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An alternative implementation of the Lanczos algorithm for wavefunction propagation

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Abstract

We reformulate the Lanczos algorithm for quantum wavefunction propagation in terms of the variational principle. By including some basis states of previous time steps in the variational subspace, the resultant accuracy increases by several orders. Numerical errors of the alternative method accumulate much slower than that of the original Lanczos method. There is almost no extra numeric cost for the gaining of the accuracy, i.e., the accuracy increase needs no extra operations of the Hamiltonian acting on state vectors, which are the major numeric cost for wavefunction propagation. A wave packet moving in a two-dimensional Hénon–Heiles model serves as an illustration. This method is suitable for small time step propagation of quantum wavefunctions in large-scale time-dependent calculations where the operations of the Hamiltonian acting on state vectors are expensive.

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1. Introduction

Propagation of quantum wavefunctions, i.e., direct integration of the time-dependent Schrödinger equation, is a fundamental numeric task. This time-dependent method exhibits many numeric advantages in first-principle calculations. For example, one is able to extract an energy spectrum efficiently from the correlation function via Fourier transformation [1] or a more advanced filter diagonalization algorithm [2]. The efficiency is more evident when one needs an excited energy spectrum in large-scale first-principle calculations.

For wavefunction propagation, the most expansive numeric operations are products of the Hamiltonian matrix and state vectors, namely, the Hamiltonian operator acting on state vectors. It is a long-standing effort to develop an efficient algorithm for wavefunction propagation that uses the minimum number of such matrix–vector product operations.

Among the popular algorithms, such as the split operator method [1, 3, 4] and the Chebyshev expansion method [5], the Lanczos method [6–8] is a robust and flexible scheme

for wavefunction propagation [9]. This method is in principle applicable to any kind of system, including the time-dependent Hamiltonian [10], and there is virtually no need for preparing knowledge about the considered system to apply the Lanczos method. Furthermore, the performance of the Lanczos method is relatively insensitive to the considered system and the initial wavefunction. In many cases, the Lanczos method is the best choice to do time-dependent calculations. For example, if one needs to compute a quantity (such as the entropy of a subsystem) changing continuously with time, and the corresponding Hamiltonian is not suitable to break into two parts to apply the split operator algorithm, one may consider employing the Lanczos method for the task.

The Lanczos algorithm transforms a Hermitian matrix into a tri-diagonal form iteratively [11]. It has many applications in first-principle calculations, see e.g. [12–15]. The basic idea of wavefunction propagation by the Lanczos method is to solve the Schrödinger equation for a given small time step in a low-dimensional subspace, namely, the Krylov subspace. The basis states of the Krylov subspace, $\{\psi_0, \ldots, \psi_m\}$, are generated by the Lanczos iteration, $H\psi_j = \beta_{j-1}\psi_{j-1} + \alpha_i\psi_i + \beta_i\psi_{i+1}$, where $\alpha_i = \langle\psi_i|H|\psi_i\rangle$ is the expectation value of the Hamiltonian H with respect to the vector $|\psi_i\rangle$, β_i is the norm of the vector $H\psi_i - \beta_{i-1}\psi_{i-1} - \alpha_i\psi_i$ with $\beta_0 = 0$ and ψ_0 being the wavefunction obtained from the previous step.

The dimension of the Krylov subspace is usually less than 10 in most cases. This dimension depends on the time step and the accuracy requirement. Higher accuracy needs either a small time step or a large Krylov subspace. For a given dimension of the Krylov subspace, the error accumulates linearly with time in the Lanczos method [9]. If one needs a wavefunction in a longer time scale, one must increase the accuracy of each time step to keep the error of the final wavefunction within the required range. This means that the numeric operations are not simply linearly proportional to the time. There is an optimal choice for the dimension of the Krylov subspace and the time step to reach the accuracy requirement of the final state. However, practical situations, e.g. calculations of correlation function, often need other time steps.

The dimension of the Krylov subspace, or the number of matrix–vector product operations in a time step, is a key factor effecting the numeric cost for the Lanczos propagation scheme. Like other algorithms, the operations of the Hamiltonian acting on the state vectors are the major numerical cost of the Lanczos propagation scheme. Higher accuracy demands more such Hamiltonian operations. From the viewpoint of efficiency, one should keep the number of Hamiltonian operations as small as possible for a given time step and accuracy requirement.

In this paper, we present an alternative to the Lanczos method. It can improve the accuracy by several orders without extra matrix–vector product operations. To this end, we reformulate the Lanczos method in terms of the variational principle with the Krylov subspace being the variational subspace. The basic idea of improvement is to enlarge the variational subspace by including basis states of previous time steps in the variational subspace. Since the required matrix elements are already calculated in previous time steps, such an enlargement of the variational subspace has virtually no extra numeric cost. In fact, including basis states of previous steps in the variational subspace is an efficient method for iteratively diagonalizing a large matrix [16–18].

2. Variational approach to the Lanczos propagation scheme

We first note that one is able to formulate the Lanczos propagation scheme from the variational principle. For short time Δt, one can approximate the evolution operator $U(t) = \exp(-\mathrm{i}H\Delta t/\hbar)$ by a polynomial of the Hamiltonian operator H. In other words,

one can approximate the wavefunction at time $t + \Delta t$, $\psi(t + \Delta t) = U(\Delta t)\psi(t)$, by a vector in the Krylov subspace spanned by $\{H^i\psi(t), i = 0, 1, \ldots, n-1\}$,

$$\psi(t + \Delta t) = \sum_{i=0}^{n-1} c_i H^i \psi(t). \tag{1}$$

The expansion coefficients c_i are yet to be determined by the variational principle,

$$\frac{\delta}{\delta c_i}\langle\psi(t + \Delta t)|\mathrm{i}\hbar\frac{\partial}{\partial t} - H|\psi(t + \Delta t)\rangle = 0. \tag{2}$$

One solves the resultant equation of motion to obtain the expansion coefficients. Instead of $\{H^i\psi(t)\}$, the basis states in the original Lanczos scheme are generated by the Lanczos iteration, and the resultant Hamiltonian matrix in the variational subspace is tri-diagonal. Of course, the subspace generated by the Lanczos iteration is the same as that spanned by states $\{H^i\psi(t)\}$.

Another way of arriving at ansatz (1) is to relate $H^i\psi(t)$ with the ith-order derivatives of the state $\psi(t)$ with respect to the time, $\mathrm{i}\hbar\frac{\partial^i}{\partial t^i}\psi(t) = H^i\psi(t)$. One can approximate the state at time $t + \Delta t$, $\psi(t + \Delta t)$, by a linear combination of the state $\psi(t)$ and its derivatives up to order n. Such an observation may be useful for time-dependent systems.

A direct way to improve the accuracy of the Lanczos propagation scheme is to enlarge the variational subspace, i.e., adding more states into the basis states of the variational subspace. This usually means more numerical operations of the matrix–vector product to obtain the basis states and the corresponding matrix elements of the Hamiltonian. However, there exists a way to enlarge the variational subspace with virtually no extra numeric cost.

We achieve this by making use of matrix–vector product operations of previous steps. To this end, we first note that one can propagate a wavefunction backward from $\psi(t)$ to $\psi(t-\Delta t)$. In other words, a wavefunction at time $t-\Delta t$, $\psi(t-\Delta t)$, is approximately a linear combination of states $\{H^i\psi(t), i = 0, \ldots, m\}$. Here m is the number of matrix–vector product operations in a time step. At time t, we already have states $H^k\psi(t - \Delta t), k = 0, 1, \ldots, m$. Each of these states is approximately equivalent to a linear combination of states $\{H^{k+i}\psi(t), i = 0, 1, \ldots, m\}$. If one includes some of these states into the variational subspace, one has effectively products of higher order power of the Hamiltonian acting on the state vector $\psi(t)$. Using the same arguments, one can also include $H^k\psi(t - 2\Delta t)$, $H^k\psi(t - 3\Delta t)$, $\ldots$, into the variational subspace.

Implementation of the above scheme is straightforward. It involves similar procedures as that of the original Lanczos propagation scheme. Each step of propagation is to solve the Schrödinger equation in the variational subspace. The variational subspace is spanned by the basis states of the original Krylov subspace, $H^i\psi(t)$, and some basis states of previous time steps, $H^i\psi(t-k\Delta t)$. The solution of the Schrödinger equation in the variational subspace determines the expansion coefficients of the next step's wavefunction with respect to the basis states of the variational subspace. The practical calculation includes the following steps:

(1) Choose the time step Δt and the dimension of the variational subspace, n, as well as the number of matrix–vector product operations, m, for each step. The basis states of the variational subspace are $\phi_k^{(i)} = H^i\psi(t - k\Delta t)$ with $i = 0, 1, \ldots, m, k = 0, 1, \ldots, K$. Here $m < n$, and $\psi(t)$ is the current state at time t. For practical applications, it is enough to set $K = 1$ and $n < 2m$, i.e., one usually needs only some of last step's basis states to form the variational subspace. In our implementation of choosing previous time steps' basis states, the order is $H^m\psi(t - \Delta t)$, $H^{m-1}\psi(t - \Delta t)$, $\ldots$. This is because that $H^m\psi(t - \Delta t)$ is closer to $H^i\psi(t)$, $(i > m)$, than other states and has less overlap with the basis states of the original Krylov subspace, $H^i\psi(t)(i \leqslant m)$.

(2) Calculate the matrix–vector products $\phi_0^{(i)} = H^i\psi(t), i = 1, \ldots, m+1$. These states and some states obtained in previous time steps form the basis states, $\phi_k^{(i)} = H^i\psi(t - k\Delta t)$, of the variational subspace. Here $\phi_0^{(m+1)}$ is only for calculation of the Hamiltonian's matrix elements in the variational subspace. Calculation of the $m+1$ matrix–vector products in this step consumes the major CPU time of the whole procedure.

(3) Calculate the matrix elements of the Hamiltonian in the variational subspace, $\mathcal{H}_{ik,jl} = \langle\Phi_k^{(i)}|H|\Phi_l^{(j)}\rangle = \langle\Phi_k^{(i)}|\phi_l^{(j+1)}\rangle$, and the overlap between the basis states, $\mathcal{S}_{ik,jl} = \langle\Phi_k^{(i)}|\Phi_l^{(j)}\rangle$. Here $\Phi_k^{(i)}$ is the normalized form of $\phi_k^{(i)}$. For indices $k > 0, l > 0$, the matrix elements of $\mathcal{H}$ and $\mathcal{S}$ are already calculated in previous time steps, one needs only to calculate the terms $\mathcal{H}_{i0,j0}$ and $\mathcal{S}_{i0,j0}$ in this step. The trade-off of reusing the previous steps' matrix elements is that the basis states are not orthogonal with each other.

(4) Solve the Schrödinger equation in the variational subspace

$$\mathrm{i}\hbar\mathcal{S}\frac{\mathrm{d}}{\mathrm{d}t}C = \mathcal{H}C \tag{3}$$

to obtain the expansion coefficients $C = \left(c_0^{(0)}, \ldots, c_k^{(i)}, \ldots\right)^T$ of the next time step's wavefunction with respect to the basis states $\Phi_k^{(i)}$. The computation cost in this step is negligibly small in comparison with other step's operations.

(5) Perform linear combination of the basis states to form the next step's wavefunction

$$\psi(t + \Delta t) = \sum_{i,k} c_k^{(i)}\Phi_k^{(i)}. \tag{4}$$

At the first time step, $t = 0$, there are no previous basis states. All the basis states are formed by states $H^i\psi_0, i = 0, 1, \ldots, n-1$, with ψ_0 being the initial state. In the next step, we remove the first $m+1$ states $\psi_0, H\psi_0, \ldots, H^m\psi_0$ from the basis states and add another $m+1$ states $\psi(\Delta t), H\psi(\Delta t), \ldots, H^m\psi(\Delta t)$ into the basis states. In following time steps, we update the basis states of the variational subspace in the same way, i.e., replacing $m+1$ oldest basis states with states $\{H^i\psi(t), i = 0, \ldots, m\}$.

In the case of $n = m + 1$, i.e., the variational subspace including no previous time step's basis states, the above procedure is essentially the same as the original Lanczos propagation scheme. In such a case, numerical cost, storage requirement and resulted accuracy are indeed the same as the original one. In the original Lanczos scheme, the Hamiltonian matrix in the variational subspace is tri-diagonal and the overlap matrix is unit. Since the dimension of the variational subspace is usually small, such a difference results in virtually no extra numerical cost. Similar to the original Lanczos scheme, the above procedure is more suitable for small time step propagation which needs only small variational subspace.

The storage requirement is also similar to the original Lanczos scheme. One needs to store the basis states of the variational subspace, as well as information about the Hamiltonian. Other information, such as matrix elements of the Hamiltonian in the variational subspace and the overlap matrix, need little memory.

For a given time step and accuracy requirement, there is an optimal choice of the dimension, n, of the variational subspace and the number, m, of the matrix–vector product operations in a time step. If m is inadequately small, i.e., one includes too many previous time steps' basis states into the variational subspace, the overlap matrix may become singular. This means that there is a limit accuracy for a given time step Δt and the number of matrix–vector product operations in a time step. We use this property of the overlap matrix to determine the dimension n for a given m and Δt.

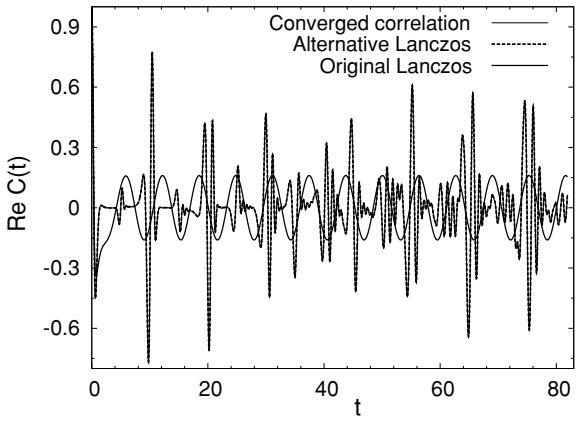

Figure 1. Real part of auto-correlation function changes with the time. The thin solid line is a well-converged result. The dashed and thick solid lines are results of the alternative and original Lanczos methods, respectively. Each time step uses two matrix–vector product operations for both dashed and thick solid lines.

3. Numerical results

We test the performance of the alternative Lanczos method via the Hénon–Heiles model. It is a particle of unit mass moving in the two-dimensional Hénon–Heiles potential [19], $v(x, y) = \frac{1}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2\right) + \lambda y(x^2 + \eta y^2)$, where $\omega_x = 1.3, \omega_y = 0.7, \lambda = -0.1, \eta = 0.1$, and the Planck constant is set to 1. This system has a chaotic classical limit. It is widely used to study the quantum-classical correspondence. Similar to [9], we estimate the accuracy of the current method by the overlap between the numeric result and the 'exact' result. We obtain the 'exact' result via the Chebyshev expansion method [5]. The Chebyshev method is a global propagator that can reach an accuracy of the machine's limit with a single time step.

In figure 1, we show the auto-correlation function $\langle\psi(t)|\psi(0)\rangle$, i.e., overlap between the initial state $\psi(0)$ and the state at time t, $\psi(t)$. The initial state is a Gaussian wave packet whose centre positions are $(2.0, 2.0)$, and centre momenta vanish. We use a 64×64 grid to represent the two-dimensional wavefunction in spatial representation. The action of momentum operator on the state is performed via fast Fourier transformation (FFT) to transform the state into momentum representation. Thus, the action of the Hamiltonian operator on a state vector needs two FFTs to transform the state back and forth between coordinate and momentum representations. Such a matrix–vector product operation is the major numerical cost of the wavefunction propagation. The thin solid line in figure 1 is a well-converged result for comparison. The dashed line is result of the alternative Lanczos method and the thick solid line is result of the original Lanczos method. Both the original and alternative Lanczos methods use two matrix–vector product operations in one time step to obtain the auto-correlation function in figure 1. The time step is $\Delta t = 0.02$. It is evident that two matrix–vector product operations are not enough to converge for the original Lanczos method. In fact, one needs at least four to five matrix–vector product operations in a time step to make the original Lanczos method converge. On the other hand, the dashed line from the alternative Lanczos method is almost indistinguishable from the well-converged result. Here we include eight previous basis states, $\{H^i\psi(t - k\Delta t), i = 0, 1, 2, k = 1, 2, 3\}$, into the variational subspace ($\psi(t - 3\Delta t)$ is not included). The total dimension of the variational subspace is 11.

By reducing the time step to $\Delta t = 0.01$, one can obtain the above converged auto-correlation with only a single matrix–vector product operation in a time step. For such a time step, we achieve similar accuracy as that in figure 1 by including five previous time steps' basis states into the variational subspace. In contrast, for such a time step and accuracy, the original Lanczos method still needs about three to four matrix–vector products in one time step.

Generally, one can increase the accuracy with virtually no extra numeric cost by including more previous basis states into the variational subspace. However, in calculation of figure 1, including more than eight previous basis states makes the overlap matrix singular, i.e., the basis states are no longer independent from each other. In fact, for a given time step Δt and the number m of matrix–vector product in a time step, there is always a limit number of previous basis states that one can include into the variational subspace. In other words, the time step Δt and the number m determine the limit of accuracy.

In our test calculations of figure 1, the overlap matrix becomes singular occasionally. When this happens, one can simply remove the non-independent basis vectors. This can be done by, e.g., the Cholesky decomposition of the overlap matrix. In our implementations, we replace each non-independent vector by one more state $H^i\psi(t)$ of the Krylov subspace. Such a treatment preserves the accuracy at the expense of one extra matrix–vector product operation.

Practical implementation of the alternative Lanczos method is indeed more stable and robust than the calculation of figure 1. In fact, the calculation of figure 1 includes several previous time steps' basis states into the variational subspace. This treatment almost reaches the accuracy limit with two matrix–vector product operations in a time step. Practically, one needs only including some of last step's basis states into the variational subspace. This can increase the accuracy by several orders with virtually no extra numeric cost. The overlap matrix, and thus the whole numeric procedures, is usually well behaved.

Figure 2 shows that the numeric errors accumulate with time for situations similar to practical calculations. The solid lines are results of the alternative Lanczos method and the dashed lines are results of the corresponding original Lanczos method which uses the same number of matrix–vector product operations. Same as [9], we use the overlap between the numeric result ψ_{numeric} and the 'exact' result ψ_{exact} as the measure of error,

$$\mathrm{E_{rr}} = 1 - \langle\psi_{\text{exact}}|\psi_{\text{numeric}}\rangle. \tag{5}$$

We obtain the 'exact' state vector by the Chebyshev expansion method with an accuracy of the machine's limit. We propagate the 'exact' states with a time step $\Delta t = 4$ and use 1024 Chebyshev polynomials to expand the evolution operator $\exp(-\mathrm{i}H\Delta t/\hbar)$. This is well beyond the accuracy requirement of the machine's limit. From our tests, 512 Chebyshev polynomials are indeed enough for a well converged result. From top to bottom of figure 2, N is the total dimension of the variational subspace for the alternative Lanczos method and m is the number of matrix–vector product operations in a time step for both methods. The time step is set to $\Delta t = 0.02$ for both methods. The initial states, as well as states' representation, are the same as that of figure 1. It is easy to see that the behaviour of the original Lanczos method is similar to that described in [9], i.e., the error accumulates about linearly with the time t and the accuracy increases quickly with the number m.

It is evident that, when including some of last step's basis states into the variational subspace, the accuracy improves drastically. We see that, for $m = 5$, the alternative method is about five orders more accurate than the original one after time $t \approx 10^3$. And for $m = 6$, the alternative method is about four orders more accurate after time $t \approx 5 \times 10^3$. The original method is well converged within the time scale $t < 10^4$ for $m = 7$. Even so, the alternative

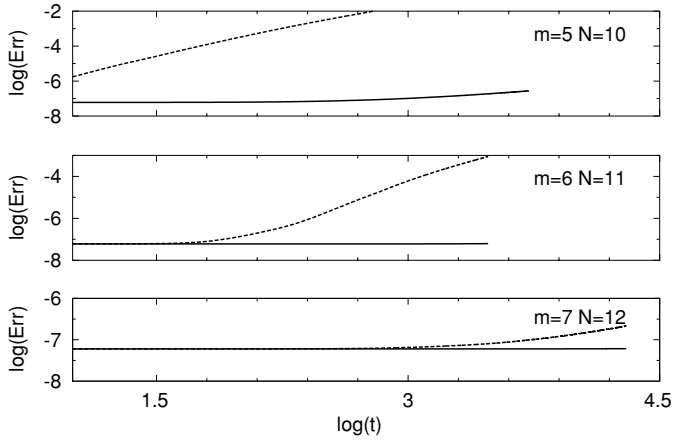

Figure 2. Logarithms, base 10, of numeric errors, Err, accumulate with the logarithmic time t. Solid and dashed lines are the alternative and original Lanczos methods, respectively. m denotes the number of matrix–vector product operations in a time step for both methods and N is the dimension of the variational subspace for the alternative method.

method is still about one order more accurate after time $t \approx 2 \times 10^4$. Another encouraging property of the alternative method is that its error accumulates much slower than the original one. This means that numeric result of the alternative method is more reliable in long time scale.

From figure 2 and other test calculations, we conclude that the alternative Lanczos method is suitable for small step wavefunction propagation. It improves the accuracy by several orders with almost no extra numeric cost. In calculation of figure 2, the variational subspace is about ten dimensional and includes only four last step's basis states. For such a setting, the resultant overlap matrix and thus the overall numeric procedure is well behaved. In fact, the included basis states, $H^i\psi(t-\Delta t)$, from the previous step play the role of high-order power of the Hamiltonian acting on the state vector, $H^i\psi(t)$, of the original Lanczos method. From the dashed lines in figure 2, we see that basis states, $H^i\psi(t)$ $(i = 0, 1, \ldots, m)$, of the original Lanczos method span the major part ($> 99\%$) of the exact wavefunction $\psi(t+\Delta t)$. Other basis states, $H^i\psi(t-\Delta t)$, included from the previous step span only a very small portion ($<1\%$) of the exact wavefunction. Thus, these included basis states $H^i\psi(t-\Delta t)$ have a relatively lower accuracy requirement to represent the high-order terms $H^i\psi(t)$ $(i > m)$. This explains the success of the alternative method.

In general, implementation of the alternative method is stable and robust, provided that the basis states $\{H^i\psi(t)\}$ span the major part of the next step's wavefunction $\psi(t+\Delta t)$. In fact, for a given time step Δt, the accuracy of both the alternative and original Lanczos methods is determined by the dimension of the variational subspace n. One chooses Δt and n in the same way as that of the original Lanczos algorithm. In the alternative implementation, one must specify additionally the number, m, of matrix–vector production in a time step. It is usually enough to set m larger than half of n, i.e., $n/2 < m < n$. If m is too small, and one includes too many basis states, $\{H^i\psi(t-k\Delta t)\}$, of previous steps into the variational subspace, these basis states may be not independent. Even if this happens, the alternative method still works. If a basis state from the previous step is linearly dependent on other basis states of the variational subspace, we replace this state by an extra state $H^i\psi(t)$ with $i > m$. This keeps the dimension of the variational subspace, and hence the accuracy of the implementation. The

expense of such a treatment is one more matrix–vector product operation for each linearly dependent state. We implement this treatment during the Cholesky decomposition of the matrix $\mathcal{S}$ which is a necessary step to solve equation (3). When the basis states are linearly dependent, the overlap matrix $\mathcal{S}$ becomes singular. The Cholesky decomposition of $\mathcal{S}$ can find all the non-independent states. By properly specifying the threshold value of the Cholesky decomposition, this numerically cheap operation can even find the states that are close to linear superposition of other basis states.

4. Conclusions

In summary, we present an alternative to the Lanczos method for quantum wavefunction propagation in terms of the variational principle. This method approximates short time evolution operator, $U(t) = \exp(-\mathrm{i}H\Delta t/\hbar)$, by a polynomial of the Hamiltonian. In other words, the wavefunction $\psi(t + \Delta t)$, resulted from a small time step propagation from $\psi(t)$, $\psi(t + \Delta t) = U(\Delta t)\psi(t)$, is approximately a vector in the Krylov subspace spanned by $\{H^i\psi(t), i = 0, \ldots, n - 1\}$. One can employ the variational principle to determine the expansion coefficients. The original Lanczos method needs to calculate all the basis states $H^i\psi(t)$ explicitly. Construction of these basis states is the major numeric cost. The alternative method needs only to calculate some of the basis states, $H^i\psi(t), i = 0, \ldots, m$, which span the major part of the wavefunction $\psi(t + \Delta t)$. We use basis states of the previous step to play the role of the other basis states, $H^i\psi(t), i > m$. Practically, it is enough to include some of last step's basis states, $H^i\psi(t - \Delta t), i \leqslant m$, into the variational subspace. The accuracy of the alternative method is several orders higher than the original Lanczos method with same matrix–vector product operations in a time step.

This alternative method is especially efficient for small time step wavefunction propagation. The error accumulation in the alternative method is much slower than that in the original Lanczos method, which increases about linearly with time. The efficiency of the alternative method comes from the fact that the basis states included from previous steps only span very small portion of the wavefunction, and thus the accuracy requirement for construction of these basis states is relatively lower. This alternative method has useful applications in large-scale time-dependent calculations in which the numeric cost for the Hamiltonian acting on state vectors is expensive.

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