Comments on Quantum Computing in Nuclear Physics

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We review recent research on quantum computing applications for calculations and simulation of nuclear physics. As systems of interacting fermions, nuclei and their quantum simulation bears much similarity to the quantum computation of chemical systems, whose studies are relatively more advanced. Hence techniques from the quantum chemsitry literature may be readily adopted. Some ways in which nuclei differ from other many-body systems, such as the strong non-perturbative interaction, are highlighted, and a selection of existing results are discussed, covering nuclear structure and reactions.

Key words: Quantum Computing; Nuclear Structure; Nuclear Reactions

1 INTRODUCTION

The ideas of quantum computing were first written down in the late 1970s and early 1980s [8, 29, 18] with the hope that the different fundamental mode of operation between quantum and classical computers would lead to new methods of solving algorithmic problems. In particular, Feynman [18] suggested that a computer whose operation meant the manipulating and processing of quantum states would be the proper way to practically model and simulate the physics of quantum systems. This idea – of simulating quantum systems with quantum computers – has been picked up widely in certain fields, most notably in quantum chemistry (see [11, 31] for reviews) and solid state systems (e.g. [10, 22, 45]).

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Nuclear physics, another archetype of a many-body quantum mechanical system, has recieved comparatively less attention than, say, quantum chemistry, by the quantum computing community. Explorations of nuclear physics on quantum computers are becoming more widespread, and it is the purpose of this short review to highlight the unique nature and challenges of the many-body quantum problem as applied to nuclei, to summarize efforts to tackle the problem on quantum computers, and to look forward to future applications. This work complements other recent reviews [25, 49], and we point out, too, the relevance of a recent US DOE white paper on quantum computing for nuclear physics [15].

2 NUCLEAR PHYSICS

Nuclear physics concerns itself with the scientific study of atomic nuclei – the bound collections of protons and neutrons that form the dense core of every atom or ion. As microscopic entities with radii of order 10^{-14} m, nuclei are subject to the laws of quantum mechanics. The consituents of nuclei, protons and neutrons (collectively called nucleons), are fermions, and as such are subject to Fermi-Dirac statistics and the Pauli exclusion principle. The underlying interaction between nucleons derives from the fact that nucleons are composite particles made up of quarks and gluons, subject to the strong nuclear force, as explained by the theory of quantum chromodynamics. At low energies, such as those sufficient to describe nuclear structure properties, it is sufficient to treat the nucleons as the basic particles, and the 'residual' strong nuclear force that leaks out from the nucleon as the basis of the nucleon-nucleon interaction [30]. The basic equation of nuclear structure is the (non-relativistic) many-body Schrödinger equation, as it is in quantum chemsitry and condensed matter systems.

The story of solving problems in theoretical nuclear physics has generally been a dual one of improving understanding and implementation of the nucleon-nucleon interaction on the one hand, and the improvement of the techniques and approximations used to solve the many-body Schrödinger equation. It is in this last aspect that quantum computing can play its role, and many techniques already developed in the quantum computing world for solutions of problems in other areas of many-body quantum mechanics can be applied. Indeed, there has been a considerable exchange of ideas over the years between sometimes isolated communities all seeking to solve what is in a broad sense the same problem, even if the details vary considerably. As an example, we mention the coupled cluster method for approximate solution of

the many-body Schrödinger equation, developed originally in nuclear physics [16], and transferred for wide use in quantum chemistry [5] and subsequently in quantum computing [34].

Nuclear physics differs in some details from quantum chemistry or solid state systems when it comes to practical solution of the Schrödinger equation. The interactions are rather different, with the short-range non-perturbative nuclear force not much resembling the long range perturbative Coulomb interaction. Nuclei are in fact subject to three-nucleon forces [24] as well as nucleon-nucleon interactions alone.

Nucleons, like the electrons interacting in chemical systems, are quantum objects with intrinsic spin of $s = \frac{1}{2}\hbar$. Since most practical implementations of real quantum computers uses the manipulation of $s = \frac{1}{2}\hbar$ sytems, the one-to-one mapping of spin of the system of interest to the qubit spin is an obvious implementation on a quantum computer. The two flavours of nucleon – proton and neutron – can formally be represented as two different isospin states of the nucleon, with isospin obeying the same mathematical properties as the spin. Hence, an isospin mapping may be efficiently applied when mapping nuclear systems to qubits on a quantum computer, or spin and isospin combined to a more general qudit.

3 VARIATIONAL QUANTUM EIGENSOLVERS

While it is of theoretical and longer term practical interest to design quantum computer algorithms of arbitrary complexity and sophisitcation, algorithms that work on the simplest, currently-avaiable quantum computers are of obvious interest. These are typically algorithms which combine classical and quantum parts [2], and the main examples which haven been implemented in nuclear physics are the class of Variational Quantum Eigensolvers (VQE) [13, 33].

The VQE algorithms rely on the general variational principle as used in quantum mechanics, which gives that the expectation value of a Hamiltonian for an arbitrary quantum state will always give a value greater than, or equal to, the true ground state energy of the system, i.e. if the true eigenstates of the Hamiltonian are denoted by $\{|\psi_n\rangle\}$ such that

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \tag{1}$$

where $\hat{H}$ is a Hamiltonian operator and E_n the eigenvalue of the Hamiltonian associated with state $|\psi_n\rangle$, then for an arbitrary state $|\phi\rangle$, the Hamiltonian

expectation value is

$$\langle\phi|\hat{H}|\phi\rangle \geq E_0. \tag{2}$$

In a variational algorithm, one uses the true Hamiltonian with a parameterised wave function ansatz. The parameter(s) in the wave function are then varied, and the lowest resulting expectation value selected as an approximation for the ground state energy E_0. The efficacy of the method relies on the fact that evaluating an expectation value on a quantum computer translates to measuring the spin of the computer's qubits, while it involves quadrature on a classical computer.

This approach has been used by Dumitrescu *et al.* [17] to calculate the binding energy of the deuteron. In that work, the authors prepare for the quantum computation by making invoking an effective field theory approach that reduces the complexities of the nuclear problem to that of a one-body operator in an oscillator basis, and with an operator of a particularly simple form. The Hamiltonian is then defined for the size of the oscillator basis N as

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n, \tag{3}$$

where T and V are the kinetic and potential energy operators respectively, $a^\dagger_n$ creates a deuteron in oscillator state $|n\rangle$ and a_n destroys a deuteron in oscillator state $|n\rangle$. The matrix element for V is non-zero only for $n' = n = 0$ and the kinetic energy matrix elements are analytically known in the oscilattor basis, so evalulation of the matrix elements is straightforward. Dumetrescu *et al.* map each deuteron state $|n\rangle$ to the n^{th} qubit, thus N qubits are needed to represent the problem for the H_N Hamiltonian. Using the standard Jordan-Wigner transform allows the Hamiltonian to be written in terms of Pauli matrices associated with each qubit (X_i, Y_i, Z_i for qubit i) using[⋆]

$$\begin{aligned} a^\dagger_n &= \frac{1}{2}\left[\prod_{j=0}^{n-1} Z_j\right](X_n - iY_n) \\ a_n &= \frac{1}{2}\left[\prod_{j=0}^{n-1} Z_j\right](X_n + iY_n). \end{aligned} \tag{4}$$

Along with a Pauli matrix representation of the Hamiltonian, a suitable wave function is needed. For this the Universal Coupled Cluster (UCC)

[⋆] N.B. Dumitrescu *et al.* give a negative sign before the Z operators, contrary to the most common common definition, but give results later on consistent with use of a positive sign.

ansatz was used, acting on the default initial uncorrelated product state to give a wave function dependent on one or more (dependent on N) rotation angles. Driven by a classical computer which varies the rotation angles, the quantum computer is asked to return expectation values of the Pauli matrix products in the Hamiltonian representation. Using cloud access to Rigetti and IBM quantum computers, $N = 2$ and $N = 3$ calcualtions were performed, including error mitigation on the quantum devices. Extrapolation to infinite N was then made using conventional methods to give a final answer, within 2% of the deuteron binding energy.

This pioneering use of the variational quantum eignensolver in nuclear physics spawned further exploration, such as in the mapping of the Hamiltonian onto qubits [35, 40, 36], and the nuclear Hamiltonian [40, 14]. These other Hamiltonians include the widely-studied non-trivial toy model due to Lipkin, Meshkov and Glick [28]. The original Dumitrescu *et al.* implementation included only s-wave states for the deuteron, which famously exhibits a large d-wave admixture. A simulated quantum computation by Siwach and Arumugam [40] highlights a method for extension to include d-waves.

4 NUCLEAR STRUCTURE

Calculation of the deuteron ground state counts as a *nuclear structure* application – the property of a single nucleus – as opposed to *nuclear reactions* – the interaction of one nucleus with another nucleus or some external probe. In this section we elaborate further on nuclear structure calculations, current and future, on quantum computers.

While the background theory in the deuteron example was rooted in rather fundamental theories of nuclear interactions, an effective one-body Hamiltonian had been derived before making use of a quantum computation. This is reminiscent of the mean-field approach, either from the Hartree–Fock (HF) method or density functional theory (DFT). Both are basic (and effectively equivalent in usual practice) approaches to nuclear structure [6], and they form the basis of recent breakthrough approaches in quantum computation in chemistry [19]. The methods are variational, with the added complication of self-consistency requiring an iterative process, but a simple demonstration of nuclear Hartree-Fock / density functional theory is achievable on today's quantum computers. The Hartree-Fock iteration could be performed by the imaginary time method, for example, as already demonstrated on quantum computers in the molecular case [32] as well as a case of two interacting nucleons [44].

Calculations of nuclear structure on classical digital computers using HF or DFT-type methods often use the mean field a starting point for further calculations. In one approach, the Generator Coordinate Method (GCM) [46] takes results of mean-field calculations and uses a combination of projection on good quantum numbers and state mixing to restore the symmetries broken by the mean field method, as well as to account for configuration mixing beyond the mean-field picture. This process is vastly more time-consuming then the initial solution of the HF equations. A recent paper by Lacroix [26] presents an algorithm whereby the projection of good quantum numbers from a mean-field state is facilitated by the quantum Fourier transform algorithm, showing promise for the next stage beyond mean-field calculations on quantum computers for nuclear structure.

The method of exact diagonalisation in a restricted model space starting from a mean-field picture is called the interacting shell model in nuclear physics, and the configuration interaction in quantum chemistry. In the latter context it has already been realised on quantum computers [3, 42]. In nuclear physics, an original breakthrough was made for efficient calculation on early digital computers, recognising that an algorithm that targetted the machine architecture well could outperform more mathametically elegant group-theroetic techniques. In his 1972 paper, Whitehead comments [48]

> The basis states may be stored in the occupation number representation in the computer by assigning a single particle orbit to each bit position in the word, a 1-bit representing an occupied orbit and a 0-bit an unoccupied one. All operations may be performed very efficiently using normal computer logic and bit handling techniques. This requires a certain amount of machine code programming [...]

The work of implementing algorithms on quantum computer follows a similar necessity of thinking at the machine level, of the qubit, not the bit, but the occupation number representation of the nuclear shell model can be built up from scratch on a quantum computer, as it has been on digital computers. The use of the Jordan-Wigner transform to associated occupation numbers with qubits is exactly in this vein, and the work of Stetcu *et al.* on preparing nuclear ground states in a shell model space [41] is an indication of how the shell model edifice can be re-built on the new technology.

5 NUCLEAR REACTIONS

Nuclear reactions complement nuclear structure and the two subfield are linked to make a full theory of nuclear physics. Nuclei feel all four of the fundamental forces and combinations of the strong nuclear force, weak nuclear force, and electromagnetism, and their interplay, are part of the landscape of nuclear physics. A formalism for nuclear reactions needs to account for changes to a system, either with explicit or implicit time-dependence. Nuclear reaction theory has been built on time-independent methods (i.e. the time-dependence is implicit). With the relative ease of implementation of real-time evolution on quantum compuers [27] explicit time-dependent methods can be examined more easily [4, 20, 23] alongside e.g. linear response approaches [37] which work in essentially the fourier-transformed representation with time replaced by energy as a variable [9].

Explicit nuclear reaction examples that have been studied on quantum computers includes response functions relevant for neutrino scattering [38, 4], neutrino oscillations [20], the interacting spins of two nucleons [23], and the preparation of excited states for dynamics studies [37].

Nuclear reactions cover a broad range of topics: fusion [39, 47], fission [7], alpha decay, beta decay, the creation of superheavy elements [1], astrophysical processes, knockout [43] and transfer [12, 21] reactions to give a partial list. The theory in each area has prosepect for quantum algorithms to impact fast computation of results, but which for now is relatively unexplored.

6 CONCLUSIONS

We have given a brief overview of some of the key topics in low energy nuclear structure theory; how the relevant algorithms can start to be tackled by quantum computers, along with some real-world examples. While nuclear physics applications lag behind other areas, particularly quantum chemistry, the field is ripe for many advances, using a combination of techniques shared with other areas, with perhaps some unique to the specialities of nuclear physics, such as the nature of the short-ranged interaction and the existence of two interacting particles, represented as nucleons of differing isospin.

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