17th International Conference on Nuclear Structure Properties (NSP2025),
June 25 – 27, 2025, Sivas Cumhuriyet University, Sivas, Türkiye

Quantum Computing for Nuclear Structure

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***Abstract*—Quantum computing methods could revolutionise many areas of human endeavour where classical computation reaches its limits of applicability. One particular area where quantum computers can be applied is in the simulation of quantum systems. In this paper, the application of quantum computation to nuclear systems made up of interacting protons and neutrons. After presenting an overview of quantum computation, we demonstrate the action of some quantum algorithms to calculate the energy levels of nuclei.**

Keywords—quantum computing, nuclear structure, nuclear models

I. INTRODUCTION

Qubits are effectively the simplest quantum mechanical system. They are two-level systems, defined in a two-dimensional Hilbert space. When n qubits interact, the resulting system state vector spans a 2^n-dimensional Hilber space in which entanglements between the interacting qubits is readily represented. Such arrays of qubits are realised in quantum computers. The ability to represent entangled high-dimensional Hilbert spaces has led to the development of methods and algorithms that promise to exceed the abilities of classical computers. The key is to find quantum algorithms whose algorithms are more efficient in a computational complexity sense than classical algorithms [1].

One class of quantum algorithms that is of widespread interest for its applicability in the physical sciences is quantum simulation. Here a physical system of interests is represented on quantum computer such that the systems own quantum degrees of freedom are mapped onto those of the quantum computer. With judicious choices of mapping and application of operations on the quantum computer, the system of interest may be directly simulated without the need for the number-crunching approximate solution of differential equations that characterises the classical computation approach to simulating quantum systems.

In this contribution, we summarise some relevant concepts in quantum computing and quantum simulation, then give some highlight results in nuclear physics problems.

II. QUANTUM COMPUTING BASIC FORMALISM

A qubit is a two-state quantum system, whose states are abstractly and conventionally labelled $|0\rangle$ and $|1\rangle$. The most common particular representation of the two states is as the eigenstates of the Pauli $Z \equiv \sigma_Z$ matrix, which are part of the full set of spin matrices (including the identity)

This work is funded by UK STFC grant no.ST/Y000358/1 and by the EU HORIZON-MSCA-2023-PF-01 project ISOON under grant number 101150471.

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

i.e. the qubit basis states are identified as

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2}$$

Systems of multiple qubits are formalized through the use of Kronecker products, so a two-qubit state can be written as

$$|01\rangle = |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ 0\begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \tag{3}$$

and similarly for matrixes, e.g.,

$$I \otimes \sigma_X = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ 0\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & 1\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{4}$$

(Multi-)qubit states are thus represented in Dirac notation or as state vectors in the σ_Z-diagonal basis, also known as *the computational basis*, and operators are given symbolically or as matrices in the same basis.

While the Pauli operators are examples of single-qubit operators, two- and higher-qubit operators exist. The basic example is the controlled NOT gate, also known as the controlled X gate. This gate acts flips the state of a target qubit if a control qubit is in the state $|1\rangle$, but leaves the target unchanged if the control qubit is in the state $|0\rangle$. Its computational basis representation is

$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{5}$$

A large collection of admissible gates, all represented as unitary matrices, are possible, as detailed in textbooks. Subsets – e.g. the Clifford+T set – form universal sets, able in combination to represent any allowable operation [2,1]. One further exemplar gate is worth mentioning: The Hadamard gate, which transforms an eigenstate in the computational basis into an equal superposition. It is a one qubit gate which can be fully described by its action on the two basis kets, or equivalently as a matrix in the computational basis:

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \qquad H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle), \qquad H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Quantum algorithms are typically representable as a series of operations on an initial quantum state, usually $|00\cdots0\rangle$, followed by a measurement of the σ_Z operator on one or all qubits. This measurement will follow the rules of quantum mechanics regarding probability. That is to say, each state will be measured with the square of the amplitude with which it appears in the state vector.

A convenient representation of a series of quantum gates on multiple qubits is in the form of a quantum circuit. An example of a two-qubit circuit is given in Figure 1.

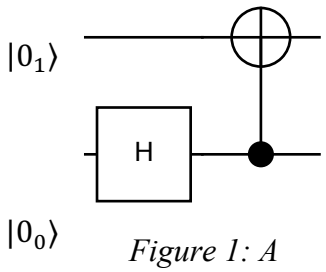

Figure 1: A sample quantum circuit, in which a Bell State is prepared

Here, one reads from left to right. The kets give the initial state of the system as $|0_1 0_0\rangle$ where we label the qubits with indices in order to be able to refer to them as qubit 1 and qubit 0. A Hadamard gate acts on qubit zero, then a controlled-NOT gate acts, with qubit 0 as the control qubit and qubit 1 as the target qubit. The resulting state from this circuit is a Bell state

$$\frac{1}{\sqrt{2}}(|0_1 0_0\rangle + |1_1 1_0\rangle).$$

This state is entangled: If one measures one of the qubit states, then one immediately knows the state of the other qubit.

III. Quantum Simulation in Nuclear Physics

Quantum computers are general devices. Algorithms of many kinds may be implemented, with famous examples being Shor's factorization algorithm [3] and Grover's search algorithm [4]. Here, though, we concentrate on the case of quantum simulation in which the Schrödinger equation-following behaviour of the qubits is used as a surrogate for the behaviour of a nuclear system. The term quantum simulation is sometimes meant to refer to just the time-evolution (i.e. the dynamics) of a quantum state. Here we use the broader definition encompassing the solution of the time-independent Schrödinger equation, which amounts to preparing the initial state for dynamic evolution.

A. A Nuclear Model

The Lipkin-Meshkov-Glick model is a simplified version of the nuclear shell model, in which two energy levels, each of degeneracy N are separated by energy ε and occupied by a total of N identical fermions [5]. The fermions interact according to the following Hamiltonian

$$H = \frac{1}{2}\varepsilon \sum_{p\sigma} \sigma a^+_{p\sigma}\, a_{p\sigma} + \frac{1}{2} V \sum_{pp'\sigma} a^+_{p\sigma}\, a^+_{p'\sigma} a_{p'-\sigma} a_{p-\sigma}. \tag{6}$$

Here $\sigma = \pm 1$ indicates the upper (+1) or lower (-1) energy level while p labels the substates within the degenerate levels. The first term gives the energy contribution from single particles occupying each orbital, while the second term, with interaction strength V scatters pairs of particles between the two levels. Depending on the total number of particles N and the interaction strength ratio V/ε, a rich

structure can be observed, with e.g. behaviour analogous to a transition between spherical and deformed states.

It is this model which we use as a test case here, as we and other authors have done in previous studies [long list]. Our strategy is to make a matrix representation of the Hamiltonian in a quasispin basis, and then to decompose the matrix into Kronecker products of Pauli matrices. Further details are given in [Hobday Thesis]. In the language of the nuclear shell model [Suhonen] this corresponds to a *J*-scheme representation, as opposed to an *m*-scheme representation. The latter scheme has its own benefits for quantum simulation, and is the most common choice for the conventional nuclear shell model on quantum computer [6,7,8,9]

From [Hobday Thesis, our VVQE paper] we take the following matrix derived from the LMG model with $N=7$ and with parameters set as $\varepsilon = 1.0, V = 0.5$:

$$H_{N=7} = \begin{pmatrix} -3.5 & -2.291 & 0 & 0 \\ -2.291 & -1.5 & -3.873 & 0 \\ 0 & -3.873 & 0.5 & -3.354 \\ 0 & 0 & -3.354 & 2.5 \end{pmatrix}. \quad (7)$$

When decomposed into tensor products of Pauli spin matrices, this becomes

$$H_{N=7} = -0.5 I_0 \otimes I_1 - 2.8225 I_0 \otimes X_1 - 1.0 I_0 \otimes Z_1 - 1.9365 X_0 \otimes X_1 \\ -1.9365 Y_0 \otimes Y_1 - 2.0 Z_0 \otimes I_1 + 0.5315 Z_0 \otimes X_1. \quad (8)$$

B. *Variational Quantum Eigensolver (VQE)*

The variational quantum eigensolver (VQE) is a widely-used hybrid quantum classical algorithm for finding ground states of Hamiltonians. It uses the textbook variational principle (see e.g. [10]) in which a wave function ansatz is guessed which one hopes is able to give a good approximation to the true ground state. The ansatz features one or more adjustable parameters, and the adjustment of these in such a way as to minimize the energy leads to an approximate (or exact, if the ansatz can manage it) ground state wave function and energy. The ansatz is prepared on a quantum computer as a circuit, and the expectation value of the Hamiltonian (that is, the energy) is obtained by measurement. Thus a quantity usually evaluated on a classical computer by quadrature is simply measured on a quantum computer. A classical computer controls the choice of parameters in the quantum circuit and directs the series of ansatzes directed towards the energy minimum according to some minimization algorithm. We detail the steps below.

A suitable ansatz to express two-qubit states is shown in figure 2. It is a parameterised circuit with three parameters, $\theta_0, \theta_1, \theta_2$. Each parameter is a rotation angle around the y-axis, applied to one or the other qubit. It is sufficiently expressive in the present case to find the ground state of the system. Choosing a suitable ansatz can be a difficult problem, and considerable literature is devoted to the art [11,12,13].

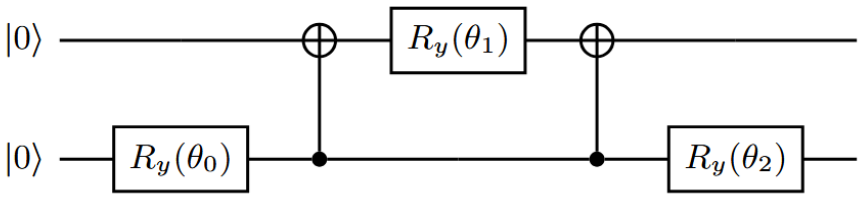

Figure 2: Two-qubit ansatz for representing LMG wave function

The steps of the VQE are

i. Choose a random starting set of parameters in the ansatz

ii. Prepare the qubits in the ansatz state

iii. Measure the expectation value of each of the Pauli terms in the Hamiltonian

iv. Combine expectation values into total energy

v. Use classical driver algorithm to use information about energy to update ansatz parameters and return to step ii, exiting when classical driver algorithm has found minimum in energy.

The classical minimization aspects of the VQE contain all the difficulties of any classical minimization problem of a function of many variables (in this case the energy as a function of all the ansatz parameters). Such difficulties typically involve getting stuck in local minima when the global minimum is sought. Different classical algorithms are then brought to bear on these difficulties, drawing on extensive experience in such problems across science areas. Details can be found in review articles on the VQE method in general [14, 15]

C. *Quantum Phase Estimation*

The variational quantum algorithms discussed so far were developed, in part, to be viable on existing quantum computers in which low circuit depth (just a few gates per quantum circuit) is preferred in order to mitigate against noise and decoherence of the qubit states. Quantum Phase Estimation is a long-proposed algorithm which neatly picks out eigenvalues from a unitary matrix, building them up binary digit by binary digit using the quantum Fourier transform. It is well-documented in textbooks [1, 2] to which we refer the reader for a detailed exposition. We note that the textbook of Wong [2], in particular, is made freely available from the author on his website.

In this algorithm, the Hamiltonian for which the eigenvalues are sought is used to define a unitary operator as

$$U = \exp(iHt/\hbar)$$

The eigenvalues of H then turn into eigenphases of U which are picked up by the quantum phase estimation algorithm. Some suitable shifting can be performed on H, along with a suitable choice of t (and setting units of t by choosing $\hbar$=1) so that the phases all lie in the range $(0,2\pi)$.

IV. RESULTS

A. *Variational Quantum Eigensolver (VQE)*

The example of the N=7 LMG model is sufficiently simple and we can directly compare results on a quantum computer to those obtained from a classical evaluation of the eigenvalues. A direct calculation of the eigenvalues of the matrix (7) gives the eigenvalues -6.208, -2.944, 1.208, 5.944, all in units of ε and to 4 significant figures.

In figure 3, we see the result of a VQE run for the Hamiltonian represented as a matrix in (7) and equivalently in its Pauli decomposition in (8). The ansatz in Figure 2 was used, and one can see the convergence to the lowest eigenstate at E/ε=-6.208 as expected, since the VQE targets the ground state.

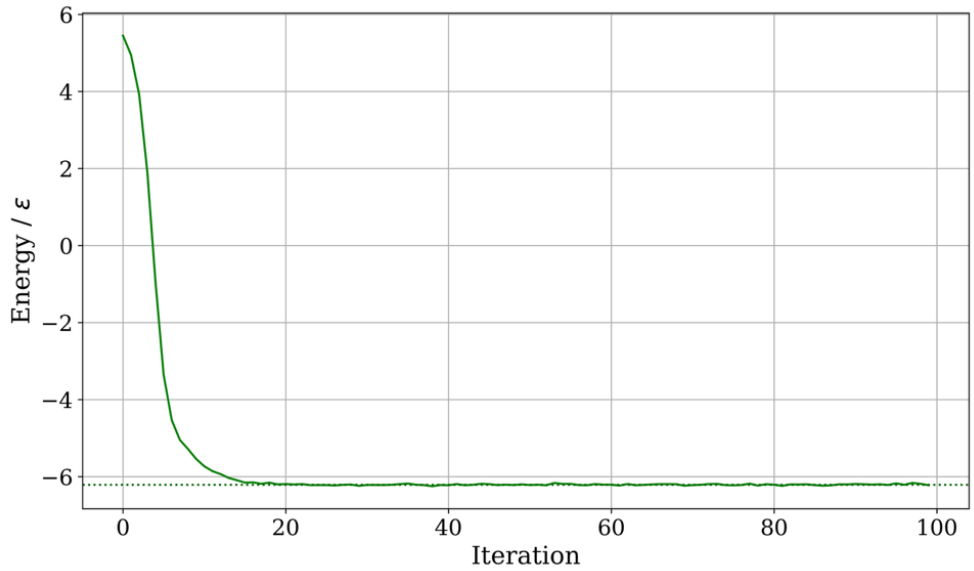

Figure 3: Energy minimization as a function of iteration using VQE

B. *Variance Variational Quantum Imaginary Time Evolution (VarVarQITE)*

Many adaptations of the basic VQE method have been made with various levels of sophistication. Though the standard variational method locates only the ground state energy and wave function, it is possible to design variational algorithms which converge to excited states. One method, broadly known as *deflation* [16], starts by finding the ground state, then removing this state from the problem, typically by adding an extra term to the Hamiltonian which pushes up the energy of the original ground state so that it is no longer the ground state of the altered Hamiltonian. One may then apply the standard variational principle to this new Hamiltonian and find the now-lowest eigenvalue, which should be the first excited state of the original Hamiltonian.

Formally, if the Hamiltonian whose eigenvalues are desired is $\widehat{H}$ with spectrum $E_n = \widehat{H}|n\rangle$ then the Hamiltonian

$$\widehat{H}' = \widehat{H} + \beta|0\rangle\langle 0|$$

has eigenvalues $E_0 + \beta, E_1, E_2, \ldots$. Hence for a suitably-chosen β, the lowest energy of $\widehat{H}'$ will be E_1.

An alternative method to find excited states is to minimize the variance of the Hamiltonian. Here, the quantity minimized is

$$\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2.$$

This quantity, the variance of the Hamiltonian, is positive semi-definite, and is zero whenever the wave function used in the expectation values is any eigenstate of the Hamiltonian. Thus, if a minimization algorithm is used in a variational quantum algorithm in which the variance is minimized, any of the eigenstates may be reached, depending on the initial set of parameters in the ansatz, and the minimization method.

Alternatives to the classically-driven minimization routines have also been developed. As an example, we show results from the *variational quantum imaginary time* minimizer, in which the variation of parameters within an ansatz is performed functionally and then implemented as a quantum circuit so that directed search for the minimum is also quantum-assisted. The idea is that e.g. since the parameters in the ansatz in Figure 2 are in R_y rotation gates, which are mathematically represented as $R_y(\theta) = \exp\left(-i\frac{\theta}{2}Y\right)$, the derivative of this operation with respect to the parameter θ is easily found as

$$\frac{\partial R_y(\theta)}{\partial \theta} = -\frac{i}{2} Y \exp\left(-i\frac{\theta}{2}Y\right) = -\frac{i}{2} Y R_y(\theta).$$

Since this derivative is a sequence of two representable operators, the encoding of the derivative, and hence a full minimization algorithm, is able to be encoded as quantum circuits. The full description is given in [17,18]. In Figure 4 we show the application of the algorithm to find all four eigenstates of the *N=7* LMG Hamiltonian.

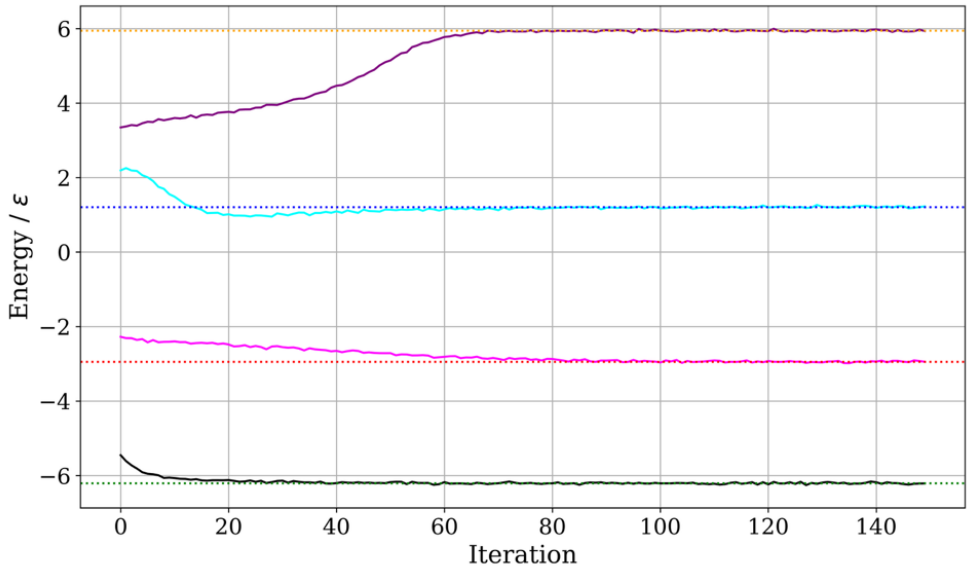

Figure 4: convergence to eigenspectrum as a function on iteration in the VarVarQITE algorithm

C. Quantum Phase Estimation

Applying the Quantum Phase Estimation as detailed in the methods chapter with a randomly-generated wave function, essentially giving a linear combination of all the eigenvalues, then extracting the phases, gives us the histogram of results shown in Figure 5. This is for the same $N=7$ LMG Hamiltonian as in the previous examples.

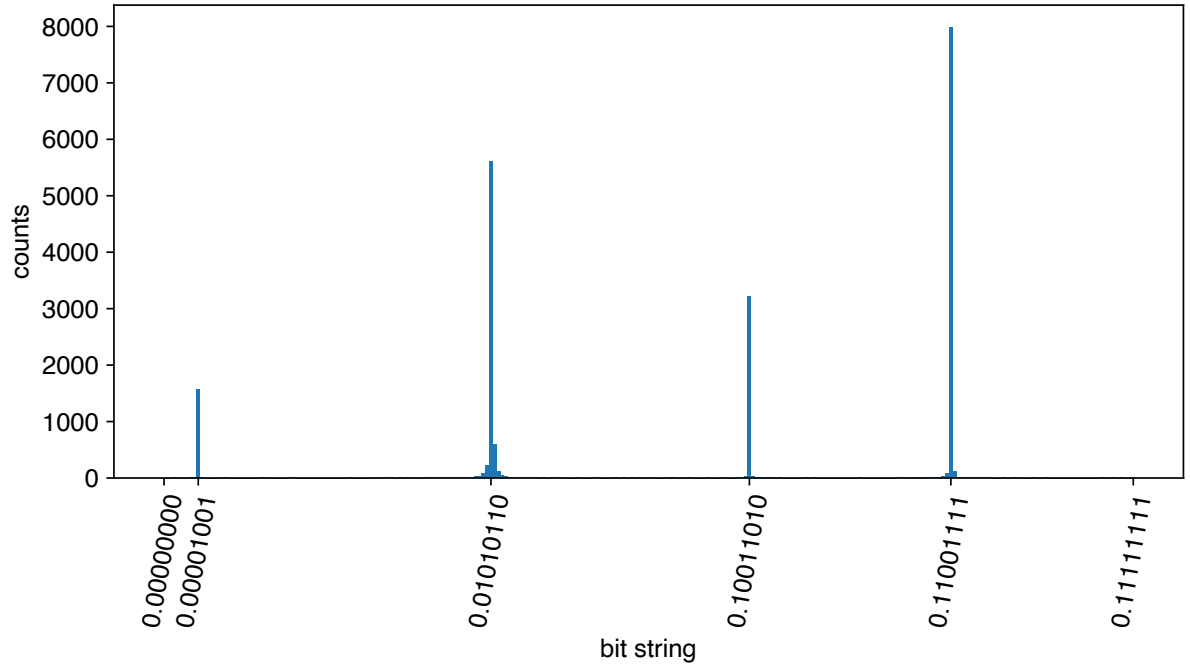

Figure 5: Spectrum of couts for each bit string in the phase. The scaling is such that the minimum bit string value is 0 and the maximum is 1, mapping to phase angles of 0 and 2π

In Figure 5 the histogram of bit strings is labelled just with the starting and ending points (0.00000000 and 0.11111111 respectively) along with the four values where strong peaks appear. To convert them into eigenvalues of H, the binary point expansions are turned into decimal numbers, multiplied by 2π, divided by the choice of t and shifted by the scaling factor. The process in shown in the table below, where the scaling value $t=0.4$ is used. As can be seen, these peaks are all in close agreement with the exact values calculated above. With this algorithm in principle one may continue to achieve increasingly accurate answers by adding extra bits to the result.

Bit string	ϕ decimal	$E = -\frac{2\pi\phi}{t} - 6.5$
0.00001001	0.03516	5.9477
0.01010110	0.33594	1.2230
0.10011010	0.60156	-2.9493
0.11001111	0.80859	-6.2013

V. CONCLUSIONS

We have presented an overview of quantum computing methods, and given some detail about their application to eigenvalue problems in nuclear structure by demonstrating the results of three algorithms: The variational quantum eigensolver (VQE), the variance-variational quantum imaginary time evolution method (VarVarQITE) and the quantum phase estimation method (QPE). The first method found the ground state of the model nuclear Hamiltonian we used, while the second and third methods found the whole spectrum of eigenvalues.

Our example Hamiltonian was one which is expressed in a small model space requiring just two qubits to represent it. Since the size of a Hilbert space increases as 2^n where n is the number of qubits, one would need only 33 qubits to represent a Hilbert space size of 10^{10}, which is at the limit of today's shell model calculations on classical computers. Since quantum computers already exist with 100+ qubits, the future is bright for such applications. What is currently missing is the sufficiently low error rates and long coherence times to allow quantum algorithms to be fully and faithfully implemented.

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