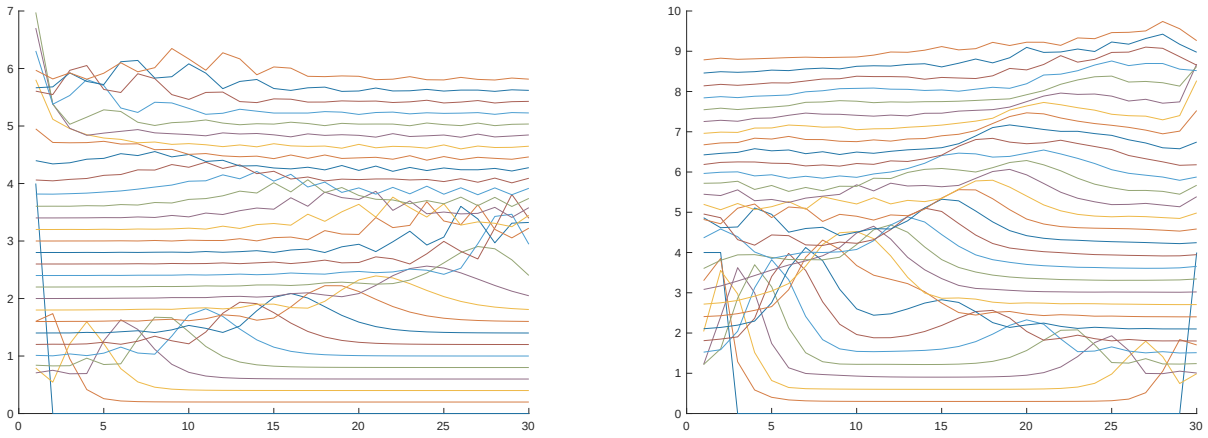


Figure 5: Plot of the real-time dynamics of a single particle released from the left edge (*left panel*), and a dimer and particle released from the left and right edges, respectively, of an $L = 30$ trap (*right panel*). We are plotting the particle density for several time snapshots, with later times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

Milestones	2020				2021				2022			
Variational Adiabatic Evolution	•	•	•	•								
Spectral Reconstruction			•	•	•	•						
Transition Matrix Elements					•	•	•	•				
Few-body Dynamics							•	•	•	•		
Scattering and Reaction Probabilities									•	•	•	•

3.3 Work Package 3 (WP3): Lattice Quantum Chromodynamics (QCD) and Quantum Information Theories

Lead Scientists: Alexei Bazavov (MSU), Huey-Wen Lin (MSU) and Andrea Shindler (MSU)

The strong interaction between quarks and gluons is described by a local quantum field theory, quantum chromodynamics (QCD). QCD also describes the properties of baryons and ultimately the interaction between them. While at high energy the smallness of the strong interaction coupling constant (asymptotic freedom) allows a perturbative expansion, at low energy one needs non-perturbative techniques. To date the only theoretically solid approach to solve QCD at low energies is to rotate from Minkowski to Euclidean and discretize space time. The theory regulated with a 4-d Euclidean lattice is called lattice QCD (LQCD). LQCD is amenable to numerical simulations and the theory can be solved numerically. Following the expectation of the Long Range Plan for Nuclear Science [62], at the Facility of Rare Isotope Beams (FRIB) we have a theoretical program to calculate the low-energy properties of nucleons and nuclei and the equilibrium properties of matter at finite temperature and density ranging from single nucleons to heavier nuclei. LQCD plays also an important role in the studies of double-beta decay of nuclei or the electric dipole moments of particles and nuclei where time-reversal symmetry is violated.

For many physical systems, the computation of the functional integral in Euclidean space defining the theory suffers from a sign problem. In general any study directly performed in Minkowski space, i.e. a real-time calculation, is plagued by a sign-problem. Quantum computing (QC) has the potential to overcome this difficulty changing completely the way the computations are performed. QC will retain the physical information contained in the quantum phase allowing a direct real-time calculation.

It has been estimated that a realistic 3+1-dimension LQCD calculation with 10^4 spatial lattice sites

on quantum computers would require around $10^5 - 10^6$ qubits [63]. Even if the hardware development is still far away to reach those numbers, there is a growing interest in the community to develop algorithmic techniques and new theoretical and numerical tools applying them to lower dimensional field theories.

Quantum electrodynamics in 1+1 dimension, i.e. the Schwinger model, serves as a test ground for simplified studies of QCD. In fact it also enjoys properties such as spontaneous breaking of chiral symmetry and confinement. The one dynamical degree of freedom of the photon remaining after the gauge fixing becomes massive. Similarly to QCD, there is a non-zero chiral condensate $\langle\bar{\psi}\psi\rangle$.

The Schwinger model is defined by the following Lagrangian density

$$\mathcal{L} = \bar{\psi}\left[iD - m\right]\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\,. \tag{15}$$

To discretize the Schwinger model we use staggered fermions [64, 65], where the 2 spinor components are distributed in neighboring sites resulting in two fermion sites per spatial sites. To obtain the form of the Hamiltonian density one uses a Jordan-Wigner transformation. To fix the gauge we set the temporal components of the gauge field to zero; one then

$$\begin{aligned} H &= \beta \sum_{n=0}^{N_{f_s}-1} \left[\sigma_n^+ L_n^- \sigma_{n+1}^- + \sigma_{n+1}^+ L_n^+ \sigma_n^-\right] \\ &+ \sum_{n=0}^{N_{f_s}-1} \left[l_n^2 + m\beta(-1)^n \sigma_n^z\right]\,, \end{aligned} \tag{16}$$

where N_{f_s} denotes the number of fermion sites and β is defined as $1/(ag)^2$ with a and g corresponding to the lattice spacing and the gauge coupling respectively. The link acting as raising or lowering operators are denoted with $L_\pm$, $L_\pm|l\rangle = |l \pm 1\rangle$ while the quantized electric flux is parameterized by the integers l_n.

The structure of the Hamiltonian in eq. (17) adapts well to the variational adiabatic method described in Sec. 3.2.1. In the strong coupling limit $\beta \to 0$ (with $m \to \infty$ and $\beta m =$ const.) it is possible to determine the ground state exactly. The form of the Schwinger Hamiltonian for $\beta = 0$ is almost identical to the initial Hamiltonian described in sec. 3.2.1. One could then tune adiabatically the coupling β to several values β_i and for each of them determine the evolved state. Following the discussion of Sec. 3.2.1, one can then apply the variational principle to determine the ground state with the target β. We plan to investigate the possibility to reduce errors generated by imperfect adiabatic evolution or the possibility to reduce the total time needed in the adiabatic evolution.

While LQCD is a very powerful tool that allows for first-principle calculations whose accuracy can be systematically improved, the Euclidean nature of the formalism makes a certain class of problems hard to solve in practice. In particular, quantities that are related to real-time dynamics, such as spectral functions of heavy quarkonia [66], transport properties of quark-gluon plasma (a recent lattice attempt can be found in Ref [67]) and the hadronic tensor [68] lead to ill-posed underdetermined inverse problems.

Here we illustrate this point with the discussion of the relation between the Euclidean meson correlators and spectral functions at finite temperature[2]. The spectral function for a given mesonic channel H in a system at temperature T can be defined through the Fourier transform of the real-time two-point functions $D^>$ and $D^<$ or equivalently as the imaginary part of the Fourier transformed retarded correlation function [69]

$$\sigma_H(p_0, \vec{p}) = \frac{1}{2\pi}(D_H^>(p_0, \vec{p}) - D_H^<(p_0, \vec{p})) = \frac{1}{\pi}\mathrm{Im}D_H^R(p_0, \vec{p}) \tag{17}$$

[2]The zero temperature limit is straightforward.

where

$$D_H^{>(<)}(p_0,\vec{p}) = \int \frac{d^4p}{(2\pi)^4} e^{ip\cdot x} D_H^{>(<)}(x_0,\vec{x}) \tag{18}$$

$$D_H^{>}(x_0,\vec{x}) = \langle J_H(x_0,\vec{x}), J_H(0,\vec{0})\rangle$$
$$D_H^{<}(x_0,\vec{x}) = \langle J_H(0,\vec{0}), J_H(x_0,\vec{x})\rangle, x_0 > 0\ , \tag{19}$$

and $J_H(t,x)$ is the local meson operators of the form $\bar{q}(t,x)\Gamma_H q(t,x)$, with q a continuous real-time fermion position operator and $\Gamma_H = 1, \gamma_5, \gamma_\mu, \gamma_5\gamma_\mu, \gamma_\mu\gamma_\nu$.

The correlators $D_H^{>(<)}(x_0,\vec{x})$ satisfy the Kubo-Martin-Schwinger (KMS) condition [69]

$$D_H^{>}(x_0,\vec{x}) = D_H^{<}(x_0 + i/T, \vec{x}). \tag{20}$$

Inserting a complete set of states and using Eq. (20), one gets the expansion

$$\sigma_H(p_0,\vec{p}) = \frac{(2\pi)^2}{Z}\sum_{m,n}(e^{-E_n/T} \pm e^{-E_m/T})|\langle n|J_H(0)|m\rangle|^2\delta^4(p_\mu - k_\mu^n + k_\mu^m) \tag{21}$$

where Z is the partition function, and $k^{n(m)}$ refers to the four-momenta of the state $|n(m)\rangle$.

In finite-temperature lattice calculations, one computes Euclidean time propagators, usually projected to a given spatial momentum:

$$G_H(\tau,\vec{p}) = \int d^3x e^{i\vec{p}.\vec{x}}\langle T_\tau J_H(\tau,\vec{x}) J_H(0,\vec{0})\rangle. \tag{22}$$

This quantity is an analytical continuation of $D_H^{>}(x_0,\vec{p})$

$$G_H(\tau,\vec{p}) = D_H^{>}(-i\tau,\vec{p}). \tag{23}$$

Using this equation and the KMS condition one can show that $G_H(\tau,\vec{p})$ is related to the spectral function, Eq. (17), by an integral equation:

$$G_H(\tau,\vec{p}) = \int_0^\infty d\omega \sigma_H(\omega,\vec{p}) K(\omega,\tau) \tag{24}$$

$$K(\omega,\tau) = \frac{\cosh(\omega(\tau - 1/2T))}{\sinh(\omega/2T)}. \tag{25}$$

This equation is the basic equation for extracting the spectral function from meson correlators.

While the left-hand side of Eq. (24) can be calculated on the lattice with a relatively small computational cost (at least, in the mesonic sector), solving the integral equation directly is not feasible, because the amount of information contained in the lattice Euclidean correlator, subject to statistical uncertainties, is insufficient for reliable reconstruction of the spectral function under the integral. Regularization is necessary and various inverse problems methods such as the Maximum Entropy Method [70], Bayesian Reconstruction Method [71], Backus-Gilbert method [72] and stochastic optimization methods [73] are often employed. The nature of this problem is tightly related to the fact that classical LQCD simulations are almost exclusively done in the Lagrangian formalism in Euclidean space-time.

The Hamiltonian form of LQCD, while not well-suited for classical computation, offers a path to access real-time dynamics. While the problem in the operator formalism is impractical for classical computers[3], this formulation is natural for quantum computers. Moreover, finding the spectrum of the Hamiltonian allows one to rely on the spectral decomposition, Eq. (21), rather than the integral equation (24).

[3]In the Hamiltonian formalism of LQCD the Hilbert space of a single gauge link is already inifinite-dimensional and the number of degrees of freedom in a realistic LQCD simulation is on the order of $O(10^6)$.

Low-dimensional quantum field theories, such as the Schwinger model with larger spaitial sites, can serve as benchmark systems for developing the Hamiltonian LQCD. Combining the formulation in Eq. (17) with the ideas of spectral decomposition in Sec 3.2.2 we propose to develop methods for determining the low-lying part of the spectrum in Hamiltonian LQCD and using it to determine the spectral functions at finite temperature. The validity of the methods will be tested with the conventional Monte Carlo as well as with the available analytical results [74]. We will test our algorithm for non-trivial low-qubit using the IBM Qiskit local simulator, before trying out the 5-qubit ibmqx4 and 16-qubit ibmqx5 machines. If successful, such methods can be generalized for multiple situations which in Euclidean QFT would lead to inverse problems arising from analytic continuation to real time.

The time line for WP3 is summarized in the table here:

Milestones	2020				2021				2022			
Spectral Functions	•	•	•	•	•	•						
Schwinger Model			•	•	•	•	•	•	•	•		
$2+1$ QFT Trails								•	•	•	•	•

3.4 Work Package 4 (WP4): Nuclear Structure, from Finite Nuclei to Infinite Nuclear Matter

Lead Scientists: Scott Bogner (MSU), Heiko Hergert (MSU), Morten Hjorth-Jensen (MSU) and Benjamin Hall (MSU Ph.D. student)

The central goal of WP4 is to perform quantum simulations of infinite nuclear matter by formulating classical many-body methods like Coupled Cluster (CC) and Similarity Renormalization Group (SRG) theory in terms of quantum algorithms. In particular, we will work on the so-called Unitary Coupled Cluster (UCC) and In-Medium SRG (IMSRG) approaches. Both methods can provide computationally affordable and systematically improvable wave functions that are suitable for implementation on current and near-term quantum computers as well as existing and future supercomputers.

We will first implement these approaches for the pairing and pairing plus particle-hole model Hamiltonians [75]. These are simplified models of nuclei that nevertheless capture important physical features. This part also links well with what is outlined in work package 1. We will then venture into calculations of the homogeneous electron gas and infinite nuclear matter based on realistic nuclear interactions. These systems have been studied with a variety of many-body methods, including standard Coupled Cluster theory and IMSRG. This offers us with ample opportunity to benchmark our quantum algorithms and allows us to set the stage for quantum computations of dynamical properties like response functions, which are at or beyond the limit of classical computers. An important example is the computation of the response function for neutrinos in nuclei and dense neutron star matter [76].

Classical vs. Quantum Simulations of Many-Body Hamiltonians. Attaining a thorough theoretical understanding of the behavior of many-body systems is a great challenge, but it provides fundamental insights into quantum mechanics and offers many potential areas of applications. However, apart from a few analytically solvable problems, the typical absence of an exactly solvable contribution to the many-particle Hamiltonian means that we ultimately need reliable numerical many-body methods. These methods should allow for controlled approximations and provide a computational scheme which accounts for successive many-body corrections in a systematic way. Typical examples of popular many-body methods, mentioned also in our introduction, are the aforementioned CC approach, various types of Monte Carlo methods, perturbative expansions, Green's function methods, the Density-Matrix Renormalization Group (DMRG), ab initio Density Functional Theory, and large-scale diagonalization methods, to mention just a few. All these methods have to face in some form or the other the problem of an exponential growth in dimensionality. This dimensional curse means that most quantum- mechanical calculations on classical computers have exponential complexity, and therefore are very hard to solve for

larger systems. In contrast quantum computer can greatly increase size of systems that can be simulated, as foreseen by Feynman [3]. It was shown early on that quantum phase estimation (QPE) provides an exponential speed-up over the best "currently" known classical algorithms for determining the ground state of a given Hamiltonian [77]. However, the use of this approach is believed to require large, error-corrected, quantum computers to surpass what is possible classically [78, 79]. A more promising path to exploring such a "quantum supremacy"[80, 81] for, say, two-body Hamiltonians on near-term quantum devices, is a quantum-classical hybrid algorithm that is referred to as the variational quantum eigensolver (VQE)[82, 83].

Unlike the quantum phase estimation, VQE requires only a short coherence time. This hybrid approach uses a quantum computer to prepare and manipulate a parameterized wave function, and embeds this in a classical optimization algorithm to minimize the energy of the state as measured on the quantum computer, i.e.,

$$E = \min_{\theta} \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle, \tag{26}$$

where θ denotes the set of parameters specifying the quantum circuit required to prepare the state $|\psi\rangle$.

From a nuclear many-body perspective, there are two key attractive aspects of the VQE framework:

1. The evaluation of the energy of a wide class of wave function ansätze which are exponentially costly classically (with currently known algorithms) requires only state preparation and measurement of Pauli operators, both of which can be carried out on a quantum processor in polynomial time. These wave function ansätze include the aforementioned UCC wave functions, [84, 82] the deep multi-scale entanglement renormalization ansatz [85], a Trotterized version of adiabatic state preparation [86], the Qubit Coupled Cluster approach (QCC) [87] and various low-depth quantum circuits inspired by the specific constraints of physical devices currently available. [88]. The IMSRG approach should also fall under this category, as we aim to demonstrate under the scope of WP4.

2. On a quantum processor, an efficient evaluation of the magnitude of the overlap between two quantum states is possible even when two states involve exponentially many determinants. Classically, this is a distinct feature only of tensor network [89] and variational Monte Carlo [90] approaches. On a quantum computer, *any* states that can be efficiently prepared will also possess this advantage.

Quantum Computations for Simplified Nuclear Models. Given the recent progress and near-term prospects in quantum computing hardware, and the uniqueness of its capabilities, it is interesting to explore these two aspects from a nuclear many-body perspective and this constitutes a major motivation of WP4.

Starting from a Hamiltonian in second-quantized form

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_s a_r \,, \tag{27}$$

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

$$\begin{aligned} a_i^\dagger &= \sigma_z^{\otimes i-1} \otimes \sigma_+ \otimes \mathbb{I}^{\otimes n-i} \\ a_i &= \sigma_z^{\otimes i-1} \otimes \sigma_- \otimes \mathbb{I}^{\otimes n-i} \,. \end{aligned} \tag{28}$$

We note that finding efficient mappings for many types of Hamiltonians and algoirthms is still very much an open problem, which this part of our project will be tightly coupled to the efforts under WP1. The next step is the application of the the time-evolution operator

$$U = e^{-iHt/\hbar} = e^{-i\sum_k H_k t/\hbar} \,, \tag{29}$$

using an approximation such as the Suzuki-Trotter

$$e^{A+B} = \lim_{n\to\infty} \left(e^{A/n} e^{B/n}\right)^n \tag{30}$$

decomposition. Finding the optimal approximation strategy for a given problem and mapping the resulting operator onto quantum gates is another active area of research, and we plan to apply our RG and many-body experience in that area. In the near term, it is especially important to construct circuits with short depth to control coherence and noise. Finally, one plugs the quantum circuit for U into an appropriate algorithm like QPE to compute the eigenvalues of a Hamiltonian, as demonstrated for the nuclear pairing model in [91].

We have recently repeated the QPE calculation for the pairing model in collaboration with MSU Ph.D. student Benjamin Hall, who also works together with MSU Ph.D. student Ryan Larose on related topics. The first near-term goal of WP4 is to extend this model to include pairing plus particle-hole excitations [75] and use VQE instead of the QPE algorithm. The quantum computer is used to prepare an initial state guess 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 an appropriate norm of the difference between the iterations of the expectation values and stops once this difference 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 using the previously attained knowledge of the ground-state energy, and repeating the algorithm. Continuing onward from these results, we will pursue the more ambitious task to design efficient quantum algorithms for the IMSRG and UCC theories that will be able to run on both existing quantum computers and classical supercomputers.

Designing Quantum Algorithms for In-Medium SRG and Unitary Coupled Cluster. Following the benchmark calculations using VQE, the next major goal of WP4 is to develop quantum algorithms that perform SRG evolutions. A quantum computer is ideally suited for this purpose because SRGs are based on continuous unitary transformations. The IMSRG, in particular, can be used to directly compute individual nuclear eigenstates [92, 93, 94]. This is achieved by solving a system of coupled non-linear ODEs. While quantum algorithms for such applications exist, the depth of the necessary quantum circuit exceeds the capabilities of current and near-term devices.

However, the IMSRG wave function that results from applying the aggregate unitary transformation to a chosen uncorrelated reference state may represent a novel type of ansatz that can be optimized using the VQE [95], as mentioned above. Using the Magnus expansion, the IMSRG wave function can be written as $|\Psi(s)\rangle = e^{\Omega(s)} |\Phi\rangle$, with a typically uncorrelated reference state $|\Phi\rangle$ and an operator $\Omega(s)$ that changes dynamically as we evolve in the flow parameter s [96]. We note that this ansatz encompasses the UCC method that has been used successfully in conjunction with the VQE to determine electronic (see, e.g., [42, 17, 97]) and nuclear ground state wave functions [98, 99]. Unitary CC is obtained as the special case in which $\Omega(s) = s(T - T^\dagger)$, where T is determined by a "global" variational optimization, and s parameterizes a trivial linear trajectory between the reference state $|\Phi\rangle$ and the UCC wave function. In contrast, the dynamically updated $\Omega(s)$ of the IMSRG approach allows more general, locally optimized trajectories in the manifold of evolving operators that should allow greater control over approximation errors (see [94] for a detailed discussion).

With its explicit flow parameter, i.e., renormalization scale, dependence the IMSRG wave function is conceptually analogous to certain types of tensor network states, in particular MERA-type states [85, 100, 101, 102, 95]. These states have not only been extremely powerful tools in real-space or lattice RG approaches, but they can also be translated into quantum circuits in a fairly easy manner (see, e.g., [95]). Instead of describing the entanglement of lattice sites under rather simple short-range interactions,

the IMSRG wave function encodes the entanglement of modes in momentum space (e.g., in a plane-wave basis) or a more general configuration space. The entanglement patterns of such modes are often more complex than those of lattice systems, especially when symmetries need to be taken into account [103], hence a quantum circuit based on the IMSRG wave function will have features that are distinct from lattice tensor network states.

Our first step in these studies is to again apply these algorithms to the simple Hamiltonians studied with VPE and QPE in the early stages of WP4. In a recent work, Babbush *et al* develop the formalism for performing quantum simulations with a plane-wave bases [104] for the homogeneous electron gas (HEG). Our final goal is to extend our quantum algorithms for the UCC and IMSRG to both the HEG and infinite nuclear matter. This will lay the foundation for the application of quantum algorithms for studies of finite nuclei and infinite nuclear matter.

Magnus Methods and Trotterization. In the Magnus formulation of the IMSRG, the unitary transformation is expressed as true operator exponential $U(s) = e^{\Omega(s)}$ rather than a Dyson series and evolutions for multiple observables are replaced by a single evolution of the anti-Hermitian operator $\Omega(s)$ [96]. Since the unitarity of the IMSRG transformation is made explicit by the Magnus ansatz, the flow equation for $\Omega(s)$ can be solved reliably with methods as simple as a first-order forward Euler integration, while taking large time steps. This is the reason why entire classes of numerical ODE integration methods are based on the Magnus expansion (see, e.g,. [105]). Continuing along those lines, we will investigate whether Magnus methods — possibly augmented with (S)RG ideas, e.g., a dynamical optimization for different time evolution scales — can be a complement or a viable alternative to Trotterization.

Preprocessing Nuclear Hamiltonians with Similarity Renormalization Group Methods. Similarity Renormalization group (SRG) methods have played an important role in enabling the enormous progress in nuclear many-body theory in the past decade, by providing systematic tools for dialing the resolution scales of interactions and quantum states [106, 92, 94, 107]. The resolution scale of the Hamiltonian will inherently affect the complexity of its quantum-gate representation and the susceptibility of the computation to noise on near-term simulators: This is immediately evident from recent quantum simulations of light nuclei based on low-resolution effective field theory interactions [98, 99] and previous realistic interactions with high inherent resolution [108].

The time line for WP4 is summarized in the following table:

Milestones	2020				2021				2022			
Develop PE algorithm for Pairing model	•	•										
Develop VQE algorithm for Pairing model	•	•										
Implement generalized two-body Hamiltonian			•	•								
UCC for the HEG and Infinite Nuclear Matter					•	•	•	•	•	•	•	•
IMSRG for the HEG and Infinite Nuclear Matter					•	•	•	•	•	•	•	•
Magnus Expansion of Time Evolution Operator									•	•	•	•

3.5 Work Package 5 (WP5): Workforce Development

The development of competences and skills in computational science, data science, quantum computing and quantum information theories, machine learning etc is an essential part of the development of a workforce for the future in the STEM (Science, Technology, Engineering and Mathematics) fields. Essentially all jobs in the STEM fields require nowadays a broad spectrum of computational capabilities.

In work package 5 we present our plans for a professional development of the Ph.D. candidates and the postdoctoral fellow. This is split in two parts, the development of scientific and professional competences and a general mentoring environment which is offered at MSU.

Scientific development The scientific development of the candidates involves several elements, of which some exist already while other ones will be developed by this project.

- Ph.D. student Ryan Larose (also together with other Ph.D. students at MSU) has developed a well-attended and widely popular seminar series on Quantum Information and Computations (QuIC) at MSU. The QuIC seminar series has had several lectures and introductions that help new students and interested researchers to get started with quantum information theory and computing. This seminar series will be an important element in the dissemination of the results reached by this project and will also serve as an arena where students learn to present and promote their results. This project aims at helping in further developing this seminar series into a sustainable series in quantum information theory and computing at MSU.

- Patrick Coles has during the last few years chaired the Los Alamos National Laboratory's (LANL) Quantum Computing Summer School. This is an immersive 10-week curriculum that includes tutorials from world-leading experts in quantum computation as well as one-on-one mentoring from LANL staff scientists who are conducting cutting-edge quantum computing research. For our Ph.D. candidates this summer school offers a unique opportunity to meet world leading experts in quantum computing.

- We will also establish a three week intensive Nuclear TALENT (Training in Advanced Low Energy Nuclear Theory) course on quantum information theory and computing tailored to nuclear physics problems. This course will be offered in the second and third years of the project with the aim to introduce potential new students to the field. The postdoctoral fellow and the Ph.D. students are both likely participants and teaching assistants as well.

- Michigan State University offers, via the newly established department for Computational Mathematics, Science and Engineering (CMSE) a dual Ph.D. program in both Physics and Computational Science. This has important consequences for the possibility to establish a proper educational path in computational skills and competences, spanning from management of large numerical projects and making sustainable code projects to important algorithms and methods. Computational skills and competences are essential to most jobs in the STEM fields, and with quantum computing and quantum information theory as emerging fields, we guarantee thus a proper professional training of our students and postdoctoral fellows. This training will also involve classical computing and classical many-body algorithms and the development of large numerical projects.

- The CMSE Department at Michigan State University plans to hire several faculty members over the few years in the areas of quantum information and quantum computing. As a part of this hiring plan there will be a concerted effort to make connections between the new quantum information/computing faculty and the existing strengths in the CMSE Department in machine learning and data analytics.

- With our collaboration partnership with IBM and other industry research venues, our Ph.D. students can take advantage of internship and job opportunities.

- The annual workshops to be held by our project group will also allow our students and postdoctoral fellow to get in contact with many of the leading experts in the field. We are also planning for the second and third year a week long Hackathon on quantum computing and quantum information theory.

Mentoring plan The mentoring of the graduate students and postdoctoral fellow participating in this project will be fully incorporated in the existing mentoring program at FRIB/NSCL. At any time there are about 20 experimental and theoretical postdoctoral fellows and approximately 100 graduate students at the FRIB/NSCL. It is an ideal research environment that enables graduate students and postdoctoral fellows to work and interact daily with other students, postdoctoral fellows and senior researchers with diverse backgrounds. A few years ago FRIB/NSCL strengthened and improved the mentoring of graduate students and postdoctoral fellows at FRIB/NSCL with the appointment of an Associate Director for Education. One of the new initiatives is a review of each postdoctoral fellow every half year. This consists of meetings with their supervisors to document progress, concerns, expectations and outlook. The Associate Director for Education also meet swith all FRIB/NSCL postdoctoral fellows on a monthly basis to keep them informed about FRIB/NSCL related news and activities. Postdoctoral fellows maintain their own website, where they share experiences and information on job openings. Postdoctoral fellows are also encouraged to participate in activities and programs offered by the university and the professional societies. Recent postdoctoral fellows have been participating in an MSU sponsored work/life-balance workshop as well as APS professional development workshops. FRIB/NSCL focuses specifically 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 interactions that connect current students and postdoctoral fellows with successful FRIB/NSCL alumni in a variety of careers. The FRIB/NSCL alumni contact list currently contains the names of 250 alumni who volunteered to be contacted by graduate students and postdoctoral fellows for career advice. The graduate students and postdoctoral fellows are an integral part of all laboratory social activities at FRIB/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 among all laboratory employees and students.

The time line for WP5 is summarized in the table here:

Milestones	2020				2021				2022			
Developing the QuIC Seminar	•	•	•	•	•	•	•	•	•	•	•	•
Nuclear TALENT Course on QI					•	•	•	•	•	•	•	•
Workshop and Hackathon					•	•	•	•	•	•	•	•

4 Timetable of Activities

We propose a three-year project to develop quantum simulation algorithms for scientific computing applications in nuclear physics. The project consists of the five work packages discussed above and this section summarizes the timetable outlined in the above tables. Our tasks include the development of classical algorithms, quantum algorithms, and software.

- Year 1: Government fiscal year 2020

  1. Project kick off meeting at MSU to coordinate logistics, discuss specific tasks, and review application targets.
  2. WP1: Cost-driven design for current QCs
  3. WP2: Variational adiabatic evolution and spectral reconstruction
  4. WP3: Spectral functions and Schwinger model
  5. WP4: Rewrite the pairing Hamiltonian in terms of quantum gates and implement QPE and VQE algorithms. Rewrite general two-body Hamiltonian in terms of quantum gates.
  6. WP5: QuIC seminar. Develop educational material which can be used at the LANL summer school.
  7. Public release of developed software tools.

8. Deliverable Year 1: Results from work packages 1-5 compiled and delivered to the program office

- Year 2: Government fiscal year 2021

1. Team hackathon meeting at MSU and coordination of logistics, discuss specific tasks and progress. Review and adjustment of targets.
2. WP1: Cost-driven design for current QCs and data-driven design for future QCs
3. WP2: Spectral reconstruction and transition matrix elements. Few-body dynamics.
4. WP3: Schwinger model and $2+1$ QFT tryout
5. WP4: Develop UCC and IMSRG codes for quantum computing, implement the VQE and PQE algorithms.
6. WP5: Develop and extend the QuIC seminar and the Nuclear TALENT Course as well as further educational material to be offered at for example the LANL summer school.
7. Public release of developed software tools.
8. Deliverable Year 2: Results from work packages 1-5 compiled and delivered to the program office.

- Year 3: Government fiscal year 2022

1. Team hackathon meeting at MSU and coordination of logistics, discuss specific tasks and progress. Review and adjustment of targets.
2. WP1: Data-driven design for future QCs
3. WP2: Few-body dynamics and scattering and reaction probabilities
4. WP3: Schwinger model and $2+1$ QFT tryout
5. WP4: Perform studies of infinite systems using developed quantum computing algorithms. Compare with existing classical coupled-cluster and IMSRG codes. Magnus Expansion of Time Evolution Operator.
6. WP5: Develop and extend the QuIC seminar. Develop educational material for intensive Nuclear TALENT courses and courses to be taught at MSU and the LANL summer school.
7. Public release of developed software tools.
8. Deliverable Year 3: Results from work packages 1-5 compiled and delivered to the program office.

5 Project Management Plan

We will manage project research activities through a combination of weekly meetings including video teleconferences, online collaborative software such as GitHub, and the teams slack channel. Every year MSU will host team workshops devoted to specific topics, including kickoff, algorithm development, and software development. The Lead Principal Investigators from each will work package provide the project leader with monthly status updates on financial and programmatic topics. The task leaders will provide the project leader and the other investigators with monthly reports on technical progress and challenges. The project leader will provide the DOE program manager with quarterly status reports via email as well as the written annual report. The structure of our project by task and personnel is described here with detailed description of individual responsibilities.

5.1 Responsibilities of Key Personnel

- Morten Hjorth-Jensen is the project leader and primary contact responsible for communications with the DOE program manager on behalf of all participants. Hjorth-Jensen will serve as Lead Principal Investigator for MSU and he will lead work package 5 **Work Force development** . He will also contribute his expertise in many-body physics and computational physics across all tasks.
- Patrick Coles is the leader of work package 1 **Quantum Simulation Algorithms**. He is a leading quantum information theorist and will provide his expertise across all work packages thus making sure that there is a proper link between quantum information theory and the three nuclear many-body problem work packages. He will also oversee the development of competencies in quantum information theories in work package 5 on work force development.
- Dean Lee is the leader of work package 2 **Quantum State Preparation and Dynamics**. He will also contribute to the other work packages with his expertise in various many-body methods, quantum information theory and computational physics. He will also oversee that there is a proper link between all work packages. He will supervise a full-time postdoctoral fellow that contributes to the work packages 1, 2 and 3.
- Alexei Bazavov is the leader of work package 3 **Lattice Quantum Chromodynamics (QCD) and Quantum Information Theories**. Bazavov will contribute his expertise in lattice QCD and computational physics and link with recent advances in quantum information theories and work packages 1, 2 and 3 as well as developing competences in quantum field theories to work package 5.
- Scott Bogner will serve as project authority with responsibility for proper conduct of the research and oversee the work force development package across tasks. He will lead work package 4 **Nuclear Structure, from Finite Nuclei to Infinite Nuclear Matter** He will contribute his expertise in the nuclear many-body physics domain to work package 4 and all other work packages.
- Heiko Hergert will contribute his expertise in the nuclear many-body physics domain to work package 4 and all other work packages.
- Andrea Shindler will contribute his expertise in the lattice QCD domain to work package 3 as well as developing competences in quantum field theories to work package 5. He will also be responsible for the link between work packages 1, 2 and 3.
- Matthew Hirn is a mathematician with expertise in machine learning and will actively contribute to the development of quantum information theories in work package 1 and oversee the development of the pertinent work force competences in work package 5.
- Huey-Wen Lin will contribute her expertise in the lattice QCD domain to work package 3 as well as developing competences in quantum field theories to work package 5. She will also be responsible for the link between work packages 1, 2 and 3.
- Jennifer Glick will serve as non-senior personnel and quantum computing scientific liasion at IBM for the researchers at Los Alamos National Laboratory and Michigan State University. She has expertise in the quantum computing platforms available at IBM Q as well as a background in nuclear physics from her time as a Ph.D. student at Michigan State University.

6 Project Objectives

- Make the grand scientific challenges of nuclear physics known and visible to the quantum computing and quantum information communities.

- Develop and optimize quantum computing algorithms to address unsolved problems in nuclear physics, especially in the areas of lattice QCD and nuclear many-body physics.
- Explore new synergies and hybrid approaches connecting quantum and classical computing paradigms while benchmarking new methods against existing techniques.
- Develop new fundamental tools designed for nuclear physics but of general character and importance that can impact the fields of quantum computing and information science.
- Build an interdisciplinary team that brings together innovators from different communities, and which recruits and develops new talent in quantum computing and nuclear physics.
- Play a formative role in the development of quantum computing in nuclear physics by contributing to the identification of key missing elements in the architecture of future quantum computing platforms and strategies.
- Share discoveries, results, and resources with the nuclear physics and quantum computing communities through comprehensive outreach activities including summer schools, publications, research talks, public lectures, and open code access.

7 Additional Perspectives

7.1 Relevance and Benefit to Society

One of the benefits of this proposal to the scientific community is the development of an open source library that can be used by researchers and serve as an educational resource for graduate students and postdoctoral fellows learning about advanced nuclear theory and quantum computing. As an example, several members of the proposal team (Bogner, Hergert, Hjorth-Jensen and Lee) have, together with graduate students and colleagues, written three chapters on applications of several different many-body methods to nuclear physics studies in a recent Lecture Notes in Physics book [109]. These chapters contain links to fully open source computer codes and benchmark calculations, thereby making the underlying science transparent and reproducible. This will be the model for the dissemination of work products associated with this proposal.

The PIs have many collaborations with academic institutions worldwide. This provides possibilities for scientific exchanges, communications, and future opportunities for the students and postdoctoral fellow. 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 of 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 and quantum information theories 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. Furthermore, the competences and skills acquired by the Ph.D. candidates and postdoctoral fellow in computational science, quantum computing and quantum information theories will lay the foundation for the education of the next generation of the scientific workforce.

7.2 Environmental Impact

This project and its realization are expected to have no significant environmental impacts.

7.3 Ethical Perspectives

This project will provide open source access to codes and data as discussed in the data management section. This has important consequences for open intellectual exchange and ensuring that scientific results are reproducible. Our published results will have a link to our repositories with codes and simulation data. This will allow researchers from other institutions to benchmark and reproduce our results, as well as help advance research progress across the field. We will strive to write our codes in a modular format, thereby making them easily adaptable for future purposes. All PIs are committed to sound ethical conduct in research. We hope to serve as an example of open and proper ethical conduct in scientific research.

7.4 Commitment to Diversity

All of the project team members are committed to diversity in science and will seek to build a diverse scientific workforce and an inclusive environment for learning and research. We plan to actively recruit students and postdoctoral candidates from diverse backgrounds, in particular, under-represented minorities and women. This will be a priority for all of the training programs as well as the research projects.

8 Institutional Commitment

All investigators in this project are committed to the responsibilities, timetables and objectives stated in the proposal. These commitments from the involved researchers are essential for the successful completion of the research work products and take the form of uncompensated efforts. In the budget we have prioritized financial support and travel for the Ph.D. students and postdoctoral fellow. We wish to prioritize their scientific growth and development. Except for travel funds for Patrick Coles (LANL) to collaborate with other team members and present results to the quantum computing and information science communities, all other principal investigators will use other funds for travel and salaries. This applies also largely to surplus materials, supplies, or equipment, and the provision of access to facilities at no cost. It implies also the mentoring and training of the Ph.D. students and postdoctoral fellow.

A Biographical Sketches

Biographical sketches of the senior personnel follow in alphabetical order.

Biographical Sketches

Alexei Bazavov
Assistant Professor
Michigan State University

Education and Training

Kiev State University, Kiev, Ukraine	Physics	B.S.	1992-1997
Florida State University, Tallahassee, FL	Physics	M.S.	2003-2005
Florida State University, Tallahassee, FL	Physics	Ph.D.	2003-2007

Research and Professional Experience

Assistant Professor	Michigan State University	2016 – present
Research Associate	Indiana University	2016
Research Associate	University of Iowa and University of California, Riverside	2013 – 2016
Research Associate	Brookhaven National Laboratory	2010 – 2013
Research Associate	University of Arizona	2007 – 2010
Junior Research Fellow	Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine	1997 – 2002

Publications

88 total refereed publications; h-index = 35 (Google Scholar)

10 selected publications relevant to the present proposal:

1. Cloët, Ian C., Dietrich, Matthew R., Arrington, John, Bazavov, Alexei, Bishof, Michael, Freese, Adam, Gorshkov, Alexey V., Grassellino, Anna, Hafidi, Kawtar, Jacob, Zubin, McGuigan, Michael, Meurice, Yannick, Meziani, Zein-Eddine, Mueller, Peter, Muschik, Christine, Osborn, James, Otten, Matthew, Petreczky, Peter, Polakovic, Tomas, Poon, Alan, Pooser, Raphael, Roggero, Alessandro, Saffman, Mark, VanDevender, Brent, Zhang, Jiehang, Zohar, Erez, *Opportunities for Nuclear Physics & Quantum Information Science*, arXiv:1903.05453
2. Alexei Bazavov, Frithjof Karsch, Swagato Mukherjee, Peter Petreczky, *Hot-dense Lattice QCD: USQCD whitepaper 2018*, arXiv:1904.09951
3. Bazavov, A., Ding, H.-T., Hegde, P., Kaczmarek, O., Karsch, F., Karthik, N., Laermann, E., Lahiri, Anirban, Larsen, R., Li, S.-T., Mukherjee, Swagato, Ohno, H., Petreczky, P., Sandmeyer, H., Schmidt, C., Sharma, S., Steinbrecher, P., *Chiral crossover in QCD at zero and non-zero chemical potentials*, arXiv:1812.08235, accepted to Physics Letters B
4. Bazavov, Alexei, Meurice, Yannick, Tsai, Shan-Wen, Unmuth-Yockey, Judah, Zhang, Jin, *Gauge-invariant implementation of the Abelian Higgs model on optical lattices*, Phys.Rev. D92 (2015) no.7, 076003, arXiv:1503.08354
5. Bazavov, Alexei, Karsch, Frithjof, Maezawa, Yu, Mukherjee, Swagato, Petreczky, Peter, *In-medium modifications of open and hidden strange-charm mesons from spatial correlation functions*, Phys.Rev. D91 (2015) no.5, 054503, arXiv:1411.3018

Synergistic Activities

1. Referee for Phys. Rev. A, B, C, D, E, Letters, Physics Letters B, Nuclear Physics A

2. Organizer of International Sympozium on Lattice Field Theory, 2018; ECT* workshop on heavy-ion physics, 2017; Extreme QCD, 2012; Workshop on Thermal Photons and Dileptons, 2011

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers

Collaborators and Co-editors: Bailey, Jon (Seoul University); Bernard, Claude (Washington University); Bhattacharya, Tanmoy (Los Alamos National Laboratory); Bouchard, Chris (University of Glasgow); Brambilla, Nora (Technical University Munich); Brown, Nathan (Washington University); Burnier, Yannis (University of Lausanne); Christ, Norman (Columbia University); DeTar, Carleton (University of Utah); Ding, Heng-Tong (Central China Normal University); Du, Daping (Syracuse University); El-Khadra, Aida (University of Illinois); Freeland, Elizabeth (School of Art Institute of Chicago); Gamiz, Elvira (University of Granada); Gottlieb, Steven (Indiana University); Gupta, Rajan (Los Alamos National Laboratory); Heller, Urs (American Physical Society); Hegde, Prasad (Central China Normal University); Hetrick, Jim (University of the Pacific); Jung, Chulwoo (Brookhaven National Laboratory); Kaczmarek, Olaf (Bielefeld University); Karsch, Frithjof (Brookhaven National Laboratory); Komijani, Javad (Technical University Munich); Kronfeld, Andreas (Fermi National Laboratory); Laermann, Edwin (Bielefeld University); Laiho, Jack (Syracuse University); Levkova, Ludmila (NAUTO); Maezawa, Yu (Kyoto University); Mackenzie, Paul (Fermi National Laboratory); Mawhinney, Robert (Columbia University); Meurice, Yannick (University of Iowa); Monahan, Chris (Rutgers University); Mukherjee, Swagato (Brookhaven National Laboratory); Neil, Ethan (Colorado University); Ohno, Hiroshi (University of Tsukuba); Osborn, James (Argonne National Laboratory); Petreczky, Peter (Brookhaven National Laboratory); Primer, Tom (University of Arizona); Schmidt, Christian (Bielefeld University); Schroeder, Chris (Lawrence Livermore National Laboratory); Sharma, Sayantan (Brookhaven National Laboratory); Simone, Jim (Fermi National Laboratory); Soltz, Ron (Lawrence Livermore National Laboratory); Soeldner, Wolfgang (Regensburg University); Sugar, Robert (University of California, Santa Barbara); Toussaint, Doug (University of Arizona); Tsai, Shan-Wen (University of California, Riverside); Unmuth-Yockey, Judah (University of Iowa); Vairo, Antonio (Technical University Munich); Vranas, Pavlos (Lawrence Livermore National Laboratory); Wagner, Matthias (NVIDIA);Van de Water, Ruth (Fermi National Laboratory); Weber, Johannes (Technical University Munich); Zhou, Ran (Fermi National Laboratory);

Graduate and Postdoctoral Advisors and Advisees: Berg, Bernd (Florida State University; Ph.D. adviser); Toussaint, Doug (University of Arizona); Karsch, Frithjof (Brookhaven National Laboratory); Meurice, Yannick (University of Iowa); Tsai, Shan-Wen (University of California, Riverside); Gottlieb, Steven (Indiana University); Chuna, Thomas (Michigan State University, Ph.D. student); Hostetler, Leon (Michigan State University, Ph.D. student); Weber, Johannes (Michigan State University, postdoctoral associate)

Scott Bogner
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Michigan State University, East Lansing, MI 48824
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Education and Training

- SUNY Stony Brook, Physics: Ph.D., 2002
- University of Cincinnati, Nuclear Engineering: B.S., 1996

Research and Professional Experience

- *Professor*, NSCL and Dept. of Physics & Astronomy, Michigan State University, 2017–
- *Associate Professor*, NSCL and Dept. of Physics & Astronomy, Michigan State University, 2012–2017
- *Assistant Professor*, NSCL and Dept. of Physics & Astronomy, Michigan State University, 2007–2012
- *Research Associate*, The Ohio State University, 2004–2007
- *Research Associate*, Institute for Nuclear Theory, University of Washington, 2002–2004

Selected Publications Relevant to this Proposal

1. S. R. Stroberg, A. Calci, H. Hergert, J. D. Holt, S. K. Bogner, R. Roth, and A. Schwenk, A Nucleus-Dependent Valence-Space Approach to Nuclear Structure, Phys. Rev. Lett. **118**, 032502 (2017).
2. H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, K. Tsukiyama, The In-Medium Similarity Renormalization Group: A New Ab Initio Method for Nuclei, Phys. Rept. **621**, 165 (2016).
3. H. Hergert, S. K. Bogner, T. D. Morris, S. Binder, A. Calci, J. Langhammer, and R. Roth, Ab-Initio Multi-Reference In-Medium Similarity Renormalization Group Calculations of Calcium and Nickel Isotopes, Phys. Rev. C **90**, 041302(R) (2014).
4. S. König, S. K. Bogner, R. J. Furnstahl, S. N. More and T. Papenbrock, Ultraviolet extrapolations in finite oscillator bases Phys. Rev. C **90**, 064007 (2014).
5. S. R. Stroberg, H. Hergert, J. D. Holt, S. K. Bogner, A. Schwenk, Ground and Excited States of Doubly Open-Shell Nuclei From Ab Initio Valence-Space Hamiltonians, Phys. Rev. C **93**, 051301(R) (2016).
6. S. K. Bogner, H. Hergert, J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, and R. Roth, Nonperturbative Shell-Model Interactions from the In-Medium Similarity Renormalization Group, Phys. Rev. Lett. **113**, 142501 (2014).
7. H. Hergert, S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, In-Medium Similarity Renormalization Group with Chiral Two- Plus Three-Nucleon Interactions, Phys. Rev. C **87**, 034307 (2013).

Selected Synergistic Activities

- *Co-organizer:* ICNT program on "Theory for open-shell nuclei near the limits of stability", East Lansing, MI, May 11 - 29, 2015
- *Lecturer/Co-organizer:* TALENT summer school in "Nuclear Density Functional Theory and Self-Consistent Methods," 2014 ECT* Trento (Italy)(UK) www.nucleartalent.org/
- *Co-Organizer:* INT Program on "Computational and Theoretical Advances for Exotic Isotopes in the Medium Mass Region", Seattle, Washington, March 25 - April 19, 2013
- *Co-Organizer:* EMMI Program on "The Extreme Matter Physics of Nuclei: From Universal Properties to Neutron-Rich Extremes", Darmstadt, Germany, April 16 - May 11, 2012

Coauthors (48 months) and Co-editors (24 months)

L. Caceres (GANIL), A. Calci (TRIUMF), R. J. Furnstahl (OSU), H. Hergert (NSCL/FRIB & U Oslo), M. Hjorth-Jensen (NSCL/FRIB & U Oslo), J. D. Holt (TRIUMF), S. More (NSCL/FRIB), T. D. Morris (UT

Knoxville/ORNL), T. Papenbrock (UT Knoxville/ORNL), N. Parzuchowski (NSCL/FRIB), R. Roth (TU Darmstadt), A. Schwenk (TU Darmstadt), O. Sorlin (GANIL), S. R. Stroberg (TRIUMF), K. Tsukiyama (Millennium Capital Management Asia Ltd.)

Advisors

- R. J. Furnstahl (OSU, Postdoctoral)
- W. Haxton (INT/UW, Postdoctoral)
- T. T. S. Kuo (Stony Brook, Doctoral)

Graduate/Postdoctoral Advisees

- Graduate students: N. Parzuchowski (Ph.D. 2017) T. Morris (Ph.D. 2016))
- Postdocs: H. Hergert(NSCL/FRIB) S. More (NSCL/FRIB)

Patrick Coles

EXPERIENCE

STAFF SCIENTIST
Los Alamos National Laboratory, T-4 division
2017 – Present, Los Alamos, NM, USA
Focus: Quantum Computing Algorithms

POSTDOCTORAL RESEARCHER
Institute for Quantum Computing,
University of Waterloo
2014 – 2017, Waterloo, Ontario, Canada
Advisor: Norbert Lutkenhaus
Focus: Quantum Cryptography and Computing

POSTDOCTORAL RESEARCHER
Centre for Quantum Technologies,
National University of Singapore
2012 – 2014, Singapore, Singapore
Advisor: Stephanie Wehner
Focus: Quantum Information Theory

POSTDOCTORAL RESEARCHER
Department of Physics,
Carnegie Mellon University
2008 – 2012, Pittsburgh, PA, USA
Advisor: Robert Griffiths
Focus: Quantum Foundations

EDUCATION

UNIVERSITY OF CALIFORNIA, BERKELEY
Ph.D. Chemical Engineering
2002 – 2008, Berkeley, CA, USA
Thesis: Spin refrigeration in semiconductors

UNIVERSITY OF CAMBRIDGE
M.Phil. Biochemistry
Churchill Scholar *(only 11 selected in USA)*
2001 – 2002, Cambridge, United Kingdom
Thesis: 3D protein structure via NMR

CASE WESTERN RESERVE UNIVERSITY
B.S. Chemical Engineering
GPA: 4.0 (highest possible GPA)
1997 – 2001, Cleveland, OH, USA

ONLINE COURSE CERTIFICATES
Machine Learning, taught by Andrew Ng
Neural Networks, taught by Geoffrey Hinton
2016 – 2017, Coursera
https://www.coursera.org/

SYNERGISTIC ACTIVITES

- School organizer for LANL Quantum Computing Summer School (2018, 2019)
- Adjunct Assistant Professor in Physics Department at University of New Mexico (2019-Present)

SELECTED PUBLICATIONS

- P. Coles, V. Katariya, S. Lloyd, I. Marvian, M. Wilde “Entropic energy-time uncertainty relation” *Physical Review Letters*. 122: 100401 (2019)
- Y. Subasi, L. Cincio, P. Coles “Entanglement spectroscopy with a depth-two quantum circuit” *Journal of Physics A: Mathematical and Theoretical*. 52: 044001 (2019)
- L. Cincio, Y. Subasi, A. Sornborger, P. Coles “Learning the quantum algorithm for state overlap” *New Journal of Physics*. 20:113022 (2018)
- A. Winick, N. Lutkenhaus, P. Coles “Reliable numerical key rates for quantum key distribution” *Quantum.* 2: 77 (2018)
- P. Coles, M. Berta, M. Tomamichel, S. Wehner “Entropic uncertainty relations and their applications” *Reviews of Modern Physics.* 89: 015002 (2017)
- P. Coles, E. Metodiev, N. Lütkenhaus “Numerical approach for unstructured quantum key

distribution" *Nature Communications.* 7: 11712 (2016)

- D. Soh, C. Brif, P. Coles, N. Lütkenhaus, R. Camacho, J. Urayama, M. Sarovar "Self-referenced continuous-variable QKD protocol" *Physical Review X.* 5: 041010 (2015)
- P. Coles, J. Kaniewski, S. Wehner "Equivalence of wave-particle duality to entropic uncertainty" *Nature Communications*. 5: 5814 (2014)
- P. Coles, M. Piani "Complementary sequential measurements generate entanglement" *Physical Review A: Rapid Communications*. 89: 010302(R) (2014), **Editors' Suggestion**
- P. Coles, R. Colbeck, L. Yu, M. Zwolak "Uncertainty relations from simple entropic properties" *Physical Review Letters*. 108: 210405 (2012)

Collaborators (in the past 48 months):
Sornborger, Andrew, Los Alamos National Laboratory; Subasi, Yigit, Los Alamos National Laboratory; Zurek, Wojciech, Los Alamos National Laboratory; Lutkenhaus, Norbert, University of Waterloo; Wehner, Stephanie, TU Delft; Tomamichel, Marco, University of Technology Sydney; Berta, Mario, Imperial College London; Wilde, Mark, Louisiana State University; Lloyd, Seth, MIT; Marvian, Iman, Duke University; Kaniewski, Jedrzej, Polish Academy of Sciences;

Graduate and Postdoctoral Advisors and Advisees:
Arrasmith, Andrew, UC Davis; Cerezo, Marco, Los Alamos National Laboratory;

Biographical Sketches

Heiko Hergert

Assistant Professor of Physics

Facility for Rare Isotope Beams and Dept. of Physics & Astronomy, Michigan State University

Education and Training

TU Darmstadt, Germany, Theoretical Nuclear Physics: Dr. rer. nat., 2004-2008

TU Darmstadt, Germany, Theoretical Nuclear Physics: Diplom, 2003-2004

Research and Professional Experience

Assistant Professor	FRIB and Dept. of Physics & Astronomy, MSU	2015-
FRIB Theory Fellow	FRIB, MSU	2014-2015
Postdoc	Dept. of Physics, The Ohio State University	2011-2014
Postdoc	NSCL, MSU	2009-2011
Postdoc	Institute for Nuclear Physics, TU Darmstadt	2008-2009

Publications

34 total refereed publications; 17 as 1st or 2nd author; h-index = 23 (Google Scholar), 21 (Publons/Web of Knowledge)

10 elected publications relevant to the present proposal:

1. *"Non-Empirical Interactions for the Nuclear Shell Model: An Update"*, S. R. Stroberg, H. Hergert, S. K. Bogner, J. D. Holt, Ann. Rev. Nucl. Part. Sci. 69, in press, arXiv: 1902.06154 [nucl-th]
2. *"Generator-coordinate reference states for spectra and 0νββ decay in the in-medium similarity renormalization group"*, J. M. Yao, J. Engel, L. J. Wang, C. F. Jiao, H. Hergert, Phys. Rev. C 98, 054311 (2018), arXiv: 1807.11053 [nucl-th]
3. *"Bogoliubov Many-Body Perturbation Theory for Open-Shell Nuclei"*, A. Tichai, P. Arthuis, T. Duguet, V. Somà, H. Hergert, R. Roth, Phys. Lett. B 786, 195 (2018), arXiv: 1806.10931 [nucl-th]
4. *"Ab Initio Electromagnetic Observables with the In-Medium Similarity Renormalization Group"*, N. M. Parzuchowski, S. R. Stroberg, P. Navrátil, H. Hergert, S. K. Bogner, Phys. Rev. C 96, 034324 (2017), arXiv: 1705.05511 [nucl-th]
5. *"Ab Initio Description of Open-Shell Nuclei: Merging No-Core Shell Model and In-Medium Similarity Renormalization Group"*, E. Gebrerufael, K. Vobig, H. Hergert, R. Roth, Phys. Rev. Lett. 118, 152503 (2017), arXiv: 1610.05254 [nucl-th]
6. *"In-Medium Similarity Renormalization Group for Closed- and Open-Shell Nuclei"*, H. Hergert, Phys. Scripta 92, 023002 (2017), arXiv: 1607.06882 [nucl-th]
7. *"A Nucleus-Dependent Valence-Space Approach to Nuclear Structure"*, S. R. Stroberg, A. Calci, H. Hergert, J. D. Holt, S. K. Bogner, R. Roth, and A. Schwenk, Phys. Rev. Lett. 118, 032502 (2017), arXiv: 1607.03229 [nucl-th]

8. *"Ground and Excited States of Doubly Open-Shell Nuclei From Ab Initio Valence-Space Hamiltonians"*, S. R. Stroberg, H. Hergert, J. D. Holt, S. K. Bogner, A. Schwenk, Phys. Rev. C 93, 051301(R) (2016), arXiv: 1511.02802 [nucl-th]
9. *"The In-Medium Similarity Renormalization Group: A New Ab Initio Method for Nuclei"*, H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, K. Tsukiyama, Phys. Rept. 621, 165 (2016), arXiv: 1512.06956 [nucl-th]
10. *"Ab-Initio Multi-Reference In-Medium Similarity Renormalization Group Calculations of Calcium and Nickel Isotopes"*, H. Hergert, S. K. Bogner, T. D. Morris, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. C 90, 041302(R) (2014), arXiv: 1408.6555 [nucl-th]

Synergistic Activities

1. *Co-Organizer:* Nuclear Structure 2018, East Lansing, MI, USA, Advances in Rare Isotope Science (ARIS) 2017, Keystone, CO, USA
2. *Co-Organizer/Instructor:* 2020 TALENT Course 4: DFT and Self-Consistent Methods (planned)
3. *Referee:* Ann. Phys., Eur. Phys. J. A, J. Phys. G, Nucl. Phys. A, Phys. Lett. B, Phys. Rev. C, Phys. Rev. Lett.
4. *Proposal Reviewer:* US Department of Energy
5. *Member:* SciDAC-4 NUCLEI Collab., DoE Double Beta Decay (DBD) Topical Collab.

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers

Collaborators and Co-editors:

P. Arthuis (U Surrey), C. Barbieri (U Surrey), S. K. Bogner (NSCL/FRIB), B. A. Brown (NSCL/FRIB), A. Calci[1] (TRIUMF), T. Duguet (CEA Saclay), J. Engel (U North Carolina–Chapel Hill), K. Fossez (ANL & NSCL/FRIB), E. Gebrerufael[1] (TU Darmstadt), M. Hjorth-Jensen (NSCL/FRIB & U Oslo), J. D. Holt (TRIUMF), C. F. Jiao (San Diego State U), V. Lapoux (CEA Saclay), E. Leistenschneider (TRIUMF), T. D. Morris (U Tennessee–Knoxville & ORNL), P. Navrátil (TRIUMF), P. Papakonstantinou (IBS Daejeon), R. Roth (TU Darmstadt), A. Schwenk (TU Darmstadt), V. Somà (CEA Saclay), S. R. Stroberg (U Washington), A. Tichai (CEA Saclay), K. Tsukiyama[1] (CNS, U Tokyo), K. Vobig[1] (TU Darmstadt), L. J. Wang (U North Carolina–Chapel Hill), J. M. Yao (NSCL/FRIB)

[1] moved to industry

Graduate and Postdoctoral Advisors and Advisees:

Advisors: R. Roth (TU Darmstadt, graduate), S. K. Bogner (NSCL/FRIB, postdoctoral), R. J. Furnstahl (OSU, postdoctoral)

Postdocs Supervised: K. Fossez, R. Wirth, J. M. Yao

Graduate Students Supervised: J. Davison, J. Hill, B. Zhu

Matthew J. Hirn

Assistant Professor, Department of Computational Mathematics, Science and Engineering (CMSE)
Assistant Professor, Department of Mathematics
Michigan State University

Education and Training

Cornell University	Ithaca, NY	Mathematics	**BA**	2004
University of Maryland	College Park, MD	Mathematics	**PhD**	2009
Yale University	New Haven, CT	Applied Math.	**Postdoc**	2009-2013
Cornell University	Ithaca, NY	Mathematics	**Visit. Asst. Prof.**	2013
École Normale Supérieure	Paris, France	Computer Science	**Postdoc**	2013-2015

Research and Professional Experience

Assistant Professor of CMSE	Michigan State University	2015-Present
Assistant Professor of Mathematics	Michigan State Uninversity	2015-Present

Publications

Ten selected publications relevant to the present proposal:

[1] Feng Gao, Guy Wolf, and Matthew Hirn. **Geometric Scattering for Graph Data Analysis**. To appear in the *36th International Conference on Machine Learning*, 2019.

[2] Xavier Brumwell, Paul Sinz, Kwang Jin Kim, Yue Qi, and Matthew Hirn. **Steerable Wavelet Scattering for 3D Atomic Systems with Application to Li-Si Energy Prediction**. In *NeurIPS Workshop on Machine Learning for Molecules and Materials*, Montreal, Canada, 2018.

[3] Michael Eickenberg, Georgios Exarchakis, Matthew Hirn, Stéphane Mallat, and Louis Thiry. **Solid Harmonic Wavelet Scattering for Predictions of Molecule Properties**. *The Journal of Chemical Physics* (Editor's Pick), vol. 148, 241732, 2018.

[4] Nicholas F. Marshall and Matthew J. Hirn. **Time Coupled Diffusion Maps**. *Applied and Computational Harmonic Analysis*, vol. 45, no. 3, pp. 709–728, 2018.

[5] Michael Eickenberg, Georgios Exarchakis, Matthew Hirn, and Stéphane Mallat. **Solid Harmonic Wavelet Scattering: Predicting Quantum Molecular Energy from Invariant Descriptors of 3D Electronic Densities**. In *Advances in Neural Information Processing Systems 30*, pp. 6543–6552, 2017.

[6] Matthew J. Hirn, Nicolas Poilvert, and Stéphane Mallat. **Wavelet scattering regression of quantum chemical energies**. *Multiscale Modeling and Simulation*, vol. 15, no. 2, pp. 827–863, 2017.

[7] Ariel Herbert-Voss, Matthew J. Hirn, and Frederick McCollum. **Computing minimal interpolants in $C^{1,1}(\mathbb{R}^d)$**. *Revista Matemática Iberoamericana*, vol. 33, no. 1, pp. 29–66, 2017.

[8] Ronald R. Coifman and Matthew J. Hirn. **Diffusion maps for changing data**. *Applied and Computational Harmonic Analysis*, vol. 36, no. 1, pp. 79–107, 2014.

[9] Matthew J. Hirn and Erwan Le Gruyer. **A general theorem of existence of quasi absolutely minimal Lipschitz extensions**. *Mathematische Annalen*, vol. 359, no. 3-4, pp. 595–628, 2014.

[10] Ronald R. Coifman and Matthew J. Hirn. **Bi-stochastic kernels via asymmetric affinity functions**. *Applied and Computational Harmonic Analysis*, vol. 35, no. 1, pp. 177–180, 2013.

SYNERGISTIC ACTIVITIES

1. **Undergraduate, Graduate, and Postdoc Education**
   - Directed an NSF REU on *Machine Learning from Quantum Computing* at MSU (Summer 2018), and an NSF REU on *High Dimensional Data Analysis* at Cornell (Summer, 2013).
   - Chair of the Undergraduate Studies Committee for the CMSE Department (2017 – Present), during which time the department developed (with the Departments of Computer Science and Statistics) and undergraduate degree in *Data Science*.
   - Scientific leader of the **C**ompl**E**x **D**ata **A**nalysis **R**esearch (CEDAR) team, whose current members include five graduate students and three postdocs.
   - Developed two new graduate courses, *Mathematical Foundations of Data Science* and *Computational Harmonic Analysis and Data Science*. Currently developing a third new graduate course, *Mathematical Foundations of Deep Learning*, which will run in the Spring 2020 semester.
2. **Conference and Seminar Organization**
   - Co-organizer of the *Machine Learning Applied to Nuclear Physics Summer School* at the Facility for Rare Isotope Beams (May 20-23, 2019).
   - Organized session on *Kernel Learning and Harmonic Analysis* for the Culminating Workshop of the IPAM program on Understanding Many-Particle Systems with Machine Learning (Dec 13, 2016).
   - Co-organizer of the 8^{th} *Whitney Problems Workshop* at CIRM (Oct 19-23, 2015).
3. **Referee Work**
   - **Journals**: Applied and Computational Harmonic Analysis, European Journal of Operational Research, IEEE Signal Processing Letters, IEEE Transactions on Circuits and Systems for Video Technology, IEEE Transactions on Information Theory, International Conference on Machine Learning, International Journal of Quantum Chemistry, Linear Algebra and Its Applications, Neural Computation, NPJ Computational Materials, Proceedings of the American Mathematical Society, SIAM Journal on Applied Dynamical Systems, Signal Processing.
   - **Agencies**: DOE, NSF/NIH.

IDENTIFICATION OF POTENTIAL CONFLICTS OF INTEREST

Collaborators and Co-editors: Andén, Joakim (Flatiron Institute); Andreux, Mathieu (ENS-Paris); Angles, Tomás (ENS-Paris); Belilovsky, Eugene (Université de Montréal); Bruna, Joan (New York University); Burkhardt, Daniel (Yale University); Cella, Carmine (UC Berkeley); Chen, William (Yale University); Eickenberg, Michael (UC Berkeley); Exarchakis, Georgios (institut de la vision); Gustafson, Adam (University of Washington-Seattle); Herbert-Voss, Ariel (Harvard University); Ivanova, Natalia (Yale University); Iwen, Mark (Michigan State University); Kim, Kwang Jin (Michigan State University); Krishnaswamy, Smita (Yale University); Le Gruyer, Erwan (INSA-Rennes); Leonarduzzi, Roberto (ENS-Paris); Lostanlen, Vincent (New York University); Marshall, Nicholas (Yale University); McCollum, Frederick (New York University); Mohammed, Kitty (University of Washington-Seattle); Moon, Kevin (Utah State University); Narayanan, Hariharan (TIFR-Mumbai); Oyallon, Edouard (Centrale Supélec); Poilvert, Nicolas (Baylabs); Qi, Yue (Michigan State University); Rochette, Gaspar (ENS-Paris); Thiry, Louis (ENS-Paris); van den Elzen, Antonia (Yale University); van Dijk, David (Yale University); Wang, Zheng (Yale University); Welp, Tobias (Yale University); Wolf, Guy (Université de Montréal); Xie, Yuying (Michigan State University); Xu, Jason (Duke University); Zarka, John (ENS-Paris); Zhang, Sixhin (Peking University).

Graduate and Postdoctoral Advisors and Advisees: Benedetto, John (University of Maryland-College Park); Brugnone, Nathan (Michigan State University); Brumwell, Xavier (Michigan State University); Coifman, Ronald (Yale University); Gao, Feng (Michigan State University); He, Jieqian (Michigan State University); LaRose, Ryan (Michigan State University); Little, Anna (Michigan State University); Mallat, Stéphane (College de France); Okoudjou, Kasso (University of Maryland-College Park); Perlmutter, Michael (Michigan State University); Sinz, Paul (Michigan State University).

Biographical Sketch for Morten Hjorth-Jensen

Education and Training:

Institution	Major/Title	Degree	Date
Norwegian University of Science and Technology, Trondheim, Norway	Physics	MSc	1983-1988
University of Oslo, Norway	Physics	PhD	1988-1993
ECT*, Trento, Italy	Postdoctoral Researcher		1994-1996
Nordita, Copenhagen, Denmark	Postdoctoral Researcher		1996-1998

Professional positions:

Position	Institution	Date
Associate Professor of Physics	University of Oslo, Norway	1999-2001
Professor of Physics	University of Oslo, Norway	2001-present
Adjunct Professor	Michigan State University/NSCL	2003-2011
Professor of Physics	Michigan State University/NSCL	2012-present
Principal investigator	Center of Mathematics for Applications, University of Oslo	2003-2013
Principal investigator	Center for Computing in Science Education, University of Oslo	2016-present

Awards and Recognitions:

Award	Date
University of Oslo award for excellence in teaching	2000
Fellow of the American Physical Society	2007
Oak Ridge National Laboratory excellence in research award	2008
Outstanding referee award of the American Physical Society	2008
University of Oslo award for excellence in teaching	2011
NOKUT (National award, Norway) award for excellence in teaching	2012
Elected member of the Norwegian Academy of Sciences and Letters	2013
Elected member of the Royal Norwegian Society of Sciences and Letters	2015
University of Oslo award for excellence in teaching for developing the Computational Physics group	2015
Olav Thon Foundation National prize for excellence in teaching award (National, Norway)	2018

Publications: 147 total refereed publications; h-index = 47 (Web of Science/Publons `https://publons.com/researcher/1751939/morten-hjorth-jensen/`). Ten publications relevant for the present proposal

1. M. Hjorth-Jensen, M. P. Lombardo, and U. van Kolck (Editors), *An Advanced Course in Computational Nuclear Physics; Bridging the Scales from Quarks to Neutron Stars*, Lecture Notes in Physics **936**, 2017

2. G. Hagen, A. Ekström, C. Forssén, G. R. Jansen, W. Nazarewicz, T. Papenbrock, K. A. Wendt, S. Bacca, N. Barnea, B. Carlsson, C. Drischler, K. Hebeler, M. Hjorth-Jensen, M. Miorelli, G. Orlandini, A. Schwenk, and J. Simonis, *Charge, neutron, and weak size of the atomic nucleus*, Nature Physics **12**, 186 (2016).

3. A. Ekström, G. R. Jansen, K. A. Wendt, G. Hagen, T. Papenbrock, B. D. Carlsson, C. Forssén, M. Hjorth-Jensen, P. Navratil, W. Nazarewicz,*Accurate nuclear radii and binding energies from a chiral interaction*, Physical Review C **91**, 051301(R) (2015).

4. G. Hagen, T. Papenbrock, A. Ekstrom, G. Baardsen, S. Gandolfi, K. A. Wendt, M. Hjorth-Jensen, and C. Horowitz, *Coupled-cluster calculations of nucleonic matter*, Physical Review C **89**, 014319 (2014).

5. T. Papenbrock, G. Hagen, M. Hjorth-Jensen, and D. J. Dean, *Coupled-cluster computations of atomic nuclei*, Reports on Progress in Physics **77**, 096302 (2014).

6. A. Ekström, G. Baardsen, C. Forssén, G. Hagen, M. Hjorth-Jensen, G. Jansen, R. Machleidt, W. Nazarewicz, T. Papenbrock, J. Sarich, and S. Wild, *Optimized Chiral Nucleon-Nucleon Interaction at Next-to-Next-to-Leading Order*, Physical Review Letters **110**, 192502 (2013).

7. K. Kowalski, D. J. Dean, M. Hjorth-Jensen, T. Papenbrock, and P. Piecuch, *Coupled cluster calculations of ground and excited states of nuclei*, Physical Review Letters **92**, 132501 (2004).

8. D. J. Dean and M. Hjorth-Jensen, *Pairing in nuclear systems: from neutron stars to finite nuclei*, Reviews of Modern Physics **75**, 607 (2003).

9. H. Heiselberg and M. Hjorth-Jensen, *Phases of dense matter in neutron stars*, Physics Reports **328**, 237 (2000).

10. M. Hjorth-Jensen, T. T. S. Kuo, and E. Osnes, *Realistic effective interactions for nuclear systems*, Physics Reports **261**, 125 (1995).

In addition I have recently finalized two textbooks on Computational Physics (one introductory and one advanced) to be published in 2019 by the Institute of Physics Publishing (IOP), UK.

Synergistic Activities

1. With colleagues at Michigan State University and Oak Ridge National Laboratory we have established a long-term activity on Computational quantum mechanics with main applications to nuclear physics and solid state physics problems. This research activity includes development of many-body theories, quantum mechanical many-body algorithms and high-performance computing activities.

2. With colleagues from the USA and other European countries, we started the Nuclear Talent initiative in 2010, see `www.nucleartalent.org`, where the main aim is provide an advanced and comprehensive training to graduate students and young researchers in low-energy nuclear theory. The network aims at developing a broad curriculum that will provide the platform for a cutting-edge theory for understanding nuclei and nuclear reactions. The Nuclear Talent initiative has been highly welcomed by the Nuclear Physics community. In the period 2012-2016 we have organized 11 advanced courses, with one more to be held in 2017. We have had almost 40 applicants per course on average. I have developed and taught two of the courses and been an organizer at two other courses, as well as being a teacher and main organizer at a course in 2017 on the nuclear shell model.

3. Since 1999 I have established an activity in computational physics at the Department of Physics at the University of Oslo. In 2015 this activity was rewarded with the University of Oslo award on excellency in teaching. I have also started from scratch and developed several courses on computational physics and many-body physics, courses I teach both at Michigan State University and at the University of Oslo. My research deals with various many-body methods and their computational aspects, with an emphasis on appplications to the nuclear many-body problem.

4. With colleagues at the University of Oslo, I have been strongly involved in revising the way we teach our science courses by including computations in physics and mathematics course from the first semester of studies. This project is called 'Computing in Science Education' and has received considerable support from the University of Oslo and the Norwegian Ministry of research and education. This activity was newly awarded as a Norwegian Center of Excellency in Education. The newly established Center of Computing in Science Education has also strong links with Michigan State University and Professor Danny Caballero, whom I collaborate with on similar projects.

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers: Collaborators and Co-editors I collaborate with Scott Bogner, Alex Brown, Heiko Hergert, Witek Nazarewicz and Andrea Shindler at Michigan State University, David Dean, Gaute Hagen, Gustav Jansen, Sam Novario and Thomas Papenbrock at University of Tennessee and Oak Ridge National Laboratory, Wick Haxton at Berkeley, Mihai Horoi at Central Michigan University, Ubirajara van Kolck at University of Arizona, Maria Paola Lombardo at INFN, Frascati, Italy, Christian Forssen and Andreas Ekström at Chalmers, Sweden, Carlo Barbieri at Surrey, UK, Francesco Pederiva at University of Trento, Takaharu Otsuka, Naofumi Tsunoda and Kazuo Takayanagi at Tokyo University, Japan, and Artur Polls at the University of Barcelona, Spain. On Computing in Science education I collaborate with Professor Danny Caballero at Michigan State Univeristy. **Graduate and Postdoctoral Advisors** Eivind Osnes (University of Oslo, Norway, PhD advisor), Ben Mottelson (ECT*, postdoctoral advisor) **Thesis Advisor and**

Postgraduate-Scholar Sponsor (2014-2019) *Graduate and Post-doctoral Advisees:* Gustav Baardsen (PhD UiO, Oslo), Gustav Jansen (PhD UiO, now ORNL), Torquil McDonald Sørenssen (PhD UiO, Oslo), Justin Lietz (PhD MSU), Sam Novario (PhD MSU), Fei Yuang (PhD MSU), Andreas Ekström (UiO and MSU, now at Chalmers, Sweden), Simen Kvaal (UiO), Sølve Selstø (UiO) Nicolas Michel (MSU, now Lanzhou China).

Biographical Sketch

Dean Lee

Education and Training

Harvard University, Cambridge, MA	Physics	A.B.	1988-1992
Harvard University, Cambridge, MA	Physics	Ph.D.	1992-1998

Research and Professional Experience

Professor	FRIB, Michigan State University	2017-present
Professor	North Carolina State University	2012-2017
Associate Professor	North Carolina State University	2007-2012
Assistant Professor	North Carolina State University	2001-2007
Postdoctoral Researcher	University of Massachusetts Amherst	1998-2001

Honors and Awards

American Physical Society Fellow, 2014
Alumni Distinguished Undergraduate Professor Award, NCSU, 2013
Outstanding Teaching Award, NCSU, 2007
Apker Award, American Physical Society, 1991

Products

Most Related to this Proposal

1. D. Lee, J. Watkins, D. Frame, G. Given, R. He, N. Li, B.-N. Lu, A. Sarkar, "Time fractals and discrete scale invariance with trapped ions, arXiv:1901.01661.
2. D. Frame, R. He, I. Ipsen, Da. Lee, De. Lee, E. Rrapaj, "Eigenvector continuation with subspace learning", Phys. Rev. Lett. **121** 032501 (2018).
3. A. Rokash, E. Epelbaum, H. Krebs and D. Lee, "Effective forces between quantum bound states," Phys. Rev. Lett. **118**, 232502 (2017).
4. S. Elhatisari, N. Li, A. Rokash, J. M. Alarcon, D. Du, N. Klein, B.-N. Lu, U.-G. Meißner, E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee, G. Rupak, "Nuclear binding near a quantum phase transition," Phys. Rev. Lett. **117**, 132501 (2016).
5. S. Elhatisari, D. Lee, G. Rupak, E. Epelbaum, H. Krebs, T. A. Lähde, T. Luu and U.-G. Meißner, "*Ab initio* alpha-alpha scattering," Nature **528**, 111 (2015).

Five Other Products

1. S. Elhatisari, E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee, N. Li, B.-N. Lu, U.-G. Meißner and G. Rupak, "*Ab initio* calculations of the isotopic dependence of nuclear clustering," Phys. Rev. Lett. **119**, 222505 (2017).
2. E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee, U.-G. Meißner and G. Rupak, "*Ab Initio* Calculation of the Spectrum and Structure of ^{16}O," Phys. Rev. Lett. **112**, 102501 (2014).

3. G. Rupak and D. Lee, "Radiative capture reactions in lattice effective field theory," Phys. Rev. Lett. **111**, no. 3, 032502 (2013).
4. E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee and U.-G. Meißner, "Viability of Carbon-Based Life as a Function of the Light Quark Mass," Phys. Rev. Lett. **110**, 112502 (2013).
5. E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee and U.-G. Meißner, "Structure and rotations of the Hoyle state," Phys. Rev. Lett. **109**, 252501 (2012).

Synergistic Activities

1. Scientific advisor to the Quantum Information Science Workshop at Michigan State University (2018)
2. Founder and organizer of the Advanced Studies Gateway at FRIB (2018-present)
3. Co-organizer of Mainz Institute for Theoretical Physics Workshop on Progress in Diagrammatic Monte Carlo Methods for Quantum Field Theories in Particle-, Nuclear-, and Condensed Matter Physics" (2017)
4. Co-organizer of Institute for Nuclear Theory Program "Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart" (2017)
5. Chair/Chair-Elect/Vice Chair APS Topical Group on Few-Body Systems and Multiparticle Dynamics (2016-present)

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers:

Collaborators and Co-editors

Jose Manuel Alarcón (Universidad Complutense de Madrid), Martin Freer (University of Birmingham), Hans-Werner Hammer (Technical University of Darmstadt), Hisashi Horiuchi (Osaka University), Yoshiko Kanada-En'yo (Kyoto University), Nico Klein (University of Bonn), Timo Lähde (Forschungszentrum Jülich), Thomas Luu (Forschungszentrum Jülich / University of Bonn), Ulf-G. Meißner (University of Bonn / Forschungszentrum Jülich), Gautam Rupak (Mississippi State University)

Graduate and Postdoctoral Advisors

Howard Georgi (Harvard University), John Donoghue (University of Massachusetts Amherst), Eugene Golowich (University of Massachusetts Amherst), Barry Holstein (University of Massachusetts Amherst)

Graduate and Postdoctoral Advisees

Joey Bonitati (Michigan State University), Serdar Elhatisari (Karamanoglu Mehmetbey University), Dillon Frame (Michigan State University), Gabriel Given (Michigan State University), Rongzheng He (Michigan State University), Caleb Hicks (Michigan State University), Ning Li (Michigan State University), Bing-Nan Lu (Michigan State University), Avik Sarkar (Michigan State University), Richard Thomson (Alcatel), Jacob Watkins (Michigan State University)

Biographical Sketch

Huey-Wen Lin
Assistant Professor
Michigan State University

Education and Training

National Taiwan University, Taiwan	Physics	B.S.	1995-1999
Columbia University, New York, New York	Physics	Ph.D.	2000-2006

Research and Professional Experience

Assistant Professor	Physics/CMSE, Michigan State University	2016-present
Visiting Assistant Professor	University of California, Berkeley	2016-2015
Research Assistant Professor	University of Washington, Seattle	2009-2014
Postdoctoral Fellow	Jefferson Lab, Newport News	2006-2009

Publications

68 total refereed publications; h-index = 43 (Google Scholar)
10 selected publications relevant to the present proposal:

1. "Parton distributions and lattice QCD calculations: a community white paper", Huey-Wen Lin et al, **Prog. Part. Nucl. Phys.** 100 (2018) 107-160 (*Impact Factor 11.229*)
2. "First Monte Carlo Global analysis of Nucleon Transversity with Lattice QCD Constraints", H-W Lin, W. Melnitchouk, A. Prokudin, N. Sato, H. Shows, **Phys. Rev. Lett**. 120 (2018) no.15, 152502
3. "Proton Isovector Helicity Distribution on the Lattice at Physical Pion Mass", H.-W. Lin, J.-W. Chen, L. Jin, Y.-S. Liu, Y. Yang, J. Zhang, Y. Zhao, **Phys. Rev. Lett.** 121, 242003 (2018).
4. "Gluon Quasi-PDF from Lattice QCD", Zhou-You Fan, Yi-Bo Yang, Adam Anthony, Huey-Wen Lin, Keh-Fei Liu, arXiv:1808.02077 [hep-lat], **Phys. Rev. Lett.** 121, 242001 (2018).
5. "Neutron Electric Dipole Moment and Tensor Charges from Lattice QCD", T. Bhattacharya, V. Cirigliano, R. Gupta, H.-W. Lin, B. Yoon, ***Phys. Rev. Lett.*** 115, 212002 (2015).
6. "Helicity and Transversity Parton Distribution from Lattice QCD", Jiunn-Wei Chen, Xiangdong Ji, Huey-Wen Lin, and Jian-Hui Zhang, invited ***Frontier Article***, Nucl.Phys. B911 (2016) 246
7. "Nuclear \sigma-terms and Scalar-Isoscalar WIMP-Nucleus Interactions from Lattice QCD", S.R. Beane, S.D. Cohen, W. Detmold, H. -W. Lin, M.J. Savage, Phys. Rev. D 89, 074505 (2014)
8. "Magnetic moments of light nuclei from lattice quantum chromodynamics", S.R. Beane, E. Chang, S. Cohen, W. Detmold, H.-W. Lin, K. Orginos, A. Parreno, M.J. Savage, B.C. Tiburzi, ***Phys. Rev. Lett.*** 113, 252001 (2014)
9. "Hyperon-Nucleon Interactions and the Composition of Dense Nuclear Matter from Quantum Chromodynamics", S. Beane, E. Chang, S.D. Cohen, W. Detmold, H.-W. Lin, T. Luu, A. Parreno, K. Orginos, M. Savage, A. Torok, A. Walker-Loud, ***Phys. Rev. Lett.*** 109, 172001

10. Evidence for a Bound H-dibaryon from Lattice QCD", S. Beane, E. Chang, W. Detmold, H.-W. Lin, T. Luu, A. Parreno, K. Orginos, M. Savage, A.Torok, A. Walker-Loud, ***Phys. Rev. Lett***. 106, 162001

Synergistic Activities

1. Elected Chair of Gordon Research Conference on Photonuclear Reactions (2020)
2. Member, International Advisory Committee for the 37th International Symposium on Lattice Field Theory (Lattice 2019)
3. Chair for the 36th International Symposium on Lattice Field Theory, Jul. 22–28, 2018, Michigan State University, East Lansing, MI, USA
4. Initiator and co-organizer for first Workshop on *Parton Distributions and Lattice Calculations in the LHC era*, Mar. 22–24, 2017, Oxford, UK
5. Lead organizer for INT program on *Intersections of BSM Phenomenology and QCD for New-Physics Search*, Institute for Nuclear Theory, Seattle, WA, Fall 2015

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers:

Collaborators and Co-editors

T. Bhattacharya (LANL), J.-W. Chen (National Taiwan U.), Vincenzo Cirigliano (LANL), W. Detmold (MIT), R. Gupta (LANL), X. Ji (Shanghai Jiaotong U. & Maryland U.), K.F. Liu (Kentucky U.), K. Orginos (JLab & William-Mary Coll.), D. Richard (JLab), M.J. Savage (INT), Y. Yang (ITP, China), B. Yoon (LANL)

Graduate and Postdoctoral Advisors

Norman Chris (Columbia University), David Richard (JLab)

Graduate and Postdoctoral Advisees

Yi-Bo Yang (ITP, China), Daniel Bolton (U. Colorado), Raul Briceno (ODU)

Biographical Sketches

Andrea Shindler
Associate Professor
FRIB – Michigan State University

Education and Training

University of Rome "Tor Vergata", Department of Physics Rome, Italy M.Sc. 1997-1998
University of Rome "Tor Vergata", Department of Physics Rome, Italy Ph.D. 1998-2002
Italian Professor Habilitation 2014

Research and Professional Experience

Associate Professor MSU 2016 - present
Postdoctoral Fellow Forschungszentrum Jülich 2013 – 2016
Heisenberg Fellow CERN – Humboldt University Berlin 2010 – 2013
Postdoctoral CSIC fellowship CERN - Universidad Autonoma Madrid 2009 – 2010
Research Associate University of Liverpool 2007 - 2009
Research Associate NIC/DESY Zeuthen 2002 - 2007

Publications

41 total refereed publications; Total number of citations 2796; 100+ papers: 13; 50-100 papers: 6 h-index = 30

10 elected publications relevant to the present proposal:

1. "Confirming the Existence of the strong CP Problem in Lattice QCD with the Gradient Flow"
   J. Dragos, T. Luu, A. Shindler, J. de Vries, A. Yousif
   Feb 8, 2019. 49 pp. e-Print: arXiv:1902.03254 [hep-lat]
2. "Three neutrons from Lattice QCD"
   J.-L. Wynen, E. Berkowitz, T. Luu, A. Shindler, J. Bulava
   Oct 30, 2018. 7 pp. Conference: C18-07-22. e-Print: arXiv: 1810.12747 [hep-lat]
3. "Massive photons: an infrared regularization scheme for lattice QCD+QED"
   M. G. Endres, A. Shindler, B. C. Tiburzi, A. Walker-Loud
   Phys.Rev.Lett. 117 (2016) no.7, 072002; e-Print: arXiv:1507.08916 [hep-lat]
4. "Nucleon electric dipole moment with the gradient flow: the θ-term contribution"
   A. Shindler, T. Luu, J. de Vries
   Phys.Rev. D92 (2015) no.9, 094518; e-Print: arXiv: 1507.02343 [hep-lat]
5. "Computation of the chiral condensate using Nf = 2 and Nf=2+1+1 dynamical flavors of twisted mass fermions"
   Krzysztof Cichy, Elena Garcia-Ramos, Karl Jansen, Andrea Shindler
   PoS LATTICE2013 (2014) 128; e-Print: arXiv: 1312.3534
6. "The epsilon regime with twisted mass Wilson fermions"
   Oliver Bär, Silvia Necco, Andrea Shindler
   JHEP 1004 (2010) 053; e-Print: arXiv: 1002.1582 [hep-lat]
7. "Light Baryon masses with dynamical twisted mass fermions"
   …, P. Dimopoulos,..., R. Frezzotti,…, G. Herdoiza, K. Jansen,…, Christopher Michael,…, A. Shindler, C. Urbach, U. Wenger
   Phys. Rev. D78 (2008) 014509; e-print: arXiv:0803.3190 [hep-lat]

8. “Twisted mass lattice QCD”
   Andrea Shindler
   Phys. Rept. 461 (2008) 37-110; e-print: arXiv:0707.4093
9. “Iterative methods for overlap and twisted mass fermions”
   T. Chiarappa, K. Jansen, K.-I. Nagai, M. Papinutto, L. Scorzato, A. Shindler, C. Urbach, U. Wenger, I. Wetzorke
   Comput. Sci. Dis. 1 (2008) 015001; e-print: hep-lat/0609023
10. “Twisted mass quarks and the phase structure of lattice QCD”
    F. Farchioni, R. Frezzotti, K. Jansen, I. Montvay, G.C. Rossi, E. Scholz, A. Shindler, N. Ukita, C. Urbach, I. Wetzorke
    Eur. Phys. J. C39 (2005) 421-433; e-print: hep-lat/0406039

Synergistic Activities

1. Coordinator lecturer and organizer of the Nuclear TALENT School “From Quarks and Gluons to Nuclear Forces and Structure”
2. Main organizer of the FRIB-TA Topical Program “Hadronic Electric Dipole Moments in the FRIB Era: from the Proton to Protoactinium”
3. Organizer of the “The 36th International Symposium on Lattice Field Theory” July 2018
4. Honors Research Seminar for undergraduates affiliated with the Honors College Fall 2017
5. Referee for JHEP (Impact factor: 6.220), Physics Letters B (Impact factor: 6.019), Physical Review D (Impact factor: 4.864), Nuclear Physics B (Impact factor: 3.946), JETP Letters (Impact factor: 1.364)

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers

Collaborators and Co-editors: Berkowitz, Evan (Forschunszentrum Jülich); Bulava, John (Southern Denmark University); Bussone, Andrea (University Autonoma of Madrid); de Vries, Jordy (Univeristy of Massachusetts); Dimopoulos, Petros (University of Rome "Roma Tre"); Dragos, Jack (Michigan State University); Endres, Michael G. (former MIT); Frezzotti, Roberto (University of Rome "Tor Vergata"); Gimenez, Vicente (University of Valencia-CSIC); Herdoiza, Gregorio (Unviersity Autonoma of Madrid); Kim, Jangho (Goethe University Frankfurt); Lubicz, Vittorio (University of Rome "Roma Tre"); Luu, Thomas (Forschungszentrum Jülich); Monahan, Christopher (University of Washington); Reyes, Jose G. (Michigan State University); Rossi, Gian Carlo (University of Rome "Tor Vergata"); Simula, Silvano (University of Rome "Roma Tre"); Tarantino, Cecilia (University of Rome "Roma Tre"); Tiburzi, Brian C. (The City College of New York); Walker-Loud, Andre (Lawrence Berkeley National Laboratory); Wynen, Jan-Lukas (Forschungszentrum Jülich); Yousif, Ahmed (Michigan State University)

Graduate and Postdoctoral Advisors and Advisees: Petronzio, Roberto (University of Rome 2 "Tor Vergata"); Garcia Ramos, Elena (Humboldt University/DESY-Zeuthen); Gonalzez Lopez, Jenifer (Humboldt University/DESY-Zeuthen); Urbach, Carsten (Frei University/DESY-Zeuthen); Rizik, Matthew D. (Michigan State University); Pederiva, Giovanni (Michigan State University)

B Current and Pending Support

Current and pending support of the senior personnel follow in alphabetical order.

Current and Pending Support

Alexei Bazavov

Current

Sponsor:	Department of Energy
Award Number:	DE-SC0012704
Project/Proposal Title:	SciDAC-4: Computing the Properties of Matter with Leadership Computing Resources
Total Award Amount:	$550,000
Person-Months:	0
Total Award Period Covered:	9/1/17 – 8/31/22
Location of Project:	Multi-institutional, led by Jefferson Laboratory, MIT and Brookhaven National Laboratory; subcontract at MSU
Brief Description of Project:	Code development for lattice QCD calculations
Overlap with Proposed Research:	none

Sponsor:	National Science Foundation
Award Number:	PHY-1812332
Project/Proposal Title:	Heavy Quarkonia as Thermometer of Quark-Gluon Plasma
Total Award Amount:	$240,000
Person-Months:	1 month SUM
Total Award Period Covered:	8/15/18 – 8/31/21
Location of Project:	MSU
Brief Description of Project:	Study of the heavy quark bound states in quark-gluon plasma applying lattice QCD
Overlap with Proposed Research:	none

Sponsor:	Department of Energy
Award Number:	DE-SC0019139
Project/Proposal Title:	Foundations of Quantum Computing for Gauge Theories and Quantum Gravity
Total Award Amount:	$127,325
Person-Months:	0 months
Total Award Period Covered:	10/1/18 – 9/30/20
Location of Project:	Multi-institutional, lead by the University of Iowa, subcontract at MSU
Brief Description of Project:	Foundational aspects of quantum computing as applied to quantum field theories and quantum gravity, study of tensor renormalization group methods with applications to quantum computing
Overlap with Proposed Research:	none

Pending

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem

Total Award Amount:	$1,000,000
Person-Months:	0.12 academic
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.
Overlap with Proposed Research:	this is the proposed project

Current and Pending Support

Scott Bogner

Current

Sponsor:	National Science Foundation
Award Number:	PHY-1713901
Project/Proposal Title:	Ab-Initio Nuclear Theory: From Nuclei to Neutron Stars
Total Award Amount:	$600,000
Person-Months:	2 summer
Total Award Period Covered:	8/1/17 – 7/31/20
Location of Project:	Michigan State University
Brief Description of Project:	Ab-initio many-body theory for nuclear structure calculations
Overlap with Proposed Research:	Shares common many-body methods (IMSRG/CC theory), but the focus is very different (the proposed research focuses on algorithms to be employed on quantum computers.)

Sponsor:	Department of Energy
Award Number:	DE-SC0015376
Project/Proposal Title:	Nuclear Theory for Double Beta Decay and Fundamental Symmetries
Total Award Amount:	$150,000
Person-Months:	0.12 academic
Total Award Period Covered:	5/1/16 – 4/20/21
Location of Project:	Michigan State University
Brief Description of Project:	Develop reliable ab-initio calculations of neutrino less double beta decay nuclear matrix elements.
Overlap with Proposed Research:	None

Sponsor:	Department of Energy
Award Number:	DE-SC0018083
Project/Proposal Title:	Nuclear Computational Low Energy Initiative (NUCLEI)
Total Award Amount:	$1,821,000
Person-Months:	0.12 academic
Total Award Period Covered:	9/1/17 – 8/31/21
Location of Project:	Michigan State University
Brief Description of Project:	Develop microscopically based energy density functionals for nuclei.
Overlap with Proposed Research:	None

Pending

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000

Person-Months:	0.12 academic
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.
Overlap with Proposed Research:	this is the proposed project

Current and Pending Support

Patrick Coles

Current

Sponsor:	LANL LDRD
Award Number:	20180628ECR
Project/Proposal Title:	Machine learning of quantum computing algorithms
Total Award Amount:	$416,000
Total Award Period Covered:	10/01/18 - 09/30/20
Person-Months:	5
Brief Description of Project:	Develop quantum computing algorithms using machine learning
Overlap with Proposed Research:	Both proposals use machine learning, but for different purposes (general toolbox versus finding quantum simulation algorithms)

Sponsor:	LANL LDRD
Award Number:	2019065DR
Project/Proposal Title:	Taming Defects on Quantum Computers
Total Award Amount:	$4,710,000
Total Award Period Covered:	10/01/18 - 09/30/21
Person-Months:	2.5
Brief Description of Project:	Develop techniques to mitigate defects on quantum computers.
Overlap with Proposed Research:	Both proposals use machine learning, but for different purposes (taming defects versus finding quantum simulation algorithms)

Sponsor:	DOE, Office of Science
Award Number:	0000022066
Project/Proposal Title:	Topological phases of quantum matter and decoherence
Total Award Amount:	$3,489,000
Total Award Period Covered:	10/01/18 - 09/30/21
Person-Months:	1
Brief Description of Project:	Work on quantum algorithm to study topologically ordered systems.
Overlap with Proposed Research:	No significant overlap with current proposal.

Sponsor:	DOE, Office of Science
Award Number:	0000014775
Project/Proposal Title:	Optimization, Verification and Engineered Reliability of Quantum Computers
Total Award Amount:	$3,489,000
Total Award Period Covered:	10/01/18 - 09/30/22
Person-Months:	3
Brief Description of Project:	Develop noise-resilient algorithms.

Overlap with Proposed Research:	Both proposals use machine learning, but for different purposes (noise resilience versus finding quantum simulation algorithms)

Pending

Sponsor:	LANL LDRD
Award Number:	20200056DR
Project/Proposal Title:	Quantum Chemistry using Quantum Computers
Total Award Amount:	$4,800,000
Total Award Period Covered:	10/01/19--09/30/22
Person-Months:	2
Brief Description of Project:	Develop quantum algorithms to study problems in quantum chemistry.
Overlap with Proposed Research:	Both proposals use machine learning, but for different purposes (chemistry versus finding quantum simulation algorithms)

Sponsor:	DOE, Office of Science
Award Number:	0000025458
Project/Proposal Title:	Quantum computing for fusion energy sciences
Total Award Amount:	$500,000k
Total Award Period Covered:	10/01/19--09/30/21
Person-Months:	1
Brief Description of Project:	Develop quantum algorithms to study problems in fusion energy.
Overlap with Proposed Research:	No significant overlap with current proposal

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000
Person-Months:	0.12
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.

Overlap with Proposed Research: this is the proposed project

Current and Pending Support

Heiko Hergert

Current

Sponsor:	Department of Energy
Award Number:	DE-SC0018083
Project/Proposal Title:	Nuclear Computational Low Energy Initiative (NUCLEI)
Total Award Amount:	$1,821,000
Person-Months:	0.12 academic
Total Award Period Covered:	9/1/17 – 8/31/21
Location of Project:	Michigan State University
Brief Description of Project:	The SciDAC-4 NUCLEI collaboration brings together experts in theoretical nuclear physics, mathematics and computer science to advance the development of nuclear physics simulations. H. Hergert's group receives support for personnel and resources to perform many-body calculations of high interest to the NSCL/FRIB experimental program, the application of renormalization group methods in nuclear physics, and the continuing improvement of the simulation software (e.g., parallelization, implementation of uncertainty quantification etc.).
Overlap with Proposed Research:	None

Sponsor:	National Science Foundation
Award Number:	PHY-1614130
Project/Proposal Title:	A Novel Many-Body Method for the Description of Open-Shell Nuclei From First Principles
Total Award Amount:	$225,000
Person-Months:	1 summer
Total Award Period Covered:	8/15/16 – 7/31/19
Location of Project:	Michigan State University
Brief Description of Project:	This award supports the reformulation of the Multireference In-Medium Similarity Renormalization Group (MR-IMSRG) with the help of the Magnus expansion techniques, and the development of basic Equation-of-Motion (EoM) technology for calculating excited states and states in odd nuclei.
Overlap with Proposed Research:	None

Sponsor:	Department of Energy
Award Number:	DE-SC0017887
Project/Proposal Title:	Advanced Many-Body Methods for Nuclear Structure
Total Award Amount:	$750,000
Person-Months:	Y1: 1 summer, Y2: 1 summer, Y3-5: 2 summer
Total Award Period Covered:	9/1/17 – 8/31/22
Location of Project:	Michigan State University

Brief Description of Project:	This award supports the development of advanced extensions of the Multireference In-Medium Similarity Renormalization Group (MR-IMSRG) framework: (i) The consistent inclusion of continuum coupling effects in the computation of ground and excited states of nuclei at the limits of stability, (ii) the treatment of nuclei with strong collective correlations, e.g., intrinsic deformation, and (iii) the application of principal component decompositions and tensor factorization to control the memory requirements and computational scaling of the method.
Overlap with Proposed Research:	None

<u>Pending</u>

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000
Person-Months:	0.12 academic
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.
Overlap with Proposed Research:	this is the proposed project

Current and Pending Support

Matthew Hirn

Current

Sponsor:	National Science Foundation
Award Number:	1845856
Project/Proposal Title:	CAREER: Understanding invariant convolutional neural networks through many particle physics
Total Award Amount:	$400,000
Person-Months:	0.5 (summer)
Total Award Period Covered:	07/01/2019 – 06/30/2024
Location of Project:	Michigan State University
Brief Description of Project:	This award will facilitate an integrated scientific and educational program at the interface of mathematics, deep learning, many particle physics and data science.
Overlap with Proposed Research:	None

Sponsor:	National Science Foundation
Award Number:	1620216
Project/Proposal Title:	Three-dimensional deep wavelet scattering for quantum energy interpolation
Total Award Amount:	$191,775
Person-Months:	1.0 (summer)
Total Award Period Covered:	09/01/2016 – 08/31/2020
Location of Project:	Michigan State University
Brief Description of Project:	The goal of this project is to understand the mathematical theory underlying multiscale, multilayer machine learning architectures for quantum many body physics.
Overlap with Proposed Research:	None

Sponsor:	Defense Advanced Research Projects Agency
Award Number:	D16AP00117
Project/Proposal Title:	Deep wavelet scattering for quantum many body physics (DARPA Young Faculty Award)
Total Award Amount:	$744,297
Person-Months:	1.0 (summer)
Total Award Period Covered:	09/15/2016 – 09/14/2019
Location of Project:	Michigan State University
Brief Description of Project:	The goal of this project is to develop machine learning algorithms for the efficient and accurate estimation of quantum many body energies.
Overlap with Proposed Research:	None

Sponsor:	Alfred P. Sloan Foundation
Award Number:	FG-2016-6607
Project/Proposal Title:	Provable machine learning algorithms for scientific computation (Sloan Fellowship)
Total Award Amount:	$55,000
Person-Months:	0.0
Total Award Period Covered:	09/15/2016 – 09/14/2020
Location of Project:	Michigan State University
Brief Description of Project:	The goal of this project is to develop provably correct machine learning algorithms to facilitate large scale scientific computation.
Overlap with Proposed Research:	None

<u>Pending</u>

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000
Person-Months:	0.12
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.
Overlap with Proposed Research:	this is the proposed project

Sponsor:	National Science Foundation (subaward from the University of Michigan)
Project/Proposal Title:	HDR DSC: Midwest immersive data science training program
Total Award Amount:	$216,288
Person-Months:	0.5 (summer)
Total Award Period Covered:	10/01/2019 – 09/30/2022
Location of Project:	Michigan State University

Brief Description of Project:	This proposal develops a data science training program between Univ. of Michigan, MSU, and Ohio State University.
Overlap with Proposed Research:	None
Sponsor:	National Science Foundation
Project/Proposal Title:	Collaborative Research: Data-driven Path Metrics for Machine Learning
Total Award Amount:	$150,000
Person-Months:	0.5 (summer)
Total Award Period Covered:	07/01/2019 – 06/30/2021
Location of Project:	Michigan State University
Brief Description of Project:	This project will investigate data dependent path metrics that are defined by the best possible path through the data, and demonstrate these metrics are both density sensitive and geometry preserving.
Overlap with Proposed Research:	None
Sponsor:	National Institutes of Health
Project/Proposal Title:	Finding emergent structure in multi-sample biological data with the dual geometry of cells and features
Total Award Amount:	$1,599,998
Person-Months:	1.0 (summer)
Total Award Period Covered:	07/01/2019 – 06/30/2023
Location of Project:	Michigan State University
Brief Description of Project:	This project will develop and validate methods for stratifying single-cell samples consisting of single-cell data and will analyze them to find structures emerging at multiple granularities.
Overlap with Proposed Research:	None

Current and Pending Support

Morten Hjorth-Jensen

Current

Sponsor:	National Science Foundation
Award Number:	PHY-1713901
Project/Proposal Title:	Ab-Initio Nuclear Theory: From Nuclei to Neutron Stars
Total Award Amount:	$600,000
Person-Months:	0.12 summer
Total Award Period Covered:	8/1/17 – 7/31/20
Location of Project:	Michigan State University
Brief Description of Project:	This project aims at developing and applying complementary many-body methods to a wide variety of nuclear systems, ranging from stable closed-shell nuclei and homogenous dense nuclear matter to exotic loosely-bound neutron and proton rich nuclei far from shell closures. The proposed research will be built around thoroughly modern\emph{ab initio} many-body methods such as coupled cluster theory and the in-medium similarity renormalization group.
Overlap:	Except for the expertise of Bogner and Hjorth-Jensen that will be used in the new proposal to link with new methods from quantum computing and quantum information theory, there is no overlap.

Pending

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000
Person-Months:	0.12 summer
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.

Overlap with Proposed Research: this is the proposed project

Current and Pending Support

Dean Lee

Current

Sponsor:	Department of Energy
Award Number:	DE-SC0018638
Project/Proposal Title:	Nuclear Theory from First Principles to Forefront Experiments
Total Award Amount:	$210,000
Person-Months:	0.12 summer
Total Award Period Covered:	5/15/18 – 5/14/20
Location of Project:	Michigan State University
Brief Description of Project:	Lattice simulations based on chiral effective field theory are used to describe nuclear structure from first principles.
Overlap with Proposed Research:	No direct overlap.

Sponsor:	Department of Energy/NNSA
Award Number:	DE-AC52-06NA25396 (subaward from LANL)
Project/Proposal Title:	Large Scale Simulations of Nuclear Reactions
Total Award Amount:	$600,000
Person-Months:	1 summer
Total Award Period Covered:	10/5/18 – 8/30/22
Location of Project:	Michigan State University
Brief Description of Project:	Lattice simulations based on chiral effective field theory are used to describe nuclear scattering and reactions from first principles.
Overlap with Proposed Research:	No direct overlap.

Pending

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000
Person-Months:	0.12 summer
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites

	researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.
Overlap with Proposed Research:	this is the proposed project
Sponsor:	National Science Foundation
Project/Proposal Title:	Time fractals and discrete scale invariance with trapped ions
Total Award Amount:	$283,508
Person-Months:	0.5 summer
Total Award Period Covered:	5/16/19 – 5/15/22
Location of Project:	Michigan State University
Brief Description of Project:	Investigations of trapped ion systems which exhibit a spectrum with discrete scale invariance.
Overlap with Proposed Research:	No direct overlap. However some test examples in the current proposal will make use of findings from this project.

Current and Pending Support
Huey-Wen Lin

Current

Sponsor:	National Science Foundation
Award Number:	1653405
Project/Proposal Title:	"CAREER: Constraining Parton Distribution Functions for New- Physics Searches"
Total Award Amount:	$425,000
Person-Months:	2 SUM
Total Award Period Covered:	2017-2022
Location of Project:	Michigan State University
Brief Description of Project:	High-performance computing using lattice QCD to study the nucleon parton distribution functions and their applications and impacts on new- physics searches
Overlap with Proposed Research:	None

Pending

Sponsor:	Research Corporation Foundation for Scientific Achievement
Project/Proposal Title:	Unveiling the Three-Dimensional Structure of Nucleons
Total Award Amount:	$100,000
Person-Months:	0.5 SUM
Total Award Period Covered:	2020-2023
Location of Project:	Michigan State University
Brief Description of Project:	High-performance computing with lattice QCD to study the three-dimensional structure of nucleons
Overlap with Proposed Research:	None

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000
Person-Months:	0.12 SUM
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that spanfrom strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.
Overlap with Proposed Research:	this is the proposed project

Current and Pending Support

Andrea Shindler

Current

Sponsor:	Michigan State University, Discretionary Funding Initiative
Award Number:	N/A, internal MSU funds
Project/Proposal Title:	Fundamental symmetries from lattice QCD
Total Award Amount:	$50,000
Person-Months:	1 summer
Total Award Period Covered:	12/5/18 – 12/4/19
Location of Project:	Michigan State University
Brief Description of Project:	Software development for the calculation of fermionic disconnected diagrams relevant for the calculation of electric dipole moment and related quantities
Overlap with Proposed Research:	No Overlap

Pending

Sponsor:	Department of Energy
Project/Proposal Title:	From Quarks to Stars; A Quantum Computing Approach to the Nuclear Many-Body Problem
Total Award Amount:	$1,000,000
Person-Months:	0.12 summer
Total Award Period Covered:	10/1/19 – 9/30/22
Location of Project:	Michigan State University
Brief Description of Project:	This proposal aims at studying and applying recent developments of algorithms and methods from quantum computing and quantum information theory to studies of complex and strongly interacting nuclear many-particle systems. The proposal aims at developing new methods for studying systems that span from strong force simulations of quarks and gluons to many-body methods applied to the equation of state of dense matter. The proposal aims at developing interdisciplinary research projects that unites researchers in quantum computing and quantum information theory with theorists working on interacting many-particle methods applied to nuclear physics.
Overlap with Proposed Research:	this is the proposed project

Sponsor:	Department of Energy
Project/Proposal Title:	Fundamental symmetries using lattice QCD with the gradient flow
Total Award Amount:	$649,000
Person-Months:	2 summer
Total Award Period Covered:	5/16/19 – 5/15/22
Location of Project:	Michigan State University

Brief Description of Project:	Calculation, in lattice QCD, using the gradient flow of the nucleon electric dipole moment from all CP-violating source
Overlap with Proposed Research:	No Overlap
Sponsor:	National Science Foundation
Project/Proposal Title:	Fundamental symmetries using lattice QCD with the gradient flow
Total Award Amount:	$679,946
Person-Months:	2 summer
Total Award Period Covered:	5/16/19 – 5/15/22
Location of Project:	Michigan State University
Brief Description of Project:	Calculation, in lattice QCD, using the gradient flow of the nucleon electric dipole moment from all CP-violating source
Overlap with Proposed Research:	No Overlap

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D Facilities, Equipment and Other Resources

This project group will have access to high performance computing resources at MSU that are listed here.

D.1 Institute for Cyber-Enabled Research

MSU's Institute for Cyber-Enabled Research (ICER), was originally launched as the High-Performance Computing Center (HPCC) in 2005, before expanding its mission in 2008 to include research consulting. ICER staff currently includes five research consultants with backgrounds in different domain sciences that can aid in the adaptation of applications to ICER's infrastructure, provide support in proposal development, etc.

ICER provides HPC services to about 1000 users from MSU faculty and other Michigan universities. It is also an XSEDE level 3 partner institution (`http://www.xsede.org`). The facility offers two types of access to its compute resources:

1. Open access for MSU faculty and faculty-sponsored users, subject to a fair-sharing policy. Users jobs are limited to running on 512 cores at any given time, although short-term exceptions can be granted if necessary.

2. Buy-in accounts give MSU faculty priority access to specific nodes in ICER's systems. Buy-in nodes are not subject to the 512-core limit. User jobs are guaranteed to begin execution within four hours of submission, allowing open-access users to run short jobs on buy-in nodes. In this way, idle time in the system is minimized.

In 2017, ICER provided a total of 107M core hours of computing time to its user base.

D.1.1 Compute Resources

Laconia is MSU's primary computing resource, operated and maintained by the Institute for Cyber-Enabled Research (ICER). The cluster consists of 400 compute nodes powered by dual 14-core Intel *Broadwell* CPUs. 45 of these nodes are equipped with four Nvidia Tesla K80 GPUs. The theoretical peak performance of the system is ∼400 teraflops from CPUs only, and 754 teraflops with GPUs. In 2016, the system was benchmarked using the LINPACK benchmark at 535 teraflops, entering the TOP500 and Green500 supercomputer lists. The majority of the nodes are equipped with 128GB RAM. 24 of the CPU nodes and the 50 GPU nodes have 256GB RAM.

Secondary resources are the **Intel18** cluster with 144 compute nodes of dual 20-core Intel Xeon Gold (*Skylake*) and 384–768GB of memory, including 7 nodes with four NVidia Volta V100 GPUs, and the **Intel14** cluster, consisting of 192 compute nodes with dual Intel *Ivy Bridge* 10-core processors and 128–256 GB memory. 40 Intel14 nodes are equipped with two Nvidia Tesla K20 GPUs, 14 with Intel Xeon Phi accelerators.

D.1.2 Storage Infrastructure

ICER's data infrastructure offers 2 PB of scratch space on a Lustre file system that is accessible by all computing resources. The facility offers 2.1PB multiply-redundant, backed-up storage, eliminating the risk of data loss. Free storage of up to 1TB is provided to all ICER user accounts, which is sufficient to meet most of the day-to-day needs of the applications that will be used for this project. An additional 1TB of project storage is offered free of charge for working groups.

E Data Management Plan

The project investigators have determined the following data to be subject to the data management plan (DMP), and includes the following list of DMP elements. 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) of Michigan State University by each member of this research group. A shared group directory will be created by the FRIB/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. More details are outlined here.

E.1 Data Types and Sources

This project will produce computational tools for quantum scientific computing and nuclear many-body physics problems, resulting in four types of data which will be made available through a project website hosted at FRIB/NSCL. Output from simulation and various numerical experiments will be organized and documented so that users elsewhere can access that output in a form that makes it easy for them to use for comparisons to their own data, or as input for related codes that they have developed. Once research results are published, source codes that produce the data will be worked on so that they are readable and well documented and then made available for downloading.

E.2 Content and Format

Our open source software will be written in standard programming languages and scripting languages, including C/C++, Fortran and Python. Software documentation will use standard tools such as Doxygen to generate much documentation automatically. Other documentation, including Manual pages, user guides, administrator guides, etc., will be written in English and made available on project website and as PDF documents. Graphs and tables will be generated using standard libraries like Matplotlib in Python, gnuplot, and others. Our publications will be made available in PDF format. Presentations will be provided in PDF formats.

E.3 Sharing and Preservation

All relevant project data will be made publicly available through a project website, database, and software repository based on the traditional software outlets immediately after being designed/generated and tested. The repository will also contain all relevant publications describing the mathematical and algorithmic techniques that either utilize or generate the stored data. Our software, documentation and publications will be made available on the project website for long-term availability. We will provide web-based tools that enable use of our tool suite on cloud computing resources. Any software will be released for free under the Apache v.2 open source license. Educational material will be placed under the Creative Commons licence. This material will be shared with any parties who agree to use the software and educational material under the terms of the open source license. All participants in this proposal will conduct research and publish the results of their work. Papers will be published in a peer-reviewed scientific journal or book that publishes in English. We will make all publications available on our website, except where prohibited by the copyright of the publisher. We will also provide access to raw data used in our publications on the web site as well as codes, and this data will be available for free to any scientists who want to use it for comparison or analysis. Publications provided on the web site may be distributed freely in academic environments and may be cited with appropriate attribution according to standard

academic practice. Although we do not envision needing to store massive data sets, we will make use of the ample storage facilities available at FRIB/NSCL.

E.4 Protection

None of the data collected during experiments and simulations will have personally identifiable information. The data pertains only to algorithm performance. When data is collected at FRIB/NSCL and DOE, we will adhere to the protection policies set in place by the facilities.

E.5 Rationale

In many cases, the data, for example output from computational simulations, may be beneficial to other physicists, engineers, mathematicians, and computer scientists. The researchers will be able to do comparative analysis, or utilize the data as inputs for related codes that they have developed. Thus, data published in journals and reports will be made available online through our public website.

E.6 Software and Codes

The software tool suite provided through the public project websites may be used as specified under the open source license Apache v.2. Raw data provided on the website may be used for analysis and comparison of scientific results.

E.7 Educational Material

All educational material developed by the project will be placed at the GitHub repository of the project under the Creative Common licence agreement.

F Letter of Support from IBM Q

Dr. Anthony J. Annunziata
IBM Q Network Global Lead
IBM TJ Watson Research Center 31-259
P.O. Box 218
Yorktown Heights, NY 10598

29 May, 2019

Dear Sir/Madam:

We are writing in support of the proposal "From Quarks to Stars: A Quantum Computing Approach to the Nuclear Many-Body" from researchers at Michigan State University and Los Alamos National Laboratory. When appropriate the IBM Q team can help facilitate in the implementation of quantum codes on the available quantum computing platforms at IBM Q.

Yours sincerely,

Anthony J. Annunziata

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