Lanczos recursion on a quantum computer for the Green's function

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The technique of quantum counting is used to obtain coefficients from a Lanczos recursion from a single ground-state wavefunction on the quantum computer. This is used to compute the continued fraction representation of a general Green's function, which can be useful in condensed matter, particle physics, and others. The wavefunction does not need to be re-prepared at each iteration. The quantum algorithm represents an exponential reduction in memory required over classical methods.

Introduction.– Quantum computers rely on a superposition of states on each qubit. Some algorithms can provide a quantum advantage in terms of the amount of time needed to run some tasks [1]. Finding a useful algorithm that can efficiently beat classical computers are highly sought, particularly those for quantum chemistry applications [2]. Many existing proposals focus on cases where a measurement from a wavefunction is used to obtain some property of a molecular system; however, the time needed to solve for a wavefunction can be prohibitively long for large systems, as demonstrated by Poulin, *et. al.* [3, 4]. Using the fewest measurements to obtain the most descriptive quantities is therefore desirable [5].

One useful quantity is the fully interacting Green's function which is approximated in current strategies on the classical computer such as dynamical mean-field theory (DMFT) [6, 7], GW [8], random-phase approximation (RPA) methods [9], and quantum field theories [10]. The Green's function contains the ground state and excitation energies notably in the imaginary part of the Green's function, known as the spectral function [11].

Recently, an excellent first step in obtaining the Green's function was to evaluate correlation functions of the form $\langle\phi(t_1)\phi(t_2)\dots\phi(t_r)\rangle$ by Rall in Ref. 12, effectively adapting techniques commonly used for matrix product states to the quantum computer [13, 14]. This form is well-suited for non-equilibrium phenomena. However, this form of the correlation function suffers from known errors. First, the finite time interval will create difficulties when evaluating a Fourier transform. A well-known uncertainty in the amount of time used to resolve the correlation function, Δt, and the spread of energies, ΔE is $\Delta t\Delta E \geq 1/2$. This implies that even long time intervals will still not be able to determine the energy down to arbitrary accuracy. In practice, this will cause properties such as peaks in the spectral function to broaden. Another source of error for time evolution is the Nyquist error when the function is over- or under-sampled in time. If the wavefunction is not efficiently available, then the repeated measurement required forces the expensive repreparation of the wavefunction [3, 4].

Computing the Green's function directly in frequency space would be highly advantageous to remove spurious effects from Fourier transforms or insufficient sampling. A form that is useful in several applications that have this property is the continued fraction representation [13].

In this work, the continued fraction representation of the Green's function is obtained through a quantum version of Lanczos recursion (QLR). For demonstration purposes, the one-body Green's function is found from the operator $\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}_{j\sigma}$, although generalization to more complicated operators is straight-forward. A quantum counting algorithm [15–17] is then used to extract the necessary coefficients which then construct the continued fraction. This algorithm leaves the wavefunction largely undisturbed and therefore it can be reused as in Ref. 5 where a recycled wavefunction for minimal prefactor (RWMP) method was introduced for the density functional. The QLR algorithm here is for zero-temperature, but extensions to finite temperature systems are possible.

Previous work by Motta, *et. al.* in Ref. 18 was focused on using a Lanczos algorithm to find the Hamiltonian in the reduced Krylov subspace. The implementation here is different since only the coefficients from quantum counting instead of time evolution. This algorithm provided here is a means to extract more data from the ground-state wavefunction, not simply find the ground state.

Lanczos recursion.– Constructing a Krylov subspace is an effective way to solve for the ground state of a quantum Hamiltonian, $\mathcal{H}$. The formatting of the following facts as theorems is to use the convention in many other physics papers even though these results are review.

Definition 1 (Krylov subspace)**.** A set of vectors known as the Krylov subspace will contain the true ground state for a Hamiltonian, $\mathcal{H}$, from an arbitrary initial state Φ by constructing the set $\{\Phi, \mathcal{H}\Phi, \mathcal{H}^2\Phi, \dots\}$.

To see this, application of $\mathcal{H}$ to Φ generates a spectral decomposition of Φ of the form $\mathcal{H}^p|\Phi\rangle = \sum_n (E_n)^p|\phi_n\rangle$ in terms of eigenvalues E_n and eigenvectors ϕ_n of $\mathcal{H}$. By including repeated application of $\mathcal{H}$ (larger p), the most extremal eigenvalues of $\mathcal{H}$ will become further from the next nearest eigenvalues [14]. Diagonalizing $\mathcal{H}$ projected into this subspace gives the ground state energy. A more exhaustive proof is omitted in favor of this intuition.

Constructing the Krylov subspace vectors by orthogonalizing against all vectors in the subspace is known as a power method. However, if all vectors are guaranteed to be orthogonal, then a 3-term recursion can be used to find the next vector in the subspace [19].

Theorem 1 (Lanczos recursion)**.** *Lanczos recursion of the form*

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

generates the Krylov subspace where $n \in \mathbb{Z}^+$, $\alpha_n = \langle\psi_n|\mathcal{H}|\psi_n\rangle$, $\beta_n^2 = \langle\psi_{n-1}|\psi_{n-1}\rangle$, $\beta_0 = 0$, $|\psi_{-1}\rangle = 0$, *and* $|\psi_0\rangle = |\Phi\rangle$.

To see this, if all previous vectors in the Krylov subspace expansion are orthonormal, then $\langle\psi_m|\mathcal{H}|\psi_n\rangle$ is identically zero if $|m-n| > 1$ since otherwise $\mathcal{H}|\psi_n\rangle$ spans the space of existing Krylov vectors, and therefore $|\psi_{n+1}\rangle$ is orthogonal to the previous states. Note that α_n does not have to be an eigenvalue of $\mathcal{H}$.

Continued fraction representation.– The method of continued fractions has been a useful way to obtain the frequency-space Green's function in a variety of applications. The coefficients of the Lanczos recursion are used to obtain the continued fraction representation.

Theorem 2 (Continued Fraction representation of the Green's function)**.** *The continued fraction representation of the Green's function,* $\mathcal{G}$*, of a Hamiltonian* $\mathcal{H}$ *for non-relativistic systems is*

$$\mathcal{G}_{i\bar{\sigma};j\sigma}(\omega) = \cfrac{\langle\Psi|\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}_{j\sigma}|\Psi\rangle}{\omega - \alpha_0 - \cfrac{\beta_1^2}{\omega - \alpha_1 - \cfrac{\beta_2^2}{\ddots}}} \tag{2}$$

where α_n *and* β_n *coefficients are defined by a Lanczos recursion algorithm from Eq.* (1)

Proof. By definition, the Green's function is [20]

$$\mathcal{G}_{i\bar{\sigma};j\sigma}(\omega) = \langle\Psi|\hat{c}^\dagger_{i\bar{\sigma}}\,(\omega - \mathcal{H} \pm i\eta)^{-1}\,\hat{c}_{i\sigma}|\Psi\rangle \tag{3}$$

for some small number η which gives the advanced $(-)$ or retarded $(+)$ Green's function. We begin with the tridiagonal representation of the Hamiltonian in terms of the Lanczos coefficients, by inspection of Eq. (1),

$$\mathcal{H} = \begin{pmatrix} \alpha_0 & \beta_1 & 0 & 0 & \cdots & 0 \\ \beta_1 & \alpha_1 & \beta_2 & 0 & \cdots & 0 \\ 0 & \beta_2 & \alpha_2 & \beta_3 & \cdots & 0 \\ 0 & 0 & \beta_3 & \alpha_3 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \beta_N \\ 0 & 0 & 0 & 0 & \beta_N & \alpha_N \end{pmatrix} \tag{4}$$

for N iterations of the Lanczos algorithm expressed in the generated in the subspace of $\{|\psi_n\rangle\}$ vectors. Note further that we can express $\omega - \mathcal{H}$ by subtracting the Hamiltonian from an identity matrix times ω.

The task is then find the inverse, where it is noted that an effective 2×2 super matrix can be formed by first isolating only the upper left entry in Eq. (4) with α_0 as

$$\omega - \mathcal{H} = \begin{pmatrix} \omega - \alpha_0 & \beta_1 \\ \beta_1 & \omega - \mathcal{H}_1 \end{pmatrix} \tag{5}$$

where the lower right $(N-1)\times(N-1)$ block into a single matrix $\mathcal{H}_1$. The upper left element denoted by (1,1) of the inverse of $\omega - \mathcal{H}$ is then

$$\left[(\omega - \mathcal{H})^{-1}\right]_{11} = \frac{1}{(\omega - \alpha_0) - \frac{\beta_1^2}{\omega - \mathcal{H}_1}} \tag{6}$$

which can be repeated iteratively (by then isolating the upper left element of $\mathcal{H}_1$ which is $\omega - \alpha_1$) to generate the continued fraction representation with $\omega \to \omega \pm i\eta$. ■

Here, division by a matrix is synonymous with the inverse in all cases since the coefficients α_n, ω, and β_n are all scalar values. Note that for relativistic Hamiltonians, the replacement by $\omega \to \omega^2$ is required since there is a second-order time derivative instead of a first-order.

The continued fraction can be evaluated out to a certain order where the coefficients are either small enough or large enough to justify leaving off the next level of the continued fraction [21]. It is also possible to construct an extrapolation of existing coefficients.

The operator used here $\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}_{j\sigma}$ is to more clearly identify with the common notation in the literature for a 2-point correlation function [20]. The more general expression would be for some unitary $\hat{\Omega}$, noting that $\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}_{j\sigma}$ is not unitary. If a unitary $\hat{\Omega}$ is required in place of $\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}_{j\sigma}$, then both of $(\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}_{j\sigma} \pm \hat{c}^\dagger_{j\sigma}\hat{c}_{i\bar{\sigma}})$ can be computed in Eq. (2) and added or subtracted. Equally, other operators such as the higher order correlation functions or pairing terms, for example $(\hat{c}^\dagger_{i\bar{\sigma}}\hat{c}^\dagger_{i\sigma} \pm \hat{c}_{i\sigma}\hat{c}_{i\bar{\sigma}})$, can be found. Note also that a representation on a grid (see discussion in Ref. 5) is used but the operators can equally be expressed in real space, $\hat{c}_\sigma(\mathbf{r})$, or in momentum space, $\hat{c}_\sigma(\mathbf{k})$.

It can also be noted that $\hat{c}_{i\sigma}$ (or $\hat{c}^\dagger_{i\sigma}$) is not unitary. One way to force a unitary operator is to require two computations : once for $\hat{\Omega}_+ = \hat{c}^\dagger_{i\sigma} + \hat{c}_{i\sigma}$ and a second time for $\hat{\Omega}_- = i(\hat{c}^\dagger_{i\sigma} - \hat{c}_{i\sigma})$ and then noting that $2c^\dagger_{i\sigma} = \hat{\Omega}_+ - i\hat{\Omega}_-$ and $2c_{i\sigma} = \hat{\Omega}_+ + i\hat{\Omega}_-$. The resulting coefficients can be combined according to these rules to generate results for $\hat{c}_{i\sigma}$ or $\hat{c}^\dagger_{i\sigma}$ if some procedure cannot directly apply $\hat{c}_{i\sigma}$.

Quantum Lanczos recursion.– QLR can determine the coefficients α_n and β_n on the quantum computer, given an initial wavefunction, Ψ [5]. Note that both α_n and β_n are stored as classical variables everywhere here.

The method known as quantum counting (also known as quantum amplitude estimation [5, 15, 17]) is used to find the coefficients α_n and β_n. The basic strategy of quantum counting is to store the energy of the initial wavefunction, E, and compare against the energy after all operations are applied, E'. If the same final state is recovered ($E = E'$) then the count is accepted, and if a recovery procedure is required ($E \neq E'$) to re-obtain the original wavefunction then the count is rejected [16]. The ratio of acceptances to total iterations is the expectation value up to a normalization. The time for the recovery

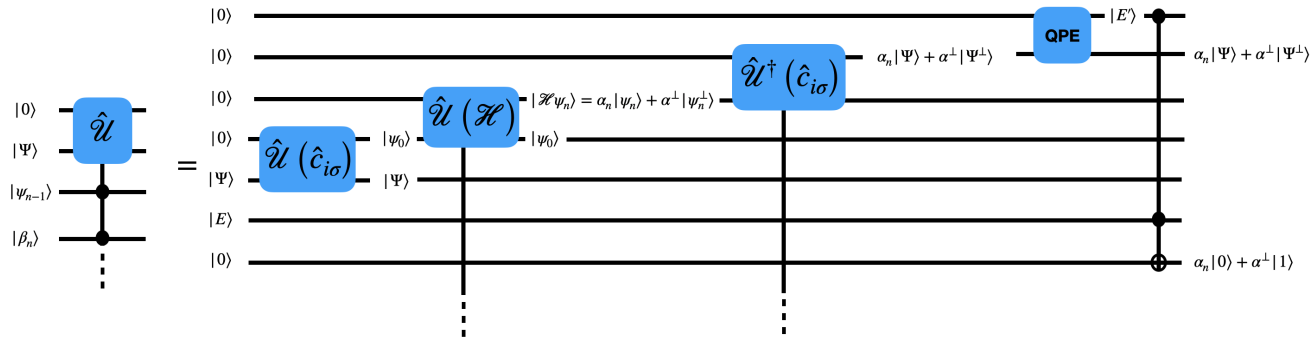

FIGURE 1. Modified quantum counting circuit to obtain α_n from input state Ψ with energy E. Vertical lines that descend below the figure account for all recursive steps including the previous α_n, β_n, and ψ_{n-1} in Eq. (1), and the application of $\hat{c}_{i\sigma}$ can be made to be unitary (see text). Quantum phase estimation (QPE) can be supplemented with qubitization [22] where applicable. The last step is a comparison of E' and the reference energy E that is converted to a single qubit.

procedure takes $\mathcal{O}(\varepsilon^{-1})$ for a precision ε [17], and the wavefunction is preserved in this process.

To start, the ground-state is given as Ψ. The next task to apply an operator $\hat{\Omega}$–which can be taken here to be $\hat{c}_{i\sigma}$ for demonstration purposes–is applied giving a state $|\Phi\rangle = \hat{c}_{i\sigma}|\Psi\rangle$. It is assumed that no error is generated in this step [17]. The first wavefunction is $|\psi_0\rangle = |\Phi\rangle$.

The counting procedure is illustrated on the first coefficient α_0 and then generalized. Applying $\mathcal{H}$ to $|\psi_0\rangle$ gives

$$\mathcal{H}|\psi_0\rangle = \alpha_0|\psi_0\rangle + \alpha^{\perp}|\psi_0^{\perp}\rangle \tag{7}$$

where all perpendicular signs ($\perp$) signify a set of states that are all orthogonal to the target state. For now, the target state is $|\psi_0\rangle$. Since the state $|\psi_0\rangle$ is not an eigenvector of $\mathcal{H}$, we must revert $|\psi_0\rangle$ back to Ψ in order to apply quantum phase estimation (QPE) and find E' since QPE acts on eigenvectors [1].

A unitary $\mathcal{U}^{\dagger}(\hat{c}_{i\sigma})$ is then applied to $|\psi_0\rangle$, which reverses all previous operations of the Lanczos recursion. At present, this is just $\hat{c}_{i\sigma}$ but will contain more operations later. The state is then $\alpha_0|\Psi\rangle + \alpha^{\perp}|\Psi^{\perp}\rangle$. Importantly, the coefficient is still denoted as α_0 here. This is because all operations are unitary, so $\Psi^{\perp}$ remains orthogonal to Ψ since unitary operations maintain orthogonality. Thus, the coefficient α_0 acting on $|\psi_0\rangle$ and $|\Psi\rangle$ are the same.

QPE can be used to obtain the ground state energy, E'. The energy is in superposition with the value found for the other perpendicular states, $\Psi^{\perp}$. The energies E and E' are compared with a series of CNOT gates to obtain a value of 0 or 1 (accept or reject) on a single pointer qubit [1, 15, 17]. The pointer qubit is measured. If the first d-bits of the energy match (the other bits are ignored since they are affected by measurement), the value is accepted and Ψ was recovered. The restriction on d is that the difference $E' - E$ is less than the difference between E and the first excited state [17].

If the reject outcome is found, then some state in $\Psi^{\perp}$ was measured and then the recovery procedure is performed until the original wavefunction is obtained, which is explained in Refs. 15 and 17. The ratio of successes to the total number of iterations is α_n. The coefficients can be output to a classical user and put back onto another register as a classical number.

The procedure for subsequent Lanczos steps ($n > 0$) is shown in Fig. 1. The only difference is that repeated applications of Eq. (1) must be applied when applying $\hat{\mathcal{U}}(\mathcal{H})$ to obtain $|\psi_n\rangle$ (before applying $\mathcal{H}$). This also implies that all previous coefficients and wavefunctions are stored on some auxiliary qubits and are reversed in $\hat{\mathcal{U}}^{\dagger}(\hat{c}_{i\sigma})$. The energy is compared as before after applying $\mathcal{H}|\psi_n\rangle$.

In order to find the β_n coefficients, note that

$$\beta_n = \langle\psi_{n-1}|\mathcal{H}|\psi_n\rangle = \langle\psi_n|\mathcal{H}|\psi_{n-1}\rangle \tag{8}$$

by direct evaluation of Eq. (1). This term can also be estimated with quantum counting. Instead of seeking the state $|\psi_n\rangle$ from $\mathcal{H}|\psi_n\rangle$, the same state $|\psi_n\rangle$ is searched from $\mathcal{H}|\psi_{n-1}\rangle$. The algorithm proceeds as before but with the appropriate inverse unitary for $|\psi_n\rangle$ after $\mathcal{H}|\psi_{n-1}\rangle$.

Figure 2 shows one cycle of the full algorithm :

Algorithm : Quantum Lanczos recursion

1. Obtain the ground state wavefunction Ψ.
2. Apply $\hat{c}_{i\sigma}$ to Ψ giving $|\psi_0\rangle = \hat{c}_{i\sigma}|\Psi\rangle$.
3. Start iteration n.
4. Add all three necessary registers from the previous steps according to Thm. 1 iteratively.
5. Use quantum counting to find $\alpha_n = \langle\psi_n|\mathcal{H}|\psi_n\rangle$.
6. Find β_n from Eq. (8) with quantum counting.
7. Repeat from Step 3, incrementing n for a certain number of iterations or until some criterion (for β_n or the energy) is reached.
8. Measure all of α_n, β_n, and $\langle\Psi|\hat{c}^{\dagger}_{i\bar{\sigma}}\hat{c}_{j\sigma}|\Psi\rangle$.

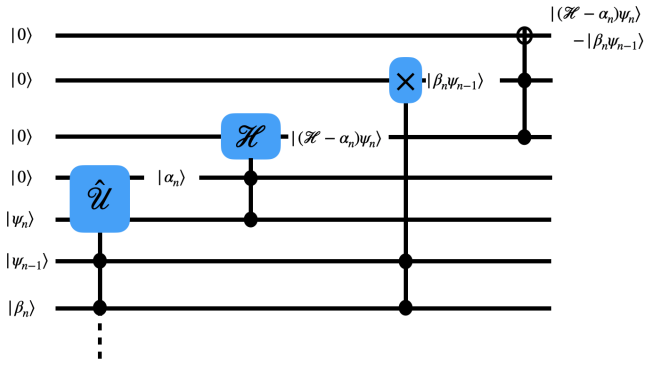

FIGURE 2. One Lanczos recursion step. The α_n coefficient is generated from quantum counting step provided in Fig. 1. The computation of β_n is omitted but shown in Eq. (8).

Since Ψ is preserved at the end of this computation, it is ready for the next computation. Another coefficient for the continued fraction, component of the Green's function can be found, or another Ψ close-by can be solved to reduce the real-time evolution steps as in the RWMP method from Ref. 5. This method could also be applied beyond scalar field theories or in other cases [21].

A stopping criteria can be applied either when the β_n coefficients become less than the specified tolerance or a specified number of iterations is accomplished. Alternatively, solving Eq. (4) shows the convergence in energy.

Comparison with classical techniques.– On the classical computer, it becomes difficult to construct a continued fraction representation that extends beyond 10 or so levels. Exact diagonalization [23] gives the Lanczos coefficients to numerical precision, but since the system sizes are limited by memory, only a few floors are possible.

The computation of continued fractions has been explored with tensor networks [13, 24] ; however, it has been found that the numerical truncation procedure decreases the normalization of the wavefunction ansatz and the reachable number of accurate floors is nearly the same as exact diagonalization [25]. The limitation comes from truncation in the singular value decomposition. Note that the method used in Ref. 12 is the most commonly used procedure to generate the Green's function with a tensor network but for a quantum computer [13, 14].

Because the quantum wavefunction will not be affected by the same limits as the classical algorithms, the quantum advantage here is an exponential reduction in memory required, not necessarily a speedup in time [26]. Although, the reduced memory may be argued to give a speedup in time since the equivalent classical wavefunctions would need to be exponentially large.

Conclusion.– Constructing the continued fraction representation of an arbitrary Green's function by implementing Lanczos recursion on a quantum computer is shown to efficiently generate the coefficients necessary with a quantum counting algorithm. This method is an exponential improvement in terms of memory storage in comparison with classical methods, and the method preserves the wavefunction for the next computation.

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