Block Lanczos method for excited states on a quantum computer

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The method of quantum Lanczos recursion is extended to solve for multiple excitations on the quantum computer. While quantum Lanczos recursion is, in principle, capable of obtaining excitations, the extension to a block Lanczos routine can resolve degeneracies with better precision and only costs $O(d^2)$ for d excitations on top of the previously introduced quantum Lanczos recursion method. Extension to non-Hermitian operators is also discussed.

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I. INTRODUCTION

For quantum computation to lead to new discoveries [1], efficient means of solving for the ground state must be understood and implemented. Some near-term algorithms that have been used in the era of noisy quantum devices have led to an increased interest in results obtained from variational quantum eigensolvers [2–10] which ultimately face noise and other limitations [11]. Looking to the long-term capabilities of a quantum computer when error correction is available, other algorithms are useful to investigate.

By far, the longest studied algorithms to obtain ground states is the implementation of real-time evolution. In this algorithm, an initial Hamiltonian $\hat{H}_0$ is defined and an initial state Ψ_0 is prepared on the quantum computer. The time-dependent Hamiltonian is

$$\hat{H}(t) = \hat{H}_0 + \lambda(t)\hat{H}_I + \mathcal{C}, \tag{1}$$

with interaction term $\hat{H}_I$, constant $\mathcal{C}$, and time-dependent coupling constant (or similar form) $\lambda(t)$ at time t. By adiabatically (slowly) increasing the interaction term in time, the wave function will eventually arrive at the ground state for the fully interacting Hamiltonian.

However, this solution strategy is known to be extremely slow for quantum chemical systems [12,13]. In order to apply the Hamiltonian, a time-evolution operator of the form $\exp[-i\hat{H}(t)\delta t]$ must be applied to the wave function. The Trotter-Suzuki decomposition of the time-evolution operator must be decomposed into many terms, $O(N^4)$, to capture the full electron-electron interaction term, although this can be reduced as $N \to \infty$ to $O(N^2)$ for the case of local basis functions [14]. However, since the time step δt must be very small depending on the strength of correlation in the system, the resulting number of operations makes the time necessary to solve for even small molecules extremely long. This is true of other classical solution techniques such as Hartree-Fock [15]. This is expected based on the complexity of solving quantum chemistry systems [16].

The question of how to obtain excited states is one that has been investigated in recent papers [6,17–28], and a direct solution would provide a means to fully manipulate the wave function. If this can be accomplished without the use of time evolutions, then avoiding the small time step necessary for those methods could be possible.

In addition to ground-state solvers, obtaining excited states is a highly valuable quantity for quantum chemistry systems. Historically, excited states have been more difficult to obtain. So, if a quantum algorithm could reliably obtain the excitations, then this would represent a major improvement over existing classical techniques [29–31].

Recently, Lanczos methods have been investigated in the context of solving quantum systems. One variety of Lanczos on the quantum computer uses even vectors of a Krylov subspace and imaginary-time evolution techniques to obtain the ground state and other quantities of interest [24,32].

Another recently introduced variety of Lanczos algorithms was introduced in Ref. [33] that circumvents any time evolution. The full Lanczos recursion can be implemented to find the ground state or the continued fraction representation of the Green's function [33]. This second Lanczos technique, called quantum Lanczos recursion (QLR), avoids the use of a time-evolution operator and therefore bypasses the computational bottleneck in terms of the number of terms in the Trotter-Suzuki decomposition.

One other advantage of the QLR is that the traditional limitations of Lanczos on the classical computer are entirely circumvented [34]. The only limitation is how accurately the operations can be applied to the wave function in practice, and this was implemented on the quantum computer as reported in Ref. [35] after the initial implementation in Ref. [33]. Since

then, other methods have used the idea of a Krylov subspace to speed up real-time evolution [7].

This paper uses similar techniques as QLR to show that the traditional Lanczos recursion can be replaced by a block Lanczos routine to resolve several excitations, leading to quantum block Lanczos recursion (QBLR), although "block" can be replaced by "banded" or some other name corresponding to a trivial change of gauge of the unitary matrices involved. While it is trivially demonstrated from QLR that excitations can be found, the performance of block Lanczos will allow for the resolving of degeneracies with greater ease. This was recently demonstrated in tensor network algorithms [36,37].

The algorithm here can also be performed with the preparation of a single initialization of starting wave functions. A full collapse of the eigenstates is avoided, meaning that a wave function can be preserved for the next computation. This is accomplished by use of a state-preserving quantum counting algorithm [33], referred to in some works as Quantum Merlin Arthur (QMA) sampling [38,39].

Some additional discussion on how errors in the Lanczos coefficients will affect the ground-state energy and otherwise is also presented. The method of slowly introducing terms into the Hamiltonian is also discussed in the context of Lanczos.

II. EXCITATIONS FROM QUANTUM LANCZOS RECURSION

The Lanczos algorithm from Ref. [33] can be used to find excitations of a given model by a simple alternative of coefficients. In this section, QLR will be reviewed and an extension to finding excited states will be shown.

A Lanczos recursion relation to find subsequent elements of the Krylov subspace, $\{\psi_0, \psi_1, \ldots, \psi_N\}$, is

$$|\psi_{n+1}\rangle = \hat{H}|\psi_n\rangle - \alpha_n|\psi_n\rangle - \beta_n|\psi_{n-1}\rangle, \tag{2}$$

where the resulting Hamiltonian in the basis of the Krylov subspace forms a tridiagonal matrix. When diagonalized, the ground state is found to a high accuracy, even if only a few n are determined.

Applying operators to wave functions. The method is from Ref. [40]. Consider a Hamiltonian which is represented as a linear combination of unitaries,

$$\hat{H} = \sum_i r_i \hat{U}_i, \tag{3}$$

where U_i is a Pauli term from a given Hamiltonian (see [40]). A unitary

$$\hat{W} = \sum_i |i\rangle\langle i| \otimes \hat{U}_i \tag{4}$$

may be constructed such that i indexes auxiliary qubits. We can prepare a state

$$|\hat{R}\rangle_c = \sum_j \sqrt{\frac{r_j}{\|\boldsymbol{r}\|}}|j\rangle\langle 0|_c \tag{5}$$

for $\boldsymbol{r} = \langle r_1, r_2, \ldots\rangle$. We note that $\langle R|\hat{W}|R\rangle = \hat{H}/\|\boldsymbol{r}\|$. One can apply the unitary $\hat{W}$ onto a state with any one of a number of operations [40–45]. This effectively applies the operator onto the wave function as a block encoding. Coefficients are measured but they are normalized to the factor $\|\boldsymbol{r}\|$.

Minimal measurements of the wave functions. In order to sample the coefficients α_n and β_n without completely measuring (and therefore destroying) the wave function, a state-preserving quantum counting algorithm can be used. The algorithm applies a generic operator $\mathcal{A}$ as in the form

$$\mathcal{A}|\Psi\rangle = p|\Psi\rangle + p^{\perp}|\Psi^{\perp}\rangle, \tag{6}$$

which signifies a superposition of eigenstates. The operator $\mathcal{A}$ is normalized and represented as a unitary such that it can be represented on the qubits [14,33]. The resulting probability p is the expectation value of $\mathcal{A}$. All states orthogonal to the original state are marked with a $\perp$ symbol. The basis of the superposition chosen here is that of the eigenbasis because this will be the natural basis to pick for quantum phase estimation (QPE) [1,40,46].

The key to finding p is to count the number of transitions from Ψ to Ψ (wave function to same wave function) after the application of $\mathcal{A}$ by the methods in Sec. II. To verify that the same state is obtained after this procedure, the energy of the state can be computed with QPE at the start of the algorithm and stored on a register. After the operator is applied, the energy is then computed on a separate register. The two registers are compared and represented on a single qubit, called a pointer qubit. The pointer qubit is then measured. If the energies match, one value is returned and the original wave function is recovered. This is counted as a "success" in the algorithm. The ratio of successes to the total times the algorithm is run is p. Once p is found, the expectation value of $\mathcal{A}$ can be determined.

If the pointer qubit demonstrates that the wrong state was recovered, then a recovery procedure is used to find the original state [14,33,39,44]. In essence, the unitary of all operations applied onto the wrong wave function and the process above is repeated until the correct wave function is found [39].

Operators for Lanczos recursion. To find the Lanczos coefficients, the following relations hold [33]:

$$\alpha_n = \langle\psi_n|\hat{H}|\psi_n\rangle \quad \text{and} \quad \beta_n = \langle\psi_{n-1}|\hat{H}|\psi_n\rangle, \tag{7}$$

and therefore provide a means to use state-preserving quantum counting to obtain the coefficients. The map between the Krylov states and the original ground state can be summarized as

$$|\psi_n\rangle = \hat{G}_n|\Psi\rangle, \tag{8}$$

where [33]

$$G_0 = \hat{H} - \alpha_0, \tag{9}$$

$$G_1 = (\hat{H} - \alpha_1)(\hat{H} - \alpha_0) - \beta_1, \tag{10}$$

and so on, where each of these operators must be scaled and shifted to create a unitary representation that gives a positive operator value measurement (POVM) [1]. For a quantum chemistry system, this can be accomplished by shifting the potential so that its minimum lies at zero energy and then normalizing the Hamiltonian appropriately. After performing a given Lanczos step, the result of the POVM, the true

value can be recovered by undoing the shifting and scaling operation.

The coefficient α_n can be regarded as applying quantum counting on the state Ψ with the operator $(\hat{G}_n^\dagger \hat{H} \hat{G}_n)$. Each operator $\hat{G}_n$ depends on coefficients from $\{0, 1, \ldots, g-1\}$ iterations and therefore the algorithm discovers the coefficients iteratively. To find β_n, the operator $(\hat{G}_{n-1}^\dagger \hat{H} \hat{G}_n)$ is used instead.

Energies from QLR. Once the Lanczos coefficients are obtained, the Hamiltonian matrix in its tridiagonal form is then known. Diagonalizing this matrix and retaining both the energies and eigenvectors makes the new ground state in terms of the Krylov basis chosen.

Defining an operator $\hat{Y}^{(g)}$ for an excitation $g \in \mathbb{Z}^+$, the operator for the gth excitation would be defined as

$$\hat{Y}^{(g)} = \sum_n \gamma_n^{(g)} \hat{G}_n, \tag{11}$$

in terms of coefficients γ_n found from the diagonalization. The summation over n is over as many elements in the Krylov basis as kept.

Thus, the QLR algorithm can access ground states ($g = 0$) or excited states ($g \geqslant 1$) by simply selecting different coefficients from the diagonalization of $\hat{H}$. At the end of this procedure, the ground state is recovered and can be used without fully repreparing it.

Note that the convergence of all algorithms discussed here is no different from the understanding of these methods on the classical computer [47–54].

A. Reduced computational complexity of applying operators

First strategy: Apply interaction incrementally. When applying an operator to a wave function, as in Sec. II, several auxiliary qubits are used.

By applying operators from the full Hamiltonian incrementally in groups of size D (for example, if there are 10 interaction terms to add into an existing Hamiltonian term, $D = 10$), the cost can be reduced.

Second strategy: Decrease strength of interaction. Note that the operator applied onto the original wave function Ψ does not need to be an operator whose eigenvectors include Ψ. This means that starting from some known state Ψ with associated operator $\hat{H}_0$,

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_I \tag{12}$$

can be defined as a new Hamiltonian. This form of the Hamiltonian has a similar form as the adiabatic evolution in Eq. (1), except that the λ coefficient can be much larger than the step size in time evolution.

The interaction term $\hat{H}_I$ can be the full interaction term or one term of that interaction. By adding the terms incrementally, the final state is closer to the provided initial state and will allow for the algorithm to find the new ground state. It is crucial that each step of this procedure begins with an eigenvector so that the QPE can be applied correctly in the quantum counting procedure.

B. Demonstration on model systems

A full demonstration on real systems by implementing a linear combination of unitaries will be delayed for a future work, but it will be shown here that Lanczos can be applied iteratively according to the suggestions in the previous paragraphs.

In order to demonstrate that only a limited number of Lanczos steps can be used to solve a model that includes a small number of extra terms from the starting wave function's Hamiltonian, a numerical study on a 10-site *XXZ* model of the form

$$\hat{H} = \sum_i J_{xy}\left(\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y\right) + J_z \hat{S}_i^z \hat{S}_{i+1}^z, \tag{13}$$

where $J_{xy} = J_z$ is the *XXZ* Hamiltonian and spin matrices $\mathbf{S} = (\hat{S}^x, \hat{S}^y, \hat{S}^z) = \frac{1}{2}\boldsymbol{\sigma}$ (with $\hbar = 1$) for the vector of Pauli matrices $\boldsymbol{\sigma}$ [55]. To start, an *XY* model,

$$\hat{H}_{\mathrm{XY}} = J_{xy} \sum_i \hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y, \tag{14}$$

will be solved for the initial wave function and a single interaction term of the form $\hat{S}_i^z \hat{S}_{i+1}^z$ will be added. In all, $D = 9$ terms will be added to the Hamiltonian. Computations were made with the DMRjulia library using the density matrix renormalization group (DMRG), Lanczos, and exact-diagonalization (ED) routines [56–58].

There are three cases of study here: $J_{xy} = J_z$ (small perturbations), $J_{xy} \ll J_z$ (large perturbations), and when the initial ψ_0 is far from the starting state.

1. Small perturbations ($J_{xy} = J_z$)

Figure 1 shows how the energy converges to the energy of the full *XXZ* model with increasing numbers of terms. In each case, using the initial wave function provided from the previous iteration, only one Lanczos iteration must be run to obtain a highly accurate energy with the new interaction term included. The small difference in energies between the DMRG solution and the Lanczos solution is shown in the lower graph of Fig. 1. There is also the possibility to add in a partial term by using a small term $d\lambda$ for each of N times such that $Nd\lambda = \lambda$. This would require more applications of the Lanczos algorithm with new Hamiltonians and may be useful for long-range interactions or other cases.

In this one-dimensional example, the convergence is aided by only adding one term. In realistic systems, the same strategy of adding interaction terms piecemeal will both allow the Lanczos algorithm to converge quickly and also reduce the time spent applying the operator with methods from Sec. II. Still, this should be expected, in general, due to the rapid convergence of Lanczos techniques.

The computational cost of each additional Lanczos operation is counted as 1 here. So, each Lanczos step will be equally costly. There are factors such as the preparation of the operator at each Lanczos iteration which are not considered. Additionally, hardware considerations are also not minded in this treatment. However, it should be noted from the results here that the convergence is so rapid that any additional cost to implementing the Lanczos step is likely to result in drastically fewer steps with regards to other algorithms that may have

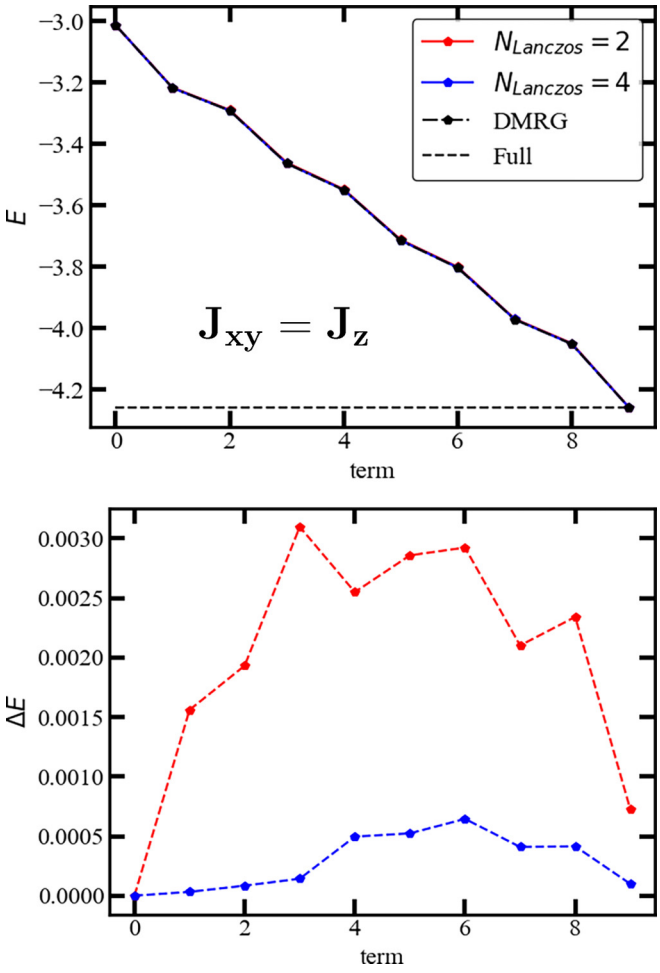

FIG. 1. Convergence in energy (E) while adding one interaction term $\hat{S}_i^z \cdot \hat{S}_{i+1}^z$ to an XY model on a 10-site lattice (9 interaction terms to add). Two solvers are used at each step. DMRG is shown as a solid blue line and a Lanczos solver is shown as a red dashed line. The initial wave function for the Lanczos algorithm is taken from the previous iteration. A black dashed line shows the energy of the full XXZ model. The lower figure shows the difference between the DMRG and Lanczos solutions. Only one Lanczos iteration was used for each added term. Lower figure: Energy differences from the exact value, ΔE. All units are such that $J = m = \hbar = 1$.

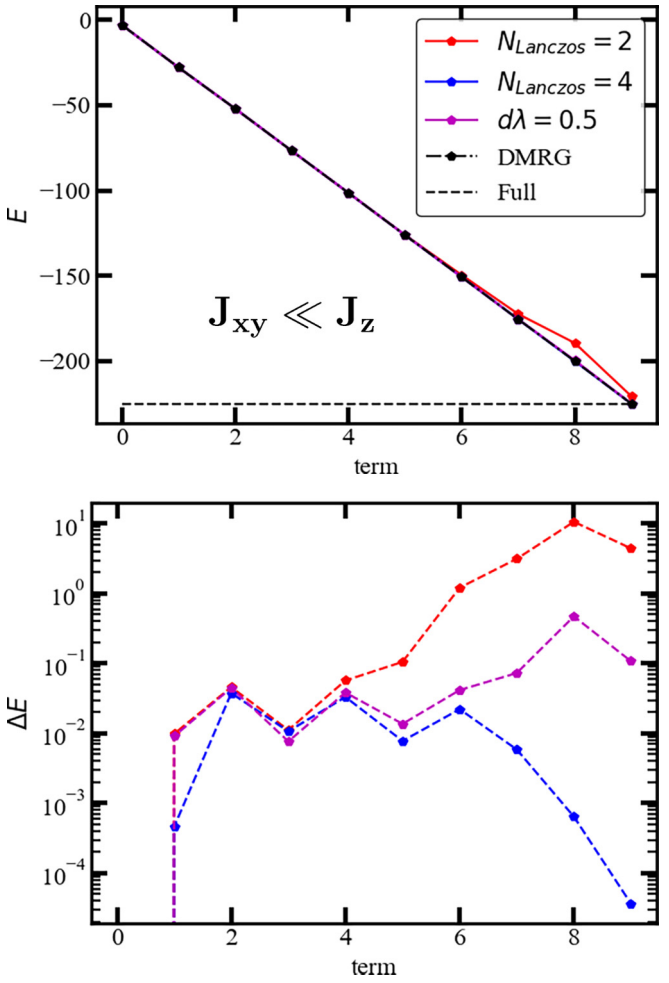

FIG. 2. Convergence in energy (E) while adding a large interaction term $J_z \hat{S}_i^z \cdot \hat{S}_{i+1}^z$ with $J_{xy} \ll J_z$. The parameters are the same as Fig. 1. By using four Lanczos steps instead of two, the accuracy is greatly improved in this case. Decreasing the incremental interaction strength $d\lambda$ (here, 0.5 with two rounds of $N_{\text{Lanczos}} = 2$) would require more than double precision (see text).

smaller costs. This makes a direct comparison between methods difficult because the rate of convergence of the Lanczos methods is so high.

2. *Large perturbations ($J_{xy} \ll J_z$)*

In this case, $100J_{xy} = J_z$ to simulate a large perturbation. For the example here, increasing the number of Lanczos iterations to four for each new added interaction term allows for the energy to be obtained to a good accuracy here. This is a large improvement over using only two Lanczos iterations, as shown by comparing the curves in Fig. 2.

It is possible to use only two Lanczos updates if one adds portions of the interaction term. In this case, $J_z/2$ is added to the Hamiltonian twice, with two Lanczos steps each (total of four Lanczos steps). The results could be improved if more Lanczos iterations were used here, but this would require greater precision in the coefficients than is available here with a double-precision classical implementation.

Note that tests with coefficients found on the classical computer will be subject to numerical instabilities that will eventually degrade the accuracy of the resulting ground state, so a full solution with this method will generate imprecise answers. For example, when increasing the number of Lanczos iterations to 10 for each step, this can occur in this example.

3. *Arbitrary starting wave function*

So far, eigenstates for the starting wave function were used. The natural question is whether the starting states can be replaced by some arbitrary state and how the convergence of the algorithm is affected. When implementing this type

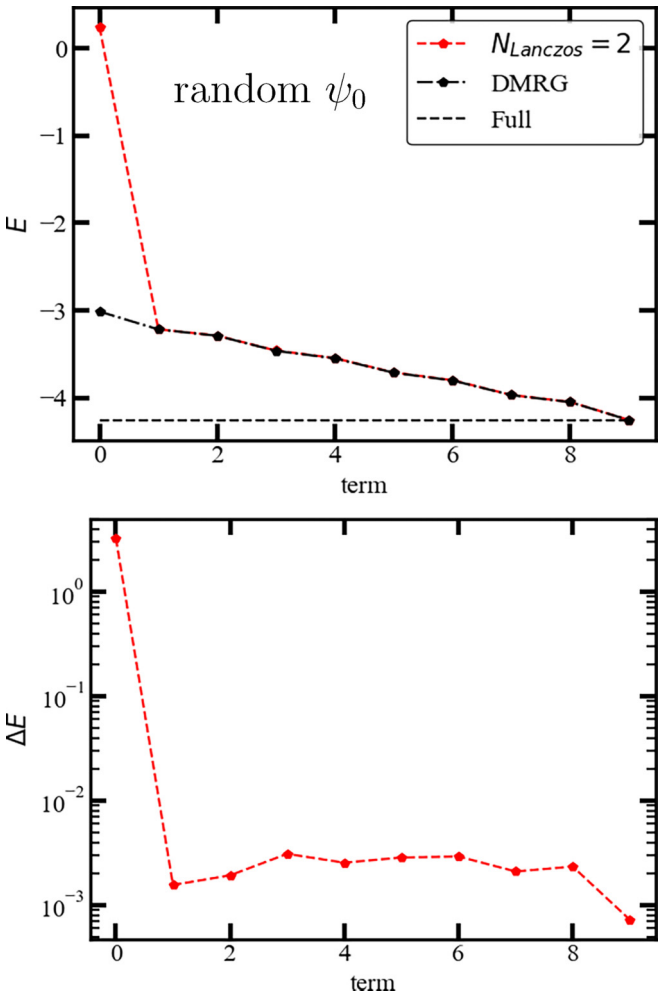

FIG. 3. Convergence in energy (E), similar to Fig. 1 except that a random starting state was used. Tests on larger systems or with more Lanczos recursion steps quickly suffer from precision errors that will not be present on the quantum computer.

of initialization on the quantum computer, the only key is to determine the energy of the wave function. If using QPE to do this, then the starting state must have an associated Hamiltonian.

For demonstration purposes, the initial state of alternating spins here is

$$|\Psi\rangle = |\psi_0\rangle = |\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle, \tag{15}$$

with $J_{xy} = J_z$ in the Hamiltonian. While the Hamiltonian, which has an eigenstate of Eq. (15), is not known and would therefore prevent the use of this state in the quantum algorithm, it is instructive to observe the convergence in this case where the initial state is not close to the final problem to solve.

Figure 3 shows the convergence for this starting wave function. The first Lanczos iteration will be the most difficult since it must change the wave function the most. Subsequent iterations converge more easily to the true ground state, just as in the previous cases.

These examples demonstrate that applying operators incrementally is possible and will yield a large cost reduction on the quantum computer. The examples here were on the ground state, but higher excited states can be found similar to the discussion around Eq. (11) once the Lanczos coefficients are known. In this example, the precision that can be found from the classical simulation is restricted [34]. The quantum computer is only limited by any errors on application of the operators.

III. QUANTUM BLOCK LANCZOS RECURSION

In principle, one should be able to discover all excitations from QLR as described above [59], but the extension of this method to a block or banded Lanczos algorithm is known to resolve degeneracies to a higher degree and generally aid convergence [36]. This would also circumvent any issues with using approximate Lanczos coefficients by still giving highly reliable wave functions from the extension presented here.

Block Lanczos is used in quantum chemistry [60], but also in physics, particularly for dynamical mean-field theory computations [61]. The scalar coefficients of the Lanczos recursion are extended to a matrix of coefficients.

To formulate the problem, consider a set of wave functions grouped as supervectors $\mathbf{\Psi}$, which is a vector of d excitations,

$$\mathbf{\Psi}_n = (|\psi_n\rangle_1, |\psi_n\rangle_2, \ldots, |\psi_n\rangle_d), \tag{16}$$

and therefore the task is to find matrices $\mathbf{A}$ and $\mathbf{B}$ which are of dimension $d \times d$ block such that Lanczos can be performed. This means that d registers, each with a wave function, are also available.

Extending the three-term recursion from Eq. (2) to a block or banded (or other) Lanczos scheme with more terms in the recursion would be possible to prepare more than one excitation at a time [61]. The expanded Lanczos recursion relation appears as [62]

$$\mathbf{\Psi}_{n+1}\mathbf{B}_{n+1} = \hat{H}\mathbf{\Psi}_n - \mathbf{\Psi}_n\mathbf{A}_n - \mathbf{\Psi}_{n-1}\mathbf{B}_n^\dagger, \tag{17}$$

for a vector of wave functions $\mathbf{\Psi}$ with matrices

$$\mathbf{A}_n = \mathbf{\Psi}_n^\dagger \hat{H} \mathbf{\Psi}_n, \tag{18}$$

and $\mathbf{B}_n$ defined recursively from

$$\mathbf{B}_n = \mathbf{\Psi}_{n-1}^\dagger \hat{H} \mathbf{\Psi}_n, \tag{19}$$

as can be most immediately seen from the tensor network diagrams in Ref. [36]. It should be understood that when applying $\hat{H}$ onto the wave-function supervector, the Hamiltonian is applied onto each wave function in the vector. The implication of Eqs. (18) and (19) is that there are simply d^2 applications of QLR to obtain QBLR.

Because the coefficients can be obtained by an operator acting on a ground state of an initial Hamiltonian, this implies that the coefficients of both $\mathbf{A}$ and $\mathbf{B}$ can be recovered by performing a state-preserving quantum counting operation on each term of the matrix. This was also true in the scalar case, and this establishes that the block Lanczos case can avoid repeated wave-function preparation as in Ref. [14]. Using the methods of that paper, each coefficient must be obtained individually: one quantum counting process for each operator. However, if operations can be performed in parallel on the quantum computer, then this could improve performance to simultaneously find all coefficients of a block.

On the classical computer, the blocks can be represented as a block-diagonal supermatrix representing the Hamiltonian

$$\hat{H} = \begin{pmatrix} \mathbf{A}_0 & \mathbf{B}_1^\dagger & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{B}_1 & \mathbf{A}_1 & \mathbf{B}_2^\dagger & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_2 & \mathbf{A}_2 & \ddots & \mathbf{0} \\ \vdots & \vdots & \ddots & \ddots & \mathbf{B}_n^\dagger \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{B}_n & \mathbf{A}_n \end{pmatrix}, \tag{20}$$

which can be diagonalized to find the energies of the excitations. From the coefficients of the eigenvectors of $\hat{\boldsymbol{H}}$ (denoted as γ_n still here too), the excitation wave functions can also be obtained.

In order to understand how best to apply the operators on the quantum computer, the block Lanczos equation can be written as

$$\sum_j B_{ij}^{(n+1)} |\psi_{n+1}\rangle_j = \hat{H}|\psi_n\rangle_i - \sum_j A_{ij}^{(n)} |\psi_n\rangle_j - \sum_j (B^*)_{ij}^{(n)} |\psi_{n-1}\rangle_j, \tag{21}$$

for a single row i of the left-hand side. This form makes clear that the d registers containing the d excitations can be acted on with the appropriate operators (sum over j) and added with the wave function on other registers with the appropriate operators. Note that the elements of $\mathbf{A}$ and $\mathbf{B}$ are stored classically and therefore the inverse of each matrix can be found. If this is done, then apply $\mathbf{B}_{n+1}^{-1}$ once the coefficients are found from Eq. (19).

The operators from Eq. (11) will be denoted as $\mathbf{G}_n$ for a given level and are extended from the scalar Lanczos case as $\hat{G}_n \to \mathbf{G}_n$. Similarly, $\psi \to \mathbf{\Psi}$ for the wave function. One additional operation is included, i.e., $\mathbf{G}$, compared with the operators listed in Ref. [33], which is that of the inverse $\mathbf{B}^{-1}$ operator. Since the operators can be determined on the classical computer, the operators can simply be prepared in a slightly different way. Again, the inverse is converted to a unitary as is standard for applying operators [14,33,41–43].

The form of the wave function on the quantum computer takes the form

$$\hat{G}_n(i, j)|\psi_0\rangle|i\rangle|j\rangle, \tag{22}$$

for elements of $(\mathbf{G}_n)_{ij} = \hat{G}_n(i, j)$. The operators $\hat{G}$ are derived from Eq. (21) for the block Lanczos case, extending the scalar Lanczos case used previously.

In all, the algorithm costs a practical amount of d^2 over the scalar Lanczos case. Each element of the matrix equations is simply one application of a set of equations slightly modified from QLR. Note that the effort expended to apply operators onto wave functions is not wasted at the end with a single measurement. The state-preserving quantum counting algorithm can be used to obtain the correct expectation values without completely measuring the wave function.

A. Algorithm summary

The following summarizes the previous discussion to demonstrate how to implement the block Lanczos on the quantum computer.

Quantum block Lanczos recursion: Algorithm for multiple excited states.

(1) A set of starting eigenfunctions, $\{|\Xi\rangle\}$, is prepared on ν registers (one for each wave function).

(2) Start a counter at $n = 0$.

(3) Construct the operator $\mathbf{G}_n$ representing the appropriate step from Eq. (17). This operator spans several excitations.

(4) $\mathbf{G}_n$ is applied onto the current state and quantum counting is used to determine the Lanczos coefficients, given by Eqs. (18) and (19).

(5) With the new coefficient(s), the algorithm returns to step (2), increments n, and finds the next step of coefficients.

(6) Storing the coefficients classically, the block-diagonal Hamiltonian from Eq. (20) can be formed and diagonalized. A set of coefficients γ_n can then be used to determine the energies.

The scaling of the method is no worse than the application of the operators at each step, albeit the number of times this must be run for d excitations is $O(d^2)$.

The coefficients of the next step are not known beforehand, so each step must be performed iteratively. Once the coefficients are obtained with the quantum counting process, they can be stored classically and used without obtaining them again, although the d^2 coefficients of a given block can be parallelized. Note, also, that the algorithm can be restarted at any time since the coefficients are stored classically.

The ground-state energy can be checked when diagonalizing Eq. (20) on the classical computer. If the ground-state energy is converged within the accuracy needed for QPE, then there are sufficient Lanczos steps run to find an accurate ground-state energy. The same applies for the excited state convergence.

B. Error analysis

In this section, a careful analysis of the relevant parameters of the system will show how uncertainty in the Lanczos coefficients will influence the resulting energies.

To investigate the effects of noise on the resulting energies, a block Hamiltonian of a particular size a is created for b such blocks. When $a = 1$, the QLR algorithm is used. When $a > 1$, QBLR is represented. A set of matrices is generated with values between [0,1] to mimic the values on the operators for the quantum computation. A noise term selected from a Gaussian distribution of width η is selected for each element.

The energies with noise E are computed with respect to the true energies without noise E_0 to find the mean absolute error (MAE) $\bar{E}$ defined as

$$\bar{E} = \frac{1}{M} \sum_{i=1}^{M} \left| E^{(i)} - E_0^{(i)} \right|, \tag{23}$$

for a number of eigenvalues M.

The MAE is shown in Fig. 4. As expected, as the noise decreases in each of the parameters, the accuracy of the energy eigenstates increases. In both cases, the error decreases linearly with the noise applied to each term. This is a straightforward but useful result. If the quantum counting obtains coefficients to a precision δ, then the resulting energy is also obtained to an error of roughly δ. The change in this trend

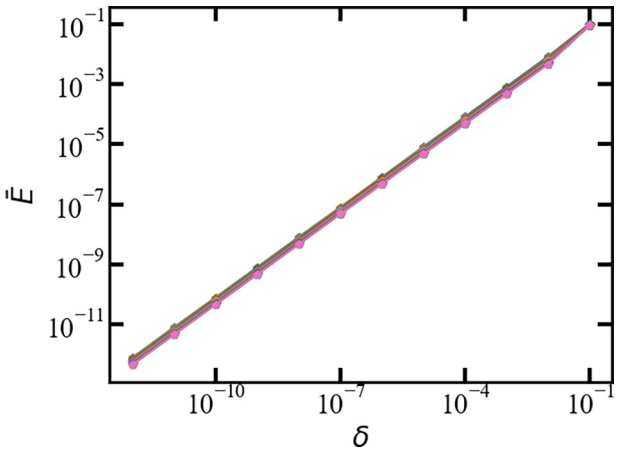

FIG. 4. Mean average error for a system of block size $d = 20$ for various numbers of iterations, $\{4, 5, 6, \ldots, 20\}$. All lines are nearly the same in magnitude. The general linear trend is mostly unchanging with the input parameters.

for other parameters that could have been picked (larger block sizes, more blocks, etc.) is very stable.

What this implies is that for a QPE to obtain the correct eigenvalue, the Lanczos coefficients must be sufficiently accurate (i.e., δ is a threshold for how accurate the coefficients will be). This is a crucial aspect to know how much precision must be obtained from the quantum counting algorithm.

C. Excitations of a spin model

Block Lanczos can be equally applied to the model used in the previous section for the ground state. To start, the ground state plus three excitations of the model will be searched for.

For the case where $J_{xy} = J_z$, the results are shown in Fig. 5. The errors in the ground state and first excitation of the model are shown to have relatively constant error. Either as the number of Lanczos iterations, N_L, is increased or the interaction strength is limited by the amount $d\lambda$ with N_L iterations applied on each operator, the error in the resulting wave function remains well controlled.

Block Lanczos is noted to be well controlled and to recover all excitations very stably for a given problem [54]. Other excitations are also recovered, but will not be shown since they are very similar to the first excitation shown here.

A model with $J_z = 100$ is possible to evaluate and gives the correct number of excitations with this strategy. The model becomes more Ising-like and gives a degeneracy in the ground state, showing that the ground-state degeneracy is captured by this method and that large perturbations are solved just as well as in the scalar case of Figs. 2 and 3.

D. Stability with degeneracies

Block Lanczos methods are known to be more stable when computing degenerate excitations. In Fig. 6, it is shown that the block Lanczos algorithm converges to the excitations and their degeneracies. The scalar Lanczos algorithm can encounter spurious degeneracies to a much greater degree. The spurious degeneracies encountered by the Lanczos algorithm are due to finite numerical precision in the simulator used for these results (i.e., it is an expression of being run on a classical computer, not an algorithmic fact). Whether noise on the quantum computer will ultimately introduce these degeneracies is a possibility and deserves further investigation on real quantum hardware.

E. Discussion

The advantages of many excitations being discovered is chiefly one of stability. The ability to resolve degeneracies and generate orthogonal wave functions is valuable in a variety of contexts and now available for the quantum computer. That this method is rapidly convergent [63,64], resolves degeneracies, and avoids repeated wave-function preparation means that this method could be a valuable alternative to time-evolution methods.

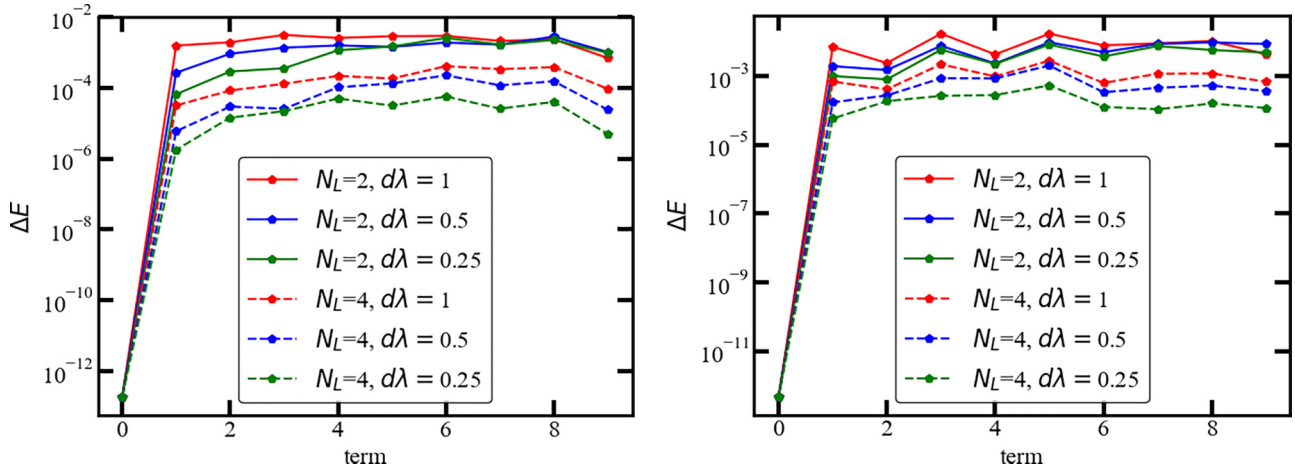

FIG. 5. Energy differences of the ground state (left) and first excitation (right) of the 10-site spin-half *XXZ* model by adding interaction terms on the free *XY* model as in Sec. II B in the case of $J_{xy} = J_z$. The block Lanczos method performs with a nearly constant error in this case. The number of Lanczos iterations is given by N_L and the operator is applied with a variable increment in terms of the interaction strength $d\lambda$. In that case, the operator $d\lambda \hat{S}_i^z \hat{S}_{i+1}^z$ is applied sufficient times to give the full interaction strength with $\lambda = 1$ (e.g., four times for $d\lambda = 0.25$).

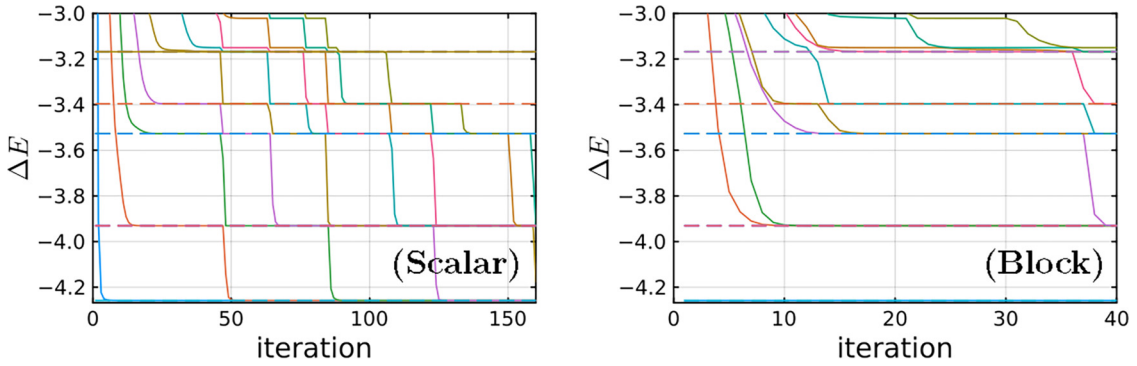

FIG. 6. Left: Lanczos plotted with a number of energies as a function of 160 iterations on a 10-site spin-half *XXZ* model. Higher excitations require more iterations, but spurious degeneracies can be encountered. Eigenvalues (solid) are seen to converge to exact energies (dashed), but spurious degeneracies appear as for the ground state around iterations 50, 90, and 125 in the figure. The initial picked state was the ground state of the model plus 0.1 times a vector of random numbers. Right: Block Lanczos run for 40 iterations (block size: four) on the same model captures degeneracies much more stably. The initial state was constructed from the same state as in the left figure with three orthogonal vectors from a Gram-Schmidt process.

The goal of QBLR is to retain the accuracy of the wave function, which is controlled directly through the gate fidelities and other quantities on the quantum computer. The quantum advantage sought here is for an exponential reduction in memory, which is a property that quantum computers exhibit under the extended Church-Turing thesis, which asks if an algorithm can be computed with significantly less memory resources over classical computing [65]. Lanczos techniques do have this property when applied on a quantum computer theoretically if perfect application of gates is assumed and with sufficient time to sample the coefficients. The typical errors on a classical computer [34,52,59,65,66] do not appear since values are retained to quantum precision.

The opportunity to obtain ground states from QLR places added emphasis on the development of state-preserving quantum counting and methods of applying operators to wave functions such as the linear combination of unitaries (and included subroutines) to obtain both the Green's function and ground state.

The possibility to discover ground states or excited states deserves more consideration since these methods are free of time steps and Trotter-Suzuki decompositions, a common feature in many other proposals. The Lanczos algorithms also do not need any notion of locality to aid convergence as would be expected for a matrix product state's relationship to local Hamiltonians [57,67,68], particularly for time-evolving block decimation (TEBD) [56]. The only instance where locality plays any role is in the writing of the application of the operators to the wave function, which could play a role in near-term implementation. It is not clear how many Lanczos coefficients would need to be obtained to find accurate ground states from this method for phase estimation to give accurate results. Further discussion would require specialization to a specific problem and is deferred to a future study [33]. Note that extensions to a fitting function for the remaining coefficients is possible in principle [69].

The QBLR algorithm is formally $O(d^2)$ applications of QLR in this formulation. However, note that formally one can add a single additional qudit of dimension d (or an equivalent number of qubits to record the number of excitations) to the quantum computer and use it to control which excitation is accessed on a single register of qubits used to record the wave function. However, the measurement of the resulting matrix coefficients will require more (albeit perhaps only moderately more) operations to obtain the same quantities using the technologies here, but it may be possible to reduce the additional cost to $O(1)$ if it can be tolerated if the number of samplings of the Lanczos coefficient values is not sampled the same number of times.

IV. NON-HERMITIAN OPERATORS

The previous discussion was for the block Lanczos algorithm that is formulated for the problem of a Hermitian operator. The extension of the above methods to non-Hermitian operators is possible without introducing too much additional computational cost. Instead, only one additional set of matrices (or in the case of scalar Lanczos, one additional set of coefficients) should be found. The procedure will be defined for the block-matrix case, but it can be reduced to the scalar case when the block size is of size 1.

Given a non-Hermitian operator $\tilde{\tilde{H}}$ with eigenvalue E, a set of two eigenvalues can be defined. One is known as the left eigenvectors (a transpose is used even if there are complex valued entries) [66],

$$\mathbf{\Psi}_L^T \tilde{\tilde{H}} = \mathbf{\Psi}_L^T E, \tag{24}$$

and the other is for the right eigenvectors,

$$\tilde{\tilde{H}} \mathbf{\Psi}_R = E \mathbf{\Psi}_R, \tag{25}$$

where block matrices $\mathbf{\Psi}_L$ and $\mathbf{\Psi}_R$ have the orthogonality relation [66]

$$\mathbf{\Psi}_L^T \mathbf{\Psi}_R = \mathbb{I}_{d\times d}, \tag{26}$$

with an identity matrix $\mathbb{I}_{d\times d}$ of dimension $d \times d$.

The block operator represented analogous to Eq. (20) appears in this case as

$$\check{\mathbf{T}}_n = \begin{pmatrix} \mathbf{A}_0 & \mathbf{C}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{B}_1 & \mathbf{A}_1 & \mathbf{C}_2 & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_2 & \mathbf{A}_2 & \ddots & \mathbf{0} \\ \vdots & \vdots & \ddots & \ddots & \mathbf{C}_n \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{B}_n & \mathbf{A}_n \end{pmatrix}. \tag{27}$$

There are two recursion relations for each of the left and right eigenvectors. They take the form of [70,71]

$$\vec{\mathbf{\Psi}}^T_{L,(n)}\tilde{H} = \check{\mathbf{T}}_n \vec{\mathbf{\Psi}}^T_{L,(n)} + \mathcal{I}_n \mathbf{C}_{n+1} \mathbf{\Psi}^T_{L,(n+1)}, \tag{28}$$

$$\tilde{H}\vec{\mathbf{\Psi}}_{R,(n)} = \vec{\mathbf{\Psi}}_{R,(n)}\check{\mathbf{T}}_n + \mathbf{\Psi}_{R,(n+1)}\mathbf{B}_{n+1}\mathcal{I}^T_n, \tag{29}$$

where

$$\vec{\mathbf{\Psi}}_{R,(n)} = \begin{pmatrix} \mathbf{\Psi}^{(0)}_R, & \mathbf{\Psi}^{(1)}_R, & \ldots, & \mathbf{\Psi}^{(n)}_R \end{pmatrix}, \tag{30}$$

$$\vec{\mathbf{\Psi}}_{L,(n)} = \begin{pmatrix} \mathbf{\Psi}^{(0)}_L, & \mathbf{\Psi}^{(1)}_L, & \ldots, & \mathbf{\Psi}^{(n)}_L \end{pmatrix}, \tag{31}$$

$$\text{and} \quad \mathcal{I}_n = (\mathbf{0}_{d\times d}, \quad \mathbf{0}_{d\times d}, \quad \ldots, \quad \mathbb{I}_{d\times d}). \tag{32}$$

The final term is an identity matrix to ensure that the dimension of the resulting matrix is consistent with all terms in the recursion. Only the last block of the matrix is nonzero where there are blocks of zero matrices, $\mathbf{0}_{d\times d}$.

Writing out the explicit terms of the recursion relation in the style of the **G** operators from earlier is lengthy, but a single operator can be written to be applied on the starting wave function just as for QLR [33]. The only additional cost is the determination of an extra block matrix **C** and double the number of registers to represent both the left and right eigenvectors.

The extension of the block Lanczos algorithm to the non-Hermitian case has therefore only introduced an extra matrix $\mathbf{C}_n$ which must also be found with the other two sets of matrices. However, this does not increase the overall computational cost of the algorithm presented here. The same forms for the operators connecting the original wave function provided to the algorithm can be derived similarly as for the Hermitian case.

In terms of non-Hermitian solution strategies, there is also the possibility to implement a full Arnoldi method with this scheme [72]. In that strategy, all the previous vectors are orthogonalized against, adding nonzero entries to the upper right portion of the matrix. However, the relatively local nature of the block Lanczos method here may create some advantages when writing out the operator on the quantum computer, keeping many terms local.

V. CONCLUSION

Lanczos recursion methods on the quantum computer were extended to solve for many excitations simultaneously. This uses a block Lanczos technique that is good at resolving degeneracies in quantum states. This comes at only a cost of the number of excitations squared sought on the quantum computer. The use of the quantum counting algorithm here allows for the wave function to not be collapsed at each step, cutting out a major cost of many other algorithms. Further, interaction terms can be applied in small groups to aid convergence and keep the process of applying those operators to the wave function less than exponentially long. The error of diagonalizing the Hamiltonian in the Krylov basis was demonstrated to scale linearly with the noise of the coefficients. The method can also be applied onto non-Hermitian operators with a moderate additional cost. Due to the feasible cost of this algorithm and the rapid convergence of Lanczos techniques, it is expected that quantum block Lanczos recursion could be an alternative to existing methods to find the ground and excited states.

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