Loschmidt echo approach to Krylov-subspace approximation error estimation

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The Krylov subspace method is a standard approach to approximate quantum evolution, allowing to treat systems with large Hilbert spaces. Although its application is general, and suitable for many-body systems, estimation of the committed error is involved. This makes it difficult to automate its use. In this paper, we solve this problem by realizing that such error can be regarded as a Loschmidt echo in a tight-binding Hamiltonian. We show that the different time-regimes of the approximation can be understood using simple physical ideas. More importantly, we obtain computationally cheap error bounds that describe with high precision the actual error in the approximation.

I. INTRODUCTION

Transmitting and processing information in quantum devices has been established in recent years [1]. Laboratories around the world are in the race to develop increasingly accurate quantum devices. To carry out this successfully, it is necessary to test their operation on classical devices. For this reason, it is important to have efficient classical algorithms to perform quantum simulation [2–3].

Several approaches for the efficient computation of quantum time-evolution have been proposed in the literature [4–8]. The cost of the simulation usually depends on specifics of the system, e.g. the initial state, or on the information that we want to know about the dynamics. For example, the cost of the simulation can be greatly reduced if the amount of entanglement developed by the system remains bounded [7–8]. Less restrictive are the well-known Krylov-subspace methods, constructed to provide approximations to the action of the exponential of a classical matrix on a vector. In the context of quantum simulation, the mechanics of the approximation is the following: an initial state that is localized at one end. The error is related to an echo between evolutions in a virtual chain, where the error in the approximation is approximated by the population in the other end of the chain. Later, Saad [12] derived computable estimates of the error using an expansion in the Krylov subspace exploiting the Lanczos algorithm. Other error bounds include involved computations making it difficult to use in an operational way [14].

The goal of this paper is to find tight and computationally inexpensive error bounds for the approximation error in Krylov schemes. We take advantage of a simple observation: the error can be regarded as a Loschmidt echo in which both the forward and backward evolutions are given by tight-binding Hamiltonians. In a virtual chain, we have an initial state that is localized at one end. The error is related to an echo between evolutions in a D site chain and a trimmed N << D chain, where N is the dimension of the truncated Krylov subspace used for the approximation. This analogy allows us to describe the time-regimes of the error using Loschmidt echo theory. In particular, we show that the error remains negligible up to some time at which it starts building up exponentially. This time is related to the effective traveling wave-packet’s tail hitting the end of the virtual chain [11]. The core of our proposal is that the error in this regime can be captured remarkably well by replacing the full-size backwards evolution with one of a chain with only an single extra site. This provides an accurate and cheap bound for the error.

Moreover, we show that one can analytically solve for the bound in the case in which the tight-binding Hamiltonian has homogeneous diagonal and off-diagonal elements. We test this solution in a 1-D Ising spin chain with transverse magnetic field. Finally, we give some physical insight explaining why this simple model works in the general case.

The paper is organized as follows. In Sec. [11] we intro-
duce the general framework of the Krylov-subspace method for quantum time evolution. Next, in Section III we describe the different time-regimes of the error, focusing on the analogy with Loschmidt echo dynamics under tight-binding Hamiltonians. In section IV, we use the connection between the error and the Loschmidt echo of tight-binding Hamiltonians to propose a bound that describes extremely well the inaccuracy of the approximate evolution in the Krylov subspace. Finally, in Section V we offer some final remarks. Appendix A provides a brief description of Lanczos algorithm and in Appendix B we describe the system used for the numerical simulations, a 1-D Ising spin chain with transverse magnetic field. In Appendix C the error bound is analytically solved for the simple case in which the tight-binding Hamiltonian has homogeneous diagonal and non-diagonal elements.

II. THE KRYLOV-SUBSPACE METHOD

Let us start by reviewing the so-called Krylov-subspace method for approximating quantum dynamics. Consider a state |ψ⟩, in a D-dimensional Hilbert space ℋ = ℂD, that evolves under a time-independent Hamiltonian H. The N-dimensional Krylov subspace associated with |ψ⟩ and H is given by

$$K_N = \text{span}\{ |ψ⟩, H|ψ⟩, \ldots, H^{N-1}|ψ⟩ \}$$

(1)

Here, without loss of generality, we consider that H and |ψ⟩ share no symmetries, i.e., such that $K_D = ℋ$. If they did share some symmetry, time evolution would occur constrained to a symmetry subspace, say $ℋ_j ⊂ ℋ$, in which case one can always redefine the problem to belong within that subspace, e.g., $ℋ ← ℋ_j$.

The Krylov approach aims at approximating the time-evolved state |ψ(t)⟩ with the best element $|ψ_N(t)⟩ ⊂ K_N$. To do so, we first have to build an orthonormal basis for $K_N$, $B_N = \{ |v_0⟩ ≡ |ψ⟩, \ldots, |v_{N-1}⟩ \}$. This is usually done using Lanczos’s algorithm, a sort of Gram-Schmidt procedure that harnesses the fact that orthonormalization only needs to be enforced with respect to the last two vectors in the basis (see Appendix A). Once we have a basis for $K_N$, we can get an approximation for $|ψ(t)⟩$ by projecting it into this basis (see Fig. 1(a) for a schematic representation of the method)

$$|ψ(t)⟩ = e^{-iHt} |ψ⟩ ≈ P_N e^{-iHt}P_N |ψ⟩$$

$$= \mathcal{V}_N e^{-i\mathcal{H}_N t} \mathcal{V}_N |ψ⟩$$

$$≡ |ψ_N(t)⟩$$

(2)

Here, $T_N = \mathcal{V}_N H \mathcal{V}_N^\dagger$ is the Hamiltonian reduced to the subspace, $\mathcal{V}_N$ and

$$\mathcal{V}_N = \begin{bmatrix}
|v_0⟩ & |v_1⟩ & |v_{N-1}⟩
\end{bmatrix}$$

(3)

are the reduction-to-the-subspace operators, and $P_N = \mathcal{V}_N^\dagger \mathcal{V}_N$ the projector onto it. By definition, $\mathcal{V}_N$ maps any initial state into the first coordinate vector of an effective N-dimensional system, $\mathcal{V}_N |ψ⟩ = (1, 0, \ldots, 0)^T ≡ |0⟩_N$. It is especially relevant to notice that the Hamiltonian reduced to a Krylov subspace is tridiagonal

$$T_N = \begin{pmatrix}
α_1 & β_1 & 0 & \cdots & 0 \\
β_1 & α_2 & β_2 & \cdots & 0 \\
0 & β_2 & α_3 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & α_N
\end{pmatrix}$$

(4)

and thus, this effective system has the form of a tight-binding model. An initial state localized in one end of an effective chain evolves according to $T_N$ (i.e. with onsite potential $α_i$ and hopping amplitude $β_i$ at the ith site) propagating the excitation and populating the rest of the lattice (see Fig. 1(b) for a schematic representation). Finally, $\mathcal{V}_N$ maps the effective evolved state back to full Hilbert space. The efficiency of the method resides in the fact that the time evolution is solved “cheaply” in the reduced space, i.e., one replaces the exponential of a $D × D$ Hermitian matrix $H$ with the much more economical exponential of a $N × N$ symmetric tridiagonal $T_N$. Of course, the assumption is that $N << D$.

The challenge in this approximate evolution scheme is to keep the error bounded by a given tolerance. This has been studied in different ways for more than three decades [11-17]. In the next Section, we show that the error as a function of time has regimes that can be well understood using physical ideas based on Loschmidt echo theory and diffusion in a tight-binding model [18].

III. TIME REGIMES OF THE ERROR

Let us review the time regimes of the error in the Krylov-subspace method. This error is given by the instantaneous infidelity between exact and approximate evolved states

$$ε_N(t) = 1 - | \langle ψ_N(t) | ψ(t) \rangle |^2$$

(5)
evolved state is where one can regard as "cutting" the chain at site (not depicted in the image). Using a truncated Lanczos basis, chain. Here, the off-diagonal elements of Lanczos tridiagonal completely localized at the leftmost end of a virtual tight-binding dynamics of \( \alpha \) sites and the diagonal elements corresponds to the diffusion of an initial state \( \psi \) on Hilbert space \( \mathcal{H} \). Any actual implementation of the approximation method has to keep track of this error. Yet, of course, it’s exact computation is out of question since it involves solving the problem one is trying to approximate, \( \psi(t) \).

A closer inspection of Eq. (5) allows for an interesting interpretation. Rewriting the overlap as

\[
|\langle \psi_N(t) | \psi(t) \rangle |^2 = | \langle \psi | \nabla_N^T e^{-iT_N t} \nabla_N e^{-iH t} | \psi \rangle |^2 = | \langle \psi | \nabla_N^T e^{-iT_N t} \nabla_N \nabla_D e^{-iT_D t} \nabla_D | \psi \rangle |^2 = | \langle \psi | \nabla_D e^{-iT_N t} e^{-iT_D t} \nabla_D | \psi \rangle |^2 = | \langle \psi | \nabla_D e^{-iT_D t} | \psi \rangle |^2
\]

where \( \hat{T}_N = \nabla_D P_N H P_N \nabla_D \) has the form

\[
\hat{T}_N = \begin{pmatrix} T_N & 0 \\ 0 & 0 \end{pmatrix}
\]

one can realize that \( 1 - \epsilon_N(t) \) has the form of a Loschmidt echo \( [18] \) in which the backwards and forward evolutions are given by tight-binding Hamiltonians. We start with \( |0\rangle \equiv \nabla_D |\psi\rangle \), a completely localized state at one end of the virtual chain. This state evolves subject to \( T_D \) for some time \( t \), then evolves backwards subject to \( T_N \) (a perturbed \( T_D \) where the effective onsite potentials and hoppings of sites \( N+1, \ldots, D \) are turned off) and is finally overlapped.

The Loschmidt echo has been widely studied as a measure of the revival occurring after a forward and backward time evolutions generated by two slightly different Hamiltonians \( [18, 20] \). As far as we know, the case of tight-binding Hamiltonians has not been explicitly considered in the literature so far. We note that one of the evolutions is done with a chain of length \( D \) and the other evolution corresponds to the case in which the chain is cut at site \( N \) (the hoppings and onsite potentials at the second part of the chain are set to zero, i.e. \( \alpha_i = 0 \) and \( \beta_i = 0 \) for \( i = N+1, \ldots, D \)).

In order to gain insight on the time regimes of the approximation, we show in Fig. 2 the Loschmidt echo \( |\langle \psi_N(t) | \psi(t) \rangle |^2 \) (top panel) and the error \( \epsilon_N(t) \) (bottom panel) for an Ising spin chain with 10 sites and a transverse magnetic field (see Sec. [14] for more details). We use a Krylov-subspace of \( N = 30 \) sites and a random initial state \( |\psi\rangle \). We can clearly see that the Loschmidt echo has two very different time regimes. Until \( t \approx t_{col} \) the echo remains roughly one, and the approximate evolution faithfully captures the exact one. After this first "faithful" regime, an abrupt decrease is observed and from there on it decays in a monotonous way.

In this first time-regime \( t < t_{col} \) where the echo practically does not change, the error has two relevant regimes. First, until some time \( t < t_{exp} \), the error is essentially zero. Then, at \( t = t_{exp} \) the error suddenly starts to build-up exponentially. This is related to the tail of the wave-packet starting to impact on the end of the chain. The interval \( t_{exp} < t < t_{col} \) is precisely the region that we have to be able to correctly approximate in order to have a good error bound. We note that the noisy plateau of \( \epsilon_N(t) \) for \( t < t_{exp} \) is due to round-off errors in the floating-point arithmetic used in the computations.

In order to understand the time regimes of Fig. 2 we plot in Fig. 3 the square of the amplitudes in the Lanczos basis for both the exact and approximate evolved states of Eq. (6), i.e. \( |\langle v_i | \psi_N(t) \rangle |^2 \) and \( |\langle v_i | \psi_D(t) \rangle |^2 \) for \( i = 1, \ldots, N \) and \( i = 1, \ldots, D \) respectively. We provide snapshots of this virtual travelling wave-packets at times \( t = 10, 25, 45 \) and 70. As mentioned before, we start with localized states at one end of the fictitious tight-binding chain. In the first panel of Fig. 3 corresponding to time \( t = 10 \), both wave-packets are travelling to the right and are essentially
equal. However, at \( t = t_{\text{exp}} \approx 25 \), the exponential tail reaches the site \( N = 30 \), and the error starts to build-up rapidly. This process continues until \( t = t_{\text{col}} \approx 42 \), where one of the packets bounces with the end of its chain and starts returning to its original position. This difference in the behavior of the wave-functions is reflected in an abrupt decay of the echo (see Fig. 2). At \( t = 60 \) and \( t = 80 \), the wave packets continuously grow apart and become more and more orthogonal.

Figure 2. **Time regimes of the echo.** Loschmidt echo \( |\langle \psi_N (t) | \psi (t) \rangle |^2 = |\langle \psi_N (t) | \psi_D (t) \rangle |^2 \) (top panel) and error \( \epsilon_N (t) \) (bottom panel) for an Ising spin chain with transverse magnetic field. We use \( N = 30 \) and \( D = 2^n = 1024 \). We have marked with dashed vertical lines the times that correspond to the snapshots shown in Fig. 3. We also highlight the relevant times \( t_{\text{exp}} \) and \( t_{\text{col}} \). The initial state \( |\psi \rangle \) is random state.

Figure 3. **Time evolution of exact and approximate states in the Lanczos basis.** We draw \( |\langle \psi_D (t) | v_i \rangle |^2 \) (black line) and \( |\langle \psi_N (t) | v_i \rangle |^2 \) (solid blue) at times \( t = 10, 25, 42, 60 \) and 80 (top to bottom). Remark: the representation in the figure takes a cubic interpolation between each site to smooth out the discrete sites effect for an easier visualization.

**IV. FROM LOSCHMIDT ECHOES TO ERROR BOUNDS**

In the previous section, we have shown that the error in the Krylov method for quantum evolution can be seen as a Loschmidt echo. Let us now show how this description can help us derive tight and computationally cheap bounds for the error, providing a fundamental tool for any practical implementation of the approximation method.

As we have previously remarked, the time-regime of the error that is relevant for a practical implementation of the approximation method is the one between \( t_{\text{exp}} \) and \( t_{\text{col}} \). In this region, the travelling packet has its center between sites 1 and \( N \), and only a small, exponentially suppressed population tail surpasses the site \( N \). With this in mind, we can ask ourselves: is it really necessary to consider the entire chain to describe the behavior of the error? Given that in the \([N + 1, D]\) region we have exponentially suppressed populations, isn’t it possible to capture the essential features of the error by considering instead an echo where we replace the full chain with one with \( K = N + i \) sites, i.e. where \( i \) is a small number of extra sites? To answer this question, in Fig. 4 we compare the echo \( |\langle \psi_D (t) | \psi (t) \rangle |^2 \) with \( |\langle \psi_N (t) | \psi_K (t) \rangle |^2 \) using \( K = N + 1 \) and \( K = N + 5 \). Here, we can see that both cases accurately capture the important region between \( t_{\text{exp}} \) and \( t_{\text{col}} \) (shaded region of Fig. 4). In the inset of Fig. 4 we plot the error \( \epsilon_{\text{K}} (t) = 1 - |\langle \psi_N (t) | \psi_K (t) \rangle |^2 \) in the shaded region to highlight this last conclusion. This remarkable fact, i.e. that only a singe extra site is enough to capture the behaviour of the error in the relevant region, will be the main building-block of our error bound proposal. Let us note that, although here we have used a spin chain model, the systematic appears to be the same for other fundamentally different systems [21]. We have tested in random Hamiltonians that belong to the Gaussian orthogonal ensamblle (GOE) and Gaussian unitary ensamble (GUE) [22].
Let us suppose that we have computed the Krylov subspace $K_N$ and want to estimate the error in this case. As we have argued in the previous paragraph, one can effectively approximate the error with $|\langle \psi_N(t) | \psi_{N+1}(t) \rangle|^2$. In order to do so, one would have to perform an extra iteration of the Lanczos algorithm, i.e. to compute this extra site approximation $|\psi_{N+1}(t)\rangle$. Alternatively, let us see if it is possible to approximate the new site in the tight-binding chain without having to do such extra iteration. One simple yet effective way of estimating the coefficients of this new site is to average over the previous sites. That is,

$$\alpha_{N+1} \approx \bar{\alpha} = \frac{1}{N} \sum_{i=1}^{N} \alpha_i, \quad \beta_{N+1} \approx \bar{\beta} = \frac{1}{N} \sum_{i=1}^{N} \beta_i \quad (8)$$

Now, we have all the elements needed to test our bound and to compare it with the established bounds in the literature, e.g. of Ref. [12]. In Fig. 5, we show the ratio between the error bounds $\tilde{\varepsilon}_N^{N+1}$ and the actual error $\varepsilon_N$ of Eq. (5). We put a bar on the bound $\tilde{\varepsilon}_N^{N+1}$ to denote that we use the averaged estimation of Eq. (8) for the coefficients of site $N+1$. In the inset of Fig. 5, we shade the region of the bound $\tilde{\varepsilon}_N^{N+1}$ in which the elements $\alpha_{N+1}$ and $\beta_{N+1}$ are the maximum of the minimum of $\alpha_i$ and $\beta_i$ with $i = 1, \ldots, N$. We also show the ratio of the bound of Ref. [12] with the actual error. It can be seen that in both of the bounds proposed the overestimation remains constant throughout the evolution, and quite lower than Ref. [12].

Interestingly, the echo $|\langle \psi_N(t) | \psi_{N+1}(t) \rangle|^2$ can be solved analytically in the particular case of homogeneous coefficients, $\alpha_i = \alpha$ and $\beta_i = \beta \forall i$, which corresponds to the Toeplitz tridiagonal matrix [23] (see appendix C). Using this analytic expression, we compute a new bound $\varepsilon_N^{N+1}$ (with a tilde) where we use Eq. (C6) with $\alpha = \bar{\alpha}$ and $\beta = \bar{\beta}$ in Eq. (8). We show in Fig. 5 that this approximation works also very well.

Let us denote that we use Eq. (8). We show in Fig. 5 that this approximation works also very well.
elegant and simple solution to the error tracking problem. Remarkably, we show that one can capture with extreme precision the behaviour of the error in the relevant region, almost without having to make any extra computations.

Typical implementations of Krylov-subspace methods usually involve a time-stepping schedule [13]. The reason for this is that Lanczos’s Algorithm suffers from instabilities when the basis is too big. Thus, the common workaround is to approximate the evolution using an iterative approach: the actual trajectory in Hilbert space is efficiently followed using a sequence of patches. That is, we build a Krylov-subspace, evolve for a small time, map back and start over. In this framework, our error bounds provide cheap and accurate way of computing optimal time intervals for the time-stepping schedule.

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Appendix A: Lanczos method

The Lanczos method (see Algorithm 1) is a well-known strategy for the construction of \(B_N = \{|v_0\}, \ldots, |v_{N-1}\}\), an orthonormal basis spanning the Krylov subspace \(K_N\). One of the most appealing features of this approach is that, unlike e.g. a Gram-Schmidt procedure where orthonormalization at each step is with respect to the whole current basis, the new candidate vector \(|x_j\rangle\) only needs to be orthonormalized with respect to the previous two basis vectors \(|v_{j-1}\rangle\) and \(|v_{j-2}\rangle\). The reason for this is that the Hamiltonian, by construction, is tridiagonal in the Lanczos Basis (see Eq. (4)).

Algorithm 1: Lanczos Algorithm. Receives state \(|\psi\rangle\) and Hamiltonian \(H\) and returns a set of \(N\) orthonormal vectors \{\(|v_i\rangle\}\) spanning the Krylov subspace \(K_N\).

1. \(|v_0\rangle = |\psi\rangle\) (assume normalized)
2. \(|x_1\rangle = H |\psi\rangle\)
3. \(|\alpha_1\rangle = \langle x_1 | v_0 \rangle\) (the component of \(|x_1\rangle\) in \(|v_0\rangle\))
4. \(|w_1\rangle = |x_1\rangle - \alpha_1 |v_0\rangle\)
5. for \(j = 1,2,\ldots\) do
6. \(\beta_j = \sqrt{\langle \omega_j | \omega_j \rangle}\)
7. if \(\beta_j > 0\) then
8. \(|v_j\rangle \leftarrow \frac{1}{\beta_j} |\omega_j\rangle\)
9. else
10. break
11. \(|x_{j+1}\rangle = H |v_j\rangle\)
12. \(|\alpha_{j+1}\rangle = \langle x_{j+1} | v_j \rangle\)
13. \(|\omega_{j+1}\rangle = |x_{j+1}\rangle - \alpha_{j+1} |v_j\rangle - \beta_j |v_{j-1}\rangle\)

\[ H = \sum_{k=1}^{N} (h_x \sigma_k^x + h_z \sigma_k^z) - J \sum_{k=1}^{N-1} \sigma_k^x \sigma_{k+1}^x, \]  

(B1)

where \(N\) is the total number of spin-1/2 sites of the chain, \(\sigma_k^x\) to the Pauli operator at site \(k = \{1,2,\ldots,N\}\) with direction \(j = \{x,y,z\}\) and \(J\) represents the interaction strength within the site \(k\) and \(k + 1\). The parameters \(h_x\) and \(h_z\) are, respectively, the strength of the magnetic field in the (transverse) \(x\) direction, and in the (parallel) \(z\) direction. We set \(\hbar = 1\), such that energies are measured in units of the interaction strength \(J\), and times in units of \(J^{-1}\).

Appendix C: Analytical solution of the error: special case of homogeneous hopping

We solve here a simplified model for the evolution on the Krylov subspace \(K_N\). Let us assume that after mapping \(|\psi\rangle\) and \(H\) to \(|0\rangle_N\) and \(T_N\), we find a homogeneous tridiagonal matrix,

\[ T_N = \alpha \sum_{n=1}^{N} |n\rangle \langle n| + \beta \sum_{n=1}^{N-1} |n\rangle \langle n+1| + \text{h.c.} \]  

(C1)

Here, \(|n\rangle \equiv |n\rangle_N\) (here and hereafter we drop de subscript) denotes the localized "site" states of the \(N\)-dimensional tight-binding chain associated with the dynamical system \((\psi,H)\). The Hamiltonian in Eq. (C1) corresponds to

Appendix B: Ising spin chain in a transverse magnetic field

Let us describe the system used in the numerical simulations. Consider a 1D Ising spin chain with transverse magnetic field and open boundary conditions, described by,
the so-called Toeplitz tridiagonal matrix \[23\], and has well documented analytical expressions for its eigenstates and eigenenergies,

\[ (n|E_k) = \sqrt{\frac{2}{N+1}} \sin \left( \frac{n k \pi}{N+1} \right), \quad \text{(C2)} \]

and

\[ E_k = \alpha + 2 \beta \cos \left( \frac{n k \pi}{N+1} \right). \quad \text{(C3)} \]

The time evolution of an arbitrary initial state \(|\psi(t=0)\rangle = \sum_{n=1}^{N} c_n |n\rangle\) is given by,

\[ |\psi(t)\rangle = \sum_{n,n'}^{N} c_n S_{n,n'}^{N}(t) |n'\rangle, \quad \text{(C4)} \]

where the transition matrix \(S_{n,n'}^{N}(t)\) is defined as,

\[ S_{n,n'}^{N}(t) = \sqrt{\frac{2}{N+1}} \sum_{k=1}^{N} \sin \left( \frac{n k \pi}{N+1} \right) \sin \left( \frac{n' k \pi}{N+1} \right) e^{i t E_k}. \quad \text{(C5)} \]

Finally, the amplitude of the echo of two time-evolutions with Toeplitz matrices of lengths \(N\) and \(N'\) yields,

\[ \langle 0 | e^{-i t T_N} e^{i t T_{N'}} | 0 \rangle = 1 - \sum_{n=1}^{N'} S_{n,1}^{N}(t) S_{n,1}^{N'}(-t). \quad \text{(C6)} \]

It is clear from Eq. (C3), that the parameter \(\alpha\) will not affect the value of the echo and \(\beta\) acts as a rescaling of time. Thus, one can limit itself to study the behavior of the chain with parameters \(\alpha = 0\) and \(\beta = 1\), and then rescale time by \(\beta t\).

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