Hamiltonian Simulation in the low energy subspace [1]

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Introduction. Simulating the dynamics of quantum systems is believed to be one of the most important and promising applications of quantum computers [2]. A useful method for Hamiltonian simulation is based on product formulas, which approximates the evolution of a Hamiltonian H by short-time evolutions under the terms that compose H [3, 4, 5, 6]. Product formulas are attractive for various reasons: they are simple, intuitive, and their implementations may not require ancillary qubits, which contrasts other sophisticated methods as those in [7, 8]. They are also the basis of classical simulation algorithms including path-integral Monte Carlo [9]. Recent works provide refined error bounds and improved complexities of product formulas [10, 11, 12, 13]. These works regard various settings, such as when H is a sum of spatially-local terms or when these terms satisfy certain Lie-algebraic properties. While these improvements are important, a number of shortcomings remain, especially when we take into account relevant physical constraints. For example, prior to this work, the best-known complexities of product formulas (and other Hamiltonian simulation methods) scale poorly with the norm of H or its terms. This can be very large or unbounded, even when the dynamics occurs in a *low-energy* sector. Further improvements will be then needed to bring quantum simulation closer to reality.

Motivated by these shortcomings, we investigate the Hamiltonian simulation problem when the initial state is supported on a low-energy subspace. This is a central problem with vast applications in many-body physics, quantum field theories, and beyond, where the interesting physics takes place in the low-energy sector. The main questions we address are:

- **Question 1:** Can we improve upon the runtime of existing simulation methods based on product formulas (and other methods) with the low-energy assumption?
- **Question 2:** For which systems can these improvements be attained and what are the resulting complexities in various regimes?

Of particular interest in our work is the simulation of local N-spin systems. In this case, each interaction term in H is of strength bounded by J and involves, at most, k spins. We do not assume that these interactions are only within neighboring spins in a lattice but instead define the degree d as the maximum number of interaction terms that involve any spin. Then, we write $H = \sum_{l=1}^{L} H_l$, where each $H_l \geq 0$ is a sum of M commuting terms [14]. The product formula approximates the evolution operator $U(t) := e^{-itH}$ as a product $\Pi_j e^{-is_j H_{l_j}}$. Each $e^{-is_j H_{l_j}}$ can be further decomposed as products of M evolutions under the local (commuting) terms in H_{l_j} with no error.

Results. Our main result is that, for a local spin Hamiltonian as above, the error induced by a p-th order product formula is $\mathcal{O}((\Delta' s)^{p+1})$, where s is a (short) time parameter and Δ' is an effective low-energy norm of H. This norm depends on Δ, which is an energy associated with the initial state, but also depends on s and other parameters that specify H. The best known error bounds for product formulas that apply to the general case depend on the $\|H_l\|$'s and are also proportional to s^{p+1} [12]. ($\|.\|$ refers to the spectral norm.) Thus, an improvement in the complexity of product formulas is possible when $\Delta' \ll \max_l \|H_l\|$, which occurs for sufficiently small values of Δ and s. Such values of s appear in low-order product formulas (e.g., first order)

Order	Previous result	Low-energy simulation
$p=1$	$\mathcal{O}(\frac{\tau^2 N}{\varepsilon})$	$\tilde{\mathcal{O}}(\frac{\tau^2}{\varepsilon}) + \mathcal{O}(\frac{\tau^{4/3}N^{2/3}}{\varepsilon^{1/3}})$
$p=2$	$\mathcal{O}(\frac{\tau^{3/2}N^{1/2}}{\varepsilon^{1/2}})$	$\tilde{\mathcal{O}}(\frac{\tau^{3/2}}{\varepsilon^{1/2}}) + \mathcal{O}(\frac{\tau^{6/5}N^{3/5}}{\varepsilon^{1/5}})$
$p=3$	$\mathcal{O}(\frac{\tau^{4/3}N^{1/3}}{\varepsilon^{1/3}})$	$\tilde{\mathcal{O}}(\frac{\tau^{4/3}}{\varepsilon^{1/3}}) + \mathcal{O}(\frac{\tau^{8/7}N^{4/7}}{\varepsilon^{1/7}})$

Table 1: Comparison between the best-known complexity [12] and the complexity of low-energy simulation for p-th order product formulas. Results show the Trotter number for constant Δ and local Hamiltonians on N spins with constant degree and strength bounded by J, and $\tau = |t|J$. ε is the approximation error. The $\tilde{\mathcal{O}}$ notation hides polylogarithmic factors in τ/ε.

or, for larger order, when the overall evolution time t is sufficiently large and/or the desired approximation error ε is sufficiently small. More precisely, our main result is:

Theorem 1. *Let $H = \sum_{l=1}^{L} H_l$ be a k-local Hamiltonian as above, $H_l \geq 0$, $\Delta \geq 0$, $0 \leq J|s| \leq 1$, and $W_p(s)$ a p-th order product formula [1]. Then,*

$$\|(U(s) - W_p(s))\Pi_{\leq\Delta}\| = \mathcal{O}((\Delta' s)^{p+1}) \,, \tag{1}$$

where $\Delta' = \Delta + \beta_1 J \log(\beta_2/(J|s|)) + \beta_3 J^2 N|s|$ and the β_i's are positive constants, $\beta_2 \geq 1$.

In general $\Pi_{\leq\Lambda}$ is a projector on the subspace of energies at most Λ. The proof of Thm. 1 is in [1], but the basic idea is as follows: There are two contributions to the error in Eq. (1). One contribution comes from approximating $U(s)$ with a p-th order product formula that involves the effective Hamiltonians $\bar{H}_l := \Pi_{\leq\Delta'} H_l \Pi_{\leq\Delta'}$ and this error is $\mathcal{O}((\Delta'|s|)^{p+1})$, which follows from standard error bounds. The other contribution comes from replacing a product formula involving the $\bar{H}_l$'s by one with the actual Hamiltonians H_l, i.e., by $W_p(s)$. Unlike $\bar{H}_l$, the evolution under each H_l allows for leakage to a subspace of higher energies $> \Delta'$. In [1] we use a result in [15] to prove that this leakage is bounded and exponentially small in $\Delta' - \Delta$. Thus, one can choose a suitable Δ' so that the second contribution to the error is also $\mathcal{O}((\Delta'|s|)^{p+1})$. This Δ' depends on Δ and s, as the support on high-energy states can increase as s increases.

To obtain the complexity of product formulas, given by the Trotter number $r = t/s$, we note that each term of Δ' in Thm. 1 can be dominant depending on s and Δ. The evolution operator is approximated as $U(t) \approx (W_p(s))^r$ and the overall error is given by the union bound; for error ε we need $r(\Delta' s)^{p+1} = \mathcal{O}(\varepsilon)$. This implies (up to logarithmic corrections)

$$r = \tilde{\mathcal{O}}\left(\frac{(t(\Delta + J))^{1+\frac{1}{p}}}{\varepsilon^{\frac{1}{p}}} + \frac{(tJ\sqrt{N})^{1+\frac{1}{2p+1}}}{\varepsilon^{\frac{1}{2p+1}}} \right) . \tag{2}$$

This is an improvement of the general case in important regimes. We summarize some of these improvements in Table 1, for low order product formulas and for local Hamiltonians of constant degree d. A more detailed analysis and the general results and improvements are in [1].

As mentioned, a key ingredient for Thm. 1 is a property of local spin systems, where we proved that the leakage to high-energy states due to the evolution under any H_l can be bounded. This result, which is given below, is not only important for improving Hamiltonian simulation methods but may encounter applications in Hamiltonian complexity and beyond.

Lemma 1 (Leakage to high energies)**.** *Let $H = \sum_{l=1}^{L} H_l$ be a k-local Hamiltonian as above, $H_l \geq 0$, and $\Lambda' \geq \Lambda \geq 0$. Then, $\forall\, s \in \mathbb{R}$ and $\forall\, l$,*

$$\|\Pi_{>\Lambda'} e^{-isH_l} \Pi_{\leq\Lambda}\| \leq e^{-\lambda(\Lambda'-\Lambda)} \left(e^{\alpha|s|M} - 1 \right) \,, \tag{3}$$

[1] For $p > 0$ integer and $s \in \mathbb{R}$, a p-th order product formula is a unitary $W_p(s) = e^{-is_q H_{l_q}} \cdots e^{-is_2 H_{l_2}} e^{-is_1 H_{l_1}}$, where each $s_j \in \mathbb{R}$ is proportional to s and $1 \leq l_j \leq L$.

where $\lambda = 1/(2Jdk)$ *and* $\alpha = eJ$.

In general, $\Pi_{>\Lambda'}$ is the projector on the subspace of energies larger thatn Λ'. Lemma 1 follows from a result in [15] on the action of a local interaction term on a quantum state of low energy, in combination with a series expansion of e^{-isH_l}. While the local interaction term could generate support on arbitrarily high-energy states, that support is suppressed by a factor that decays exponentially in $\Lambda' - \Lambda$.

Another key ingredient for Thm. 1 is the ability to replace evolutions under the H_l's in a product formula by those under their effective low-energy versions with bounded error:

Lemma 2. *Let* $H = \sum_{l=1}^{L} H_l$ *be a* k*-local Hamiltonian as above,* $H_l \geq 0$*, and* $\Delta' \geq \Lambda' \geq \Lambda \geq 0$*. Then,* $\forall\ s \in \mathbb{R}$ *and* $\forall\ l$*,*

$$\|\Pi_{\leq\Lambda'}(e^{-is\bar{H}_l} - e^{-isH_l})\Pi_{\leq\Lambda}\| \leq e^{-\lambda(\Lambda'-\Lambda)}(e^{\alpha|s|M} - 1) \tag{4}$$

and

$$\|\Pi_{>\Lambda'}e^{-is\bar{H}_l}\Pi_{\leq\Lambda}\| \leq 3e^{-\lambda(\Lambda'-\Lambda)}(e^{\alpha|s|M} - 1)\ , \tag{5}$$

where $\lambda = 1/(2Jdk)$ *and* $\alpha = eJ$.

Lemma 2 also follows from [15] and other analyses.

Impact and Outlook. The problem of low-energy Hamiltonian simulation is central in physics and has vast applications, including the simulation of many-body systems for studying quantum phase transitions [16], the simulation of quantum field theories [17], the simulation of adiabatic quantum state preparation [18, 19], and more. Our work investigates the complexity of Hamiltonian simulation methods under the low-energy constraint, where we showed improved error bounds and complexities for product formulas that approximate the evolution operator. This is the first significant improvement of this kind. Product formulas are at the root of various quantum and classical methods that simulate quantum systems and our results may be translated into complexity improvements of such methods as well. We also analyzed potential complexity improvements of other, more sophisticated methods for quantum simulation [7, 8], but the improvements we obtained were not nearly as significant.

Our work opens up new questions as well: The obtained complexity improvements are useful as long as the energy Δ of the initial state is sufficiently small. However, the assumption $H_l \geq 0$ is needed and may be in conflict with ensuring small values of Δ. It will be important to resolve this issue if possible, which may be related to the fact that, for general Hamiltonians ($H_l \ngeq 0$), an improvement in the low-energy simulation could imply an improvement in the high-energy simulation by considering $-H$ instead. Indeed, certain spin models possess a symmetry that connects the high-energy and low-energy subspaces via a simple transformation. Whether such (high-energy) improvement is possible or not remains open. Additionally, known complexities of product formulas are polynomial in $1/\varepsilon$. This is an issue if precise computations are required as in the case of quantum field theories or QED. Whether this complexity can be improved as in [20, 7, 8, 21] is also open. Furthermore, even if some of our assumptions (e.g., $H_l \geq 0$) are not valid for certain Hamiltonians, the simulations may still be improved. Such assumptions yield sufficient but not necessary conditions for an improvement. Our work is an initial attempt to this problem and we expect to inspire further studies on improved Hamiltonian simulation methods in this setting.

References

[1] B. Şahinoğlu and R. D. Somma, *Hamiltonian simulation in the low energy subspace*, *arXiv preprint arXiv:2006.02660* (2020).

[2] R. P. Feynman, *Simulating physics with computers*, *International Journal of Theoretical Physics* **21** (1982), no. 6–7 467–488.

[3] M. Suzuki, *Fractal decomposition of exponential operators with applications to many-boyd theories and monte carlo simulations*, *Phys. Lett. A* **146** (1990) 319–323.

[4] M. Suzuki, *General theory of fractal path integrals with applications to many-body theories and statistical physics*, *J. Math. Phys.* **32** (1991) 400–407.

[5] D. Berry, G. Ahokas, R. Cleve, and B. Sanders, *Efficient quantum algorithms for simulating sparse hamiltonians*, *Comm. Math. Phys.* **270** (2007) 359.

[6] N. Wiebe, D. Berry, P. Hoyer, and B. Sanders, *Higher order decompositions of ordered operator exponentials*, *J. Phys. A: Math. Theor.* **43** (2010) 065203.

[7] D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, and R. D. Somma, *Simulating hamiltonian dynamics with a truncated taylor series*, *Phys. Rev. Lett.* **114** (2015) 090502.

[8] G. Low and I. Chuang, *Optimal hamiltonian simulation by quantum signal processing*, *Phys. Rev. Lett.* **118** (2017) 010501.

[9] M. Newman and G. Barkema, *Monte Carlo Methods in Statistical Physics*. Oxford University Press, 1998.

[10] R. D. Somma, *A trotter-suzuki approximation for lie groups with applications to hamiltonian simulation*, *Journal of Mathematical Physics* **57** (2016), no. 6 062202.

[11] A. M. Childs and Y. Su, *Nearly optimal lattice simulation by product formulas*, *Phys. Rev. Lett.* **123** (2019) 050503.

[12] A. M. Childs, Y. Su, M. C. Tran, N. Wiebe, and S. Zhu, *A theory of trotter error*, *arXiv: 1912.08854* (2019).

[13] L. Clinton, J. Bausch, and T. Cubitt, *Hamiltonian simulation algorithms for near-term quantum hardware*, *arXiv:2003.06886* (2020).

[14] R. L. Brooks, *On colouring the nodes of a network*, in *Mathematical Proceedings of the Cambridge Philosophical Society*, vol. 37, pp. 194–197, Cambridge University Press, 1941.

[15] I. Arad, T. Kuwahara, and Z. Landau, *Connecting global and local energy distributions in quantum spin models on a lattice*, *Journal of Statistical Mechanics: Theory and Experiment* **2016** (2016), no. 3 033301.

[16] S. Sachdev, *Quantum Phase Transitions, 2nd Edition*. Cambridge University Press, Cambridge, 2011.

[17] S. P. Jordan, K. S. Lee, and J. Preskill, *Quantum algorithms for quantum field theories*, *Science* **336** (2012) 1130.

[18] E. Farhi, J. Goldstone, S. Gutmann, and M. Sipser, *Quantum computation by adiabatic evolution*, *arXiv:quant-ph/0001106* (2000).

[19] S. Boixo, E. Knill, and R. Somma, *Fast quantum algorithms for traversing paths of eigenstates*, *arXiv:1005.3034* (2010).

[20] D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, and R. D. Somma, *Exponential improvement in precision for simulating sparse Hamiltonians*, in *Proc. of the 46th ACM Symposium on Theory of Computing*, pp. 283–292, 2014.

[21] G. H. Low, V. Kliuchnikov, and N. Wiebe, *Well-conditioned multiproduct hamiltonian simulation*, *arXiv:1907.11679* (2019).