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A note on Hamiltonian simulation in the Pauli basis

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Abstract. In this note, we consider a multiqubit quantum system with a Hamiltonian which can be decomposed into a few parts in such a way that each of these parts is a finite linear combination of pairwise anticommuting Pauli operators. It turns out that such a decomposition allows one to enhance both quantum and classical algorithms for Hamiltonian simulation, at least for Hamiltonians that are sparse in the Pauli basis. The advantage is achieved due to the possibility to represent in a simple closed form the exponential of a linear combination of pairwise anticommuting Pauli operators. We consider two illustrative models, which demonstrate the quantum computational advantage for the Trotter-Suzuki algorithm. We also show how an anticommutatively decomposed Hamiltonian can be efficiently simulated on a classical computer.

Keywords: Hamiltonian simulation, anticommuting operators, n-qubit quantum system, Pauli basis, operator exponential

MSC numbers: 81-08, 81R05

1 Introduction

The problem of simulating the time evolution of a quantum systems was at the core of the idea that has led to the emergence of the theory of quantum computing [1, 2, 3, 4]. Any realization of a computational process based on the principles of quantum mechanics involves the use of a certain model and an appropriate physical device. Typically, a real quantum system is modeled by another quantum system, which is usually artificial and simpler, since it consists of qubits, and its evolution is governed by a simple Hamiltonian. Simulation is a satisfactory implementation of computations for a given model on a quantum or classical device in order to correctly reproduce the main features of the modeled real system. For example, the Hamiltonian of a system of qubits and then the corresponding unitary transformation can be implemented at the hardware level by a suitable quantum circuit.

In this note, we will always be dealing with a quantum system of n pairwise distinguishable qubits, which is mathematically described by means of the Hilbert space $\mathcal{H}_n = \mathcal{H}^{\otimes n}$, where $\mathcal{H}$ is the Hilbert space of a qubit and thus $\dim_{\mathbb{C}}\mathcal{H} = 2$. Let $L(\mathcal{H}_n) = \mathcal{H}_n \otimes \mathcal{H}_n^{\dagger}$ be the associative algebra of linear operators on $\mathcal{H}$ and $\mathcal{H}^{\dagger}$, which act on ket and bra state vectors by the left and right contractions, respectively. The dimensions of $\mathcal{H}_n$ and $L(\mathcal{H}_n)$ are

$$\dim_{\mathbb{C}}\mathcal{H}_n = \dim_{\mathbb{C}}\mathcal{H}_n^{\dagger} = N, \quad \dim_{\mathbb{C}}L(\mathcal{H}_n) = N^2, \quad N = 2^n.$$

In fact, only two classes of operators are needed in quantum computing (this is generally not true in quantum theory), namely, the (real) linear space $H(\mathcal{H}_n) \subset L(\mathcal{H}_n)$ of Hermitian operators and the unitary groups $SU(N) \subset U(N) \subset L(\mathcal{H}_n)$; $H(\mathcal{H}_n)$ is not a real subalgebra in $L(\mathcal{H}_n)$, but is a Jordan algebra under the anticommutation operation. In general, a state of an n-qubit quantum system is mathematically described by a density operator $\rho \in H(\mathcal{H}_n)$, which is positive (has no negative eigenvalues) and has unit trace. In quantum theory, observables are also Hermitian operators, while unitary operators determine the evolution of a system.

Nowadays, it is believed that a universal quantum computer [5, 6] demonstrating quantum supremacy should have a large number of qubits, say $n \geq 100$. Thus the number of basis states is $N = 2^n > 10^{30}$ in $\mathcal{H}_n$ and $N^2 = 4^n > 10^{60}$ in $L(\mathcal{H}_n)$, so that the matrix representation of states and operators is not practically acceptable. Both universal quantum computers and quantum computers with small number of qubits ($n \sim 100$) that will be available in the near term have be employed together with a classical computer, and, in both cases, multiqubit quantum computations are very sensitive to the choice of a computational basis [7, 8, 9]. We will use the Pauli basis in $L(\mathcal{H}_n)$.

Our aim is to consider in detail the following two issues: (i) preliminary simulation of a multiqubit quantum system on a classical computer for some special but important case when the Hamiltonian of the system can be decomposed into a

few parts in such a way that each of these part consists of pairwise anticommuting Pauli operators; (ii) a quantum computational advantage (using the Trotter-Suzuki algorithm as an example) that can be achieved by such a decomposition. We will understand the term "simulating" in a wide sense assuming that for a real quantum many-body system modeled by a multiqubit quantum system, the simulation process replicates (approximately, but with good accuracy) its eigenstates, time evolution, and thermodynamics properties. Then in both cases of quantum and classical simulation, the problem consists of computing the exponentials of linear operators in finite-dimensional spaces.

In Sec. 2, we briefly consider some general aspects of setting the problem of Hamiltonian simulation. Sec. 3 is devoted to the discussion of the related properties of the Pauli basis. In Sec. 4, we discuss the notion of sparse Hamiltonian in the Pauli basis. In Sec. 5, we give two model examples of anticommutatively decomposed Hamiltonians. Throughout the text we use the system of units with $\hbar = c = k_B = 1$, where k_B is the Boltzmann constant.

2 Statement of the Hamiltonian simulation problem

The general formulation of the problem can be represented as an efficient computation of exponentials of the form $\mathrm{e}^{-\beta\hat{H}}$, where $\hat{H}$ is an arbitrary Hermitian operator which is further regarded as a Hamiltonian. A weaker statement of the problem requires only an approximation with the desired accuracy. There are two special cases of interest in quantum theory. If $\beta = it$ or, in a more general context when the Hamiltonian $\hat{H}$ is time-dependent and $\beta = i$, the exponential $\mathrm{e}^{-it\hat{H}}$ or, respectively, $\mathrm{e}^{-i\hat{H}(t)}$ describes the unitary dynamics of the corresponding quantum system. In another case, β denotes the inverse temperature of a "large" isolated quantum system that has a fixed energy and number of particles — such system is commonly referred to as the environment, — and $\hat{H}$ denotes the Hamiltonian of a "small" subsystem weakly coupled to the environment. We will also assume, for simplicity, that the number of particles in the subsystem is fixed, but at the same time the subsystem can exchange some portions of energy with the environment. Then, if the environment has reached its thermal equilibrium, the subsystem is described by the Gibbs state

$$\hat{\rho} = \frac{\mathrm{e}^{-\beta\hat{H}}}{Z}, \qquad Z = \operatorname{tr} \mathrm{e}^{-\beta\hat{H}}.$$

Functions of operators arise naturally as formal solutions to a number of problems in physics and applied mathematics and have been widely studied earlier in the equivalent formulation of functions of matrices [10, 11]. The operator formulation is commonly used in simulating quantum Hamiltonian dynamics, quantum machine learning, quantum computing. A preliminary classical calculation of the Hamiltonian exponential is useful both for testing quantum algorithms and for the inverse problem of choosing the model Hamiltonians itself [12]; however, the com-

putational complexity is exponential in the number of qubits. Moreover, we have no universal algorithm that would be computationally efficient for all types of Hamiltonians at once. We have Trotter-Suzuki decomposition [13], Magnus expansion [14], and — see review [10] — Padé approximation, Jordan-Schur decomposition (not suitable for time-dependent Hamiltonians) For bounded linear operators in a normed vector space, the exponential of an operator can be defined by the Taylor expansion,

$$\mathrm{e}^{-\beta\hat{H}} = \sum_{k=0}^{\infty}(-1)^k \frac{\beta^k}{k!}\,\hat{H}^n \quad (\hat{H}^0 = \hat{I}\,), \tag{1}$$

and can be computed approximately using truncated Taylor series [15]. In this paper, our attention is restricted to finite dimensional Hilbert spaces, and even more specifically, to quantum systems consisting of a finite number of qubits. If $\hat{H} \in L(\mathcal{H}_n)$, then this series converges absolutely for any $\beta \in \mathbb{C}$ (and converges uniformly for β taking values in a bounded domain) with respect to the Frobenius norm. The expansion (1) provides us with the simplest algorithm for computing operator exponentials using truncated Taylor series, but it should be kept in mind that the results will, in general, not be unitary. An exception is the case when the series can be summed exactly to obtain the result in the form of an explicit closed-form expression.

3 Properties of the Pauli basis

First of all, we need to introduce in detail some special properties of the n-qubit Pauli basis. The choice of a basis in $L(\mathcal{H}_n)$ is equally important for both quantum computing and its emulation on a classical computer. There are two general possibilities for choosing a basis, and which one is more efficient depends on both a given algorithm and a particular type of quantum computer. First, we can use a standard orthonormal basis in the based Hilbert space and then construct a suitable basis in the algebra of linear operators. However, this approach turns out to be inconvenient and unnatural in the consideration of problems related to mixed states, graph states, tensor networks, and more generally, to all cases where measurements are not projective [6, 17, 18]. The second possibility deals directly with a basis in the operator algebra, and in this case the basis elements usually cannot be separated into a tensor product of some ket and bra vectors; the Pauli basis is considered to be the best choice. A systematic algebraic overview of the Pauli basis in multiqubit systems is given, for example, in [19, 20].

We assume that $L(\mathcal{H}_n)$ is equipped with the Hilbert-Schmidt inner product and the corresponding Frobenius norm:

$$\langle \hat{A}, \hat{B}\rangle = \mathrm{tr}(\hat{A}^\dagger \hat{B}), \qquad \|\,\hat{A}\,\| = \langle \hat{A}, \hat{A}\rangle^{1/2}, \qquad \hat{A}, \hat{B} \in L(\mathcal{H}_n).$$

The set of the Pauli operators $\{\hat{\sigma}_k\}_{k=0}^3$ (the identity operator $\hat{\sigma}_0$ is included) is usually chosen as an Hermitian orthogonal basis in the one-qubit algebra $L(\mathcal{H})$. In

the operator (non-matrix) representation, $\hat{\sigma}_k$ can be written as the expansion on the standard basis in the form

$$\hat{\sigma}_0 = |0\rangle\langle 0| + |1\rangle\langle 1|, \qquad \hat{\sigma}_1 = |0\rangle\langle 1| + |1\rangle\langle 0|,$$

$$\hat{\sigma}_2 = -i|0\rangle\langle 1| + i|1\rangle\langle 0|, \quad \hat{\sigma}_3 = |0\rangle\langle 0| - |1\rangle\langle 1|,$$

Let us consider the set $K_4 = \{0, 1, 2, 3\}$ as the Klein group with the multiplication rules

$$0{*}k = k, \quad k{*}k = 0, \quad k{*}l = m, \quad k, l, m \in \{1, 2, 3\},$$

where m is defined by the condition that klm is a permutation of 123. Defining the function $s : K_4 \times K_4 \to \{1, i, -i\}$ as

$$\begin{aligned} &s(0,0) = s(0,k) = s(k,0) = s(k,k) = 1, \\ &s(k,l) = \epsilon_\pi i, \quad k, l \in \{1, 2, 3\}, \end{aligned} \tag{2}$$

where ϵ_π is the sign of the permutation $\pi(123) = klm$, $m = k{*}l$, we can write the well-known expressions for composition of these operators as

$$\hat{\sigma}_k \hat{\sigma}_l = s(k,l)\hat{\sigma}_m, \quad m = k{*}l, \quad k, l \in \{0, 1, 2, 3\}.$$

As stated above, qubits in a quantum system are distinguishable and therefore can be numbered from 1 to n. We will consider the qubit system to be ordered and hence do not use a qubit position index; mathematically, the location in the tensor product distinguishes qubits from each other. In other words, we assume in what follows that their numbers correspond to the ordinal numbers of the one-qubit Pauli operators in their tensor product, so that no additional labels for the operators are required. Thus, the lowercase indices in Pauli strings will always denote the Pauli operator number from the set $\{0, 1, 2, 3\}$. Keeping this in mind, we can introduce the set of N^2 pairwise orthogonal operators (also commonly called Pauli operators or, alternatively, Pauli strings),

$$\left\{\hat{\sigma}_{k_1 \ldots k_n}\right\}_{k_1,\ldots,k_n \in \{0,1,2,3\}}, \quad \hat{\sigma}_{k_1 \ldots k_n} = \hat{\sigma}_{k_1} \otimes \ldots \otimes \hat{\sigma}_{k_n} \in L(\mathcal{H}_n), \tag{3}$$

which, in turn, is the Pauli basis in $L(\mathcal{H}_n)$.

It is easy to prove [16, 17] that there exists a unitary transformation from the Pauli basis, to the corresponding computational basis $\{|u\rangle\langle v|\}$, where $|u\rangle$ and $|v\rangle$ are binary strings of length n. We will also use the notation $\hat{\sigma}_K$ for the operator $\hat{\sigma}_{k_1 \ldots k_n}$, where K is the decimal representation of the Pauli string $k_1 \ldots k_n$ which is considered as a number in base 4. Note, in particular, that $\hat{\sigma}_0 = \hat{\sigma}_{0\ldots0}$ is the identity operator in $L(\mathcal{H}_n)$.

Recall, first, that the Pauli operators $\hat{\sigma}_K$ are Hermitian and unitary at the same time, and satisfy the relations

$$\operatorname{tr} \hat{\sigma}_0 = N, \quad \operatorname{tr} \hat{\sigma}_K\big|_{K \neq 0} = 0, \quad \hat{\sigma}_K^2 = \hat{\sigma}_0, \;\; 0 \leq K \leq N^2 - 1, \quad \| \hat{\sigma}_K \| = \sqrt{N}. \tag{4}$$

Second, we need an explicit formula for the composition of n-qubit Pauli operators, since it is an important part of the complete algorithm. Third, let $\hat{\sigma}_K$ and $\hat{\sigma}_L$ be Pauli operators. Using (2) – (3), one finds for $K = k_1 \dots k_n$ and $L = l_1 \dots l_n$ the key expressions

$$\hat{\sigma}_K \hat{\sigma}_L = S(K, L)\hat{\sigma}_M, \quad M = K * L = m_1 \dots m_n, \quad 0 \le K, L \le N^2 - 1, \tag{5}$$

where

$$S(K, L) = s(k_1, l_1)s(k_2, l_2) \cdots s(k_n, l_n), \tag{6}$$

and the operation $*$ is extended to the Pauli strings in such a way that $m_\alpha = k_\alpha * l_\alpha$ for all $\alpha = 1, \dots, n$. This algorithmic rule can be interpreted more intuitively as follows.

Proposition 1. *Let us consider the set of pairs (k_α, l_α) such that $k_\alpha, l_\alpha \in \{1, 2, 3\}$ and $k_\alpha \neq l_\alpha$. Let $\mathfrak{n}_e$ and $\mathfrak{n}_o$ be the numbers of such pairs for which the triple $k_\alpha l_\alpha m_\alpha$, where $m_\alpha = k_\alpha * l_\alpha$, is an even and, respectively, an odd permutation of the string 123. Then $\hat{\sigma}_K$ and $\hat{\sigma}_L$ commute if $\mathfrak{n}_e$ and $\mathfrak{n}_o$ have the same parity, and anticommute otherwise.*

The proof follows directly from (2) and (6). We have

$$S(K, L) = i^{\mathfrak{n}_e}(-i)^{\mathfrak{n}_o} = i^{\mathfrak{n}_e + \mathfrak{n}_o}(-1)^{\mathfrak{n}_o}, \tag{7}$$

so that $S(K, L) = S(L, K)$ if and only if $\mathfrak{n}_e$ and $\mathfrak{n}_o$ are both either even or odd; in this case, $\hat{\sigma}_K$ and $\hat{\sigma}_L$ commute. Otherwise, $S(K, L) = -S(L, K)$ and these operators anticommute.

Finally recall that the set

$$\left\{ i\hat{\sigma}_K \middle| \, 0 \le K \le N^2 - 1 \right\}$$

of the anti-Hermitian operators is a basis in the real Lie algebra $\mathfrak{u}(N)$ of the unitary group $U(N)$, and is a basis in the algebra $\mathfrak{su}(N)$ of the group $SU(N)$ if K is restricted to the set $\{1, \dots, N^2 - 1\}$. Indeed, relations (5) and (7) imply that $[i\hat{\sigma}_K, i\hat{\sigma}_L] = C_{KL} i\hat{\sigma}_M$, where the structure constants $C_{KL} = iS(K, L) - iS(L, K)$ are real.

4 Sparse quantum states and Hamiltonians

The Pauli basis is particularly useful for representing density operators and Hamiltonians. A quantum state (a density operator) is a Hermitian positive operator of the form

$$\hat{\rho} = \frac{1}{2^n} \sum_{k_1, \dots, k_n \in \{0,1,2,3\}} a_{k_1 \dots k_n} \hat{\sigma}_{k_1 \dots k_n} \equiv \frac{1}{2^n} \sum_{K=0}^{4^n - 1} a_K \hat{\sigma}_K, \tag{8}$$

where $a_{k_1\ldots k_n} \in \mathbb{R}$ and

$$a_{0\ldots0} = 1\,, \quad |a_{k_1\ldots k_n}| \leqslant 1, \qquad \sum_{k_1,\ldots,k_n\,\in\,\{0,1,2,3\}} (a_{k_1\ldots k_n})^2 \leqslant 2^n. \tag{9}$$

Conditions (9) guarantee that $\hat{\rho}^\dagger = \hat{\rho}$, $\operatorname{tr}\hat{\rho} = 1$, and $\operatorname{tr}\hat{\rho}^2 \leqslant 1$. For quantum computation, it is important that all coefficients in the state (8) are real and each of them, except $a_{0\ldots0}$, is exactly the result of a local measurement with one of the basis operators (3), $a_K \equiv a_{k_1\ldots k_n} = \operatorname{tr}\bigl(\hat{\rho}\hat{\sigma}_{k_1\ldots k_n}\bigr)$. All the quantum (pure and mixed) states constitute a convex set (closed manifold, since it is the preimage of 1 under the map $\operatorname{tr} : H(\mathcal{H}_n) \to \mathbb{R}$) of real dimension $4^n - 1$ in the real linear manifold $\mathcal{S}_n \subset H(\mathcal{H}_n)$, while the pure states are placed on the boundary of $\mathcal{S}_n$ and make up a real submanifold of dimension $2^{n+1} - 2$.

Next we consider the representation of a Hamiltonian $\hat{H} \in L(\mathcal{H}_n)$ in the form

$$\hat{H} = \sum_{K\in\mathcal{T}} h_K\hat{\sigma}_K, \quad h_K \in \mathbb{R}, \quad \mathcal{T} \subset \{1, 2, \ldots, N^2 - 1\}, \tag{10}$$

where we assume, without loss of generality, that the Hamiltonian is traceless, that is, $\hat{\sigma}_0$ is not included in this expansion.

A Hamiltonian represented in the form of the expansion (10) will be said to be *sparse* in the Pauli basis if the following two conditions are fulfilled. First, the condition $|\mathcal{T}| \ll N^2$ is satisfied, and second, the set $\sigma_{\hat{H}} = \bigl\{\hat{\sigma}_K \bigm| K \in \mathcal{T}\bigr\}$ in (10) is closed under composition.

The first condition should be understood only as the necessity to relate the length of expansion (10) to the available computational resources. The second condition is also not too restrictive in practice, since the set $\sigma_{\hat{H}}$ can usually be extended to be closed (by successively adding to this set all operators of the form $\hat{\sigma}_M = \hat{\sigma}_K\hat{\sigma}_L/S(K,L)\big|_{K,L\in\mathcal{T}}$ that are not contained in it) while maintaining the first condition. On the other hand, there exist Hamiltonians that cannot be extended in this way to short ones. For example, the Hamiltonian of the quantum Heisenberg XY model is obviously not short, since we will get $|\mathcal{T}| = N^2$ as a result of this procedure. Note that the property of being sparse can be applied not only to Hamiltonians, but also to density operators and unitary operators. For example, the expansion for the density operator of the so-called uniform quantum superposition,

$$\hat{\rho}_s = \frac{1}{N}\sum_{k,l=0}^{N-1} |k\rangle\langle l| = \frac{1}{N}\sum_{K\in\{0,1\}^n} \hat{\sigma}_K,$$

has N^2 terms in the standard (computational) basis, and only N terms in the corresponding Pauli basis; hence, in certain cases, the density operator $\hat{\rho}_s$ can be considered as a sparse operator.

Below it is assumed that all Hamiltonians under consideration are sparse.

5 Anticommutatively decomposed Hamiltonians

This section is based on the following

Proposition 2. *If all the operators $\hat{\sigma}_K$ in the Pauli expansion (10),*

$$\hat{H} = \sum_{K\in\mathcal{T}} h_K \hat{\sigma}_K,$$

anticommute pairwise, $\{\hat{\sigma}_K, \hat{\sigma}_L\} = 2\delta_{K,L}\hat{\sigma}_0$, then

$$\mathrm{e}^{-\beta\hat{H}} = \cosh(h\beta)\,\hat{\sigma}_0 - \frac{\sinh(h\beta)}{h}\,\hat{H}, \quad h = \left(\sum_{K\in\mathcal{T}} h_K^2\right)^{1/2}. \tag{11}$$

The coefficients h_K can be time-depended.

To prove this proposition, it is sufficient to note that

$$\hat{H}^2 = h^2\hat{\sigma}_0, \quad \hat{H}^{2k} = h^{2k}\hat{\sigma}_0, \quad \hat{H}^{2k+1} = h^{2k}\hat{H}, \quad k\in\mathbb{N},$$

and then substitute these equalities in the Taylor series (1).

For example, let us consider the model Hamiltonian[1]

$$\hat{H} = a_1\hat{\sigma}_{123} + a_2\hat{\sigma}_{231} + a_3\hat{\sigma}_{312}, \tag{12}$$

in which $\{\hat{\sigma}_{123}, \hat{\sigma}_{231}\} = \{\hat{\sigma}_{312}, \hat{\sigma}_{231}\} = \{\hat{\sigma}_{123}, \hat{\sigma}_{312}\} = 0$, and a_k $(k = 1, 2, 3)$ are real. According to the general formula (11), we have

$$\mathrm{e}^{-\beta\hat{H}} = \cosh(p\beta)\,\hat{\sigma}_{000} - \frac{\sinh(p\beta)}{p}\,\hat{H}, \quad p = \sqrt{a_1^2 + a_2^2 + a_3^2}. \tag{13}$$

Then the dynamics of this three-qubit system, assumed to be closed, is determined by the unitary operator

$$\mathrm{e}^{-it\hat{H}} = \cos(pt)\,\hat{\sigma}_{000} - i\frac{\sin(pt)}{p}\,\hat{H}.$$

In a more general case, the Hamiltonian of a multiqubit system is assumed to be decomposed into the sum (such a Hamiltonian is said to be *anticommutatively decomposed*)

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \ldots + \hat{H}_m, \quad \hat{H}_k = \sum_{K\in\mathcal{T}_k} h_K\hat{\sigma}_K, \quad k = 1, 2, \ldots, m,$$

where each set $\{\hat{\sigma}_K\}_{K\in\mathcal{T}_k}$ consists of pairwise anticommuting Pauli operators, and, in accordance with expression (10),

$$\mathcal{T}_1 \cup \mathcal{T}_2 \cup \ldots \cup \mathcal{T}_m = \mathcal{T}, \quad \mathcal{T}_i \cap \mathcal{T}_j\big|_{i\neq j} = \varnothing, \quad i, j = 1, 2, \ldots, m.$$

[1] In the system of units with $\hbar = c = k_B = 1$, energy (coefficients a, b, c in the present case) is measured in inverse units of length, and t and β are measured in units of length. Everywhere we suppose that the unit of length is fixed in some convenient way.

For simplicity, we consider the sum with $m = 2$, that is, $\hat{H} = \hat{H}_1 + \hat{H}_2$, but generalization to the case $m > 2$ is obvious. It turns out that the anticommutative decomposition of a Hamiltonian allows one to optimise the approximate methods listed in 2. This assertion can be explicitly illustrated on the example of the well-known Trotter-Suzuki algorithm [13]. For example, the Lie-Trotter symmetrized formula takes the form

$$\mathrm{e}^{-it\hat{H}} = \lim_{s\to\infty} \big(\hat{U}_{12}(s,t)\big)^s, \tag{14}$$

where

$$\begin{aligned}\hat{U}_{12}(s,t) &= \frac{1}{2}\left(\mathrm{e}^{-(it/s)\hat{H}_1}\mathrm{e}^{-(it/s)\hat{H}_2} + \mathrm{e}^{-(it/s)\hat{H}_2}\mathrm{e}^{-(it/s)\hat{H}_1}\right)\\ &= \cos\frac{pt}{s}\,\cos\frac{qt}{s}\,\hat{\sigma}_0 - \frac{1}{2pq}\sin\frac{pt}{s}\,\sin\frac{qt}{s}\,\{\hat{H}_1,\hat{H}_2\}\\ &\qquad - \frac{i}{p}\sin\frac{pt}{s}\,\cos\frac{qt}{s}\,\hat{H}_1 - \frac{i}{q}\sin\frac{qt}{s}\,\cos\frac{pt}{s}\,\hat{H}_2,\end{aligned} \tag{15}$$

and (n is the number of qubits)

$$p = \left(2^{-n}\operatorname{tr}\hat{H}_1^2\right)^{1/2}, \quad q = \left(2^{-n}\operatorname{tr}\hat{H}_2^2\right)^{1/2}.$$

The unitary operator $\hat{U}_{12}$ can be easily implemented using a quantum circuit, and its multiple repetition yields the exponential $\mathrm{e}^{-\beta\hat{H}}$ with a good accuracy. We have restricted our consideration to the simplest first-order formula, but the generalization of the algorithm to the second order,

$$\mathrm{e}^{-\beta\hat{H}} = \left(\mathrm{e}^{-(\beta/2s)\hat{H}_1}\mathrm{e}^{-(\beta/s)\hat{H}_2}\mathrm{e}^{-(\beta/2s)\hat{H}_1}\right)^s + O(\beta^3/s^2),$$

as well as to higher orders, can be done directly.

In the next example, we take the Hamiltonian (11) as $\hat{H}_1$ and set for $\hat{H}_2$ the operator

$$\hat{H}_2 = b_1\hat{\sigma}_{301} + b_2\hat{\sigma}_{013} + b_3\hat{\sigma}_{130}, \quad q = \sqrt{b_1^2 + b_2^2 + b_3^2},$$

where all Pauli operators anticommute, and b_k ($k=1,2,3$) are real. It is convenient to introduce the notations

$$\boldsymbol{\alpha} = \frac{1}{p}(a_1\,a_2\,a_3), \quad \boldsymbol{\beta} = \frac{1}{q}(b_1\,b_2\,b_3), \quad \hat{\mathbf{A}} = \big(\hat{\sigma}_{123}\,\hat{\sigma}_{231}\,\hat{\sigma}_{312}\big), \quad \hat{\mathbf{B}} = \big(\hat{\sigma}_{301}\,\hat{\sigma}_{013}\,\hat{\sigma}_{130}\big).$$

Denoting by a dot the formal inner product (as in $\mathbb{R}^3$), we have

$$\hat{H}_1 = p\boldsymbol{\alpha}\cdot\hat{\mathbf{A}}, \quad \hat{H}_2 = q\boldsymbol{\beta}\cdot\hat{\mathbf{B}}, \tag{16}$$

$$(\boldsymbol{\alpha}\cdot\hat{\mathbf{A}})^2 = (\boldsymbol{\beta}\cdot\hat{\mathbf{B}})^2 = (\boldsymbol{\beta}\cdot\hat{\mathbf{A}})^2 = (\boldsymbol{\alpha}\cdot\hat{\mathbf{B}})^2 = \hat{\sigma}_{000}. \tag{17}$$

It is also easy to find that

$$\{\boldsymbol{\alpha}\cdot\hat{\mathbf{A}},\boldsymbol{\beta}\cdot\hat{\mathbf{B}}\}=2(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})\,\hat{\sigma}_{222},\qquad \{\boldsymbol{\alpha}\cdot\hat{\mathbf{B}},\boldsymbol{\beta}\cdot\hat{\mathbf{A}}\}=2(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})\,\hat{\sigma}_{222}, \tag{18}$$

$$\{\hat{\sigma}_{222},\boldsymbol{\alpha}\cdot\hat{\mathbf{A}}\}=\boldsymbol{\alpha}\cdot\hat{\mathbf{B}},\qquad \{\hat{\sigma}_{222},\boldsymbol{\beta}\cdot\hat{\mathbf{B}}\}=\boldsymbol{\beta}\cdot\hat{\mathbf{A}}, \tag{19}$$

$$\{\hat{\sigma}_{222},\boldsymbol{\alpha}\cdot\hat{\mathbf{B}}\}=\boldsymbol{\alpha}\cdot\hat{\mathbf{A}},\qquad \{\hat{\sigma}_{222},\boldsymbol{\beta}\cdot\hat{\mathbf{A}}\}=\boldsymbol{\beta}\cdot\hat{\mathbf{B}}. \tag{20}$$

The operator $\hat{U}_{12}$ takes the form

$$\hat{U}_{12}=\cos\frac{pt}{s}\,\cos\frac{qt}{s}\,\hat{\sigma}_{000}-\sin\frac{pt}{s}\,\sin\frac{qt}{s}\,(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})\,\hat{\sigma}_{222}$$
$$-i\sin\frac{pt}{s}\,\cos\frac{qt}{s}\,\boldsymbol{\alpha}\cdot\hat{\mathbf{A}}-i\sin\frac{qt}{s}\,\cos\frac{pt}{s}\,\boldsymbol{\beta}\cdot\hat{\mathbf{B}}.$$

Using the expressions (16) – (20), one can obtain a (cumbersome) recurrence formula for even powers of this operator.

In the simple case when $\boldsymbol{\alpha}\cdot\boldsymbol{\beta}=\pm1$, it is easy to find a closed expression for an arbitrary power of $\hat{U}_{12}$. By direct calculation, regardless of the sign of $\boldsymbol{\alpha}\cdot\boldsymbol{\beta}$, we obtain

$$\hat{U}_{12}^{k}=\cos\frac{kpt}{s}\,\cos\frac{kqt}{s}\,\hat{\sigma}_{000}-\sin\frac{kpt}{s}\,\sin\frac{kqt}{s}\,(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})\,\hat{\sigma}_{222}$$
$$-i\sin\frac{kpt}{s}\,\cos\frac{kqt}{s}\,\boldsymbol{\alpha}\cdot\hat{\mathbf{A}}-i\sin\frac{kqt}{s}\,\cos\frac{kpt}{s}\,\boldsymbol{\beta}\cdot\hat{\mathbf{B}}.$$

Thus, $\hat{U}_{12}^{s}=\hat{U}_{12}$ for $k=s$. In the limit $s\to\infty$, we get (for $\boldsymbol{\alpha}\cdot\boldsymbol{\beta}=\pm1$)

$$\mathrm{e}^{-it(\hat{H}_1+\hat{H}_2)}=\cos pt\,\cos qt\,\hat{\sigma}_{000}-\sin pt\,\sin qt\,(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})\,\hat{\sigma}_{222}$$
$$-i\sin pt\,\cos qt\,\boldsymbol{\alpha}\cdot\hat{\mathbf{A}}-i\sin qt\,\cos pt\,\boldsymbol{\beta}\cdot\hat{\mathbf{B}}.$$

This result, which is a very special case of the general formulae (14) and (15), could be obtained by direct summation of the Taylor series (1) with $\beta=it$ and $\hat{H}=\hat{H}_1+\hat{H}_2$. Indeed, $\hat{H}_1\hat{H}_2=pq(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})-ipq(\boldsymbol{\alpha}\times\boldsymbol{\beta})=pq(\boldsymbol{\alpha}\cdot\boldsymbol{\beta})$ if $\boldsymbol{\alpha}$ is proportional to $\boldsymbol{\beta}$, and consequently $\left[\hat{H}_1,\hat{H}_2\right]=0$.

Finally, we consider the case when the system is in the state of thermal equilibrium with the environment. Setting, for definiteness, $\boldsymbol{\alpha}\cdot\boldsymbol{\beta}=1$ and returning to the previous notations, we obtain the partition function and the density operator in the form

$$Z=\mathrm{tr}\,\mathrm{e}^{-\beta(\hat{H}_1+\hat{H}_2)}=8\cosh p\beta\,\cosh q\beta$$

$$\rho=\frac{\mathrm{e}^{-\beta(\hat{H}_1+\hat{H}_2)}}{Z}=\frac{1}{8}\,\hat{\sigma}_{000}+\tanh p\beta\,\tanh q\beta\,\hat{\sigma}_{222}$$
$$-\frac{1}{p}\tanh p\beta\,\hat{H}_1-\frac{1}{q}\tanh q\beta\,\hat{H}_2.$$

The partition function determines the mean value of the energy and the entropy of the system as follows:

$$\langle E\rangle = \mathrm{tr}\{\rho(\hat{H}_1+\hat{H}_2)\} = -\partial_\beta \ln Z = -p\tanh p\beta - q\tanh q\beta,$$

$$S = \ln Z + \beta\langle E\rangle =$$

$$\ln 2 + \ln(\mathrm{e}^{p\beta}+\mathrm{e}^{-p\beta}) + \ln(\mathrm{e}^{q\beta}+\mathrm{e}^{-q\beta}) - p\beta\tanh p\beta - q\beta\tanh q\beta.$$

It is interesting to consider the behavior of the model at temperatures close to zero, since modern quantum gadgets operate in this temperature range (μK÷mK). We have $Z\to\infty$ and

$$\langle E\rangle = -(p+q) + O\big(\mathrm{e}^{-2(p+q)\beta}\big) \quad S = \ln 2 + O\big(\mathrm{e}^{-2(p+q)\beta}\big), \quad \beta\to\infty. \tag{21}$$

This result is consistent with the third law of thermodynamics, which states that the entropy of a system approaches a constant value as the temperature of the system (and of its environment) adiabatically goes to absolute zero. Note also that the Helmholtz free energy,

$$F = -\frac{1}{\beta}\ln Z = -(p+q) + O\big(\beta^{-1}\big), \quad \beta\to\infty, \tag{22}$$

approaches to $\langle E\rangle$ as the temperature goes to zero.

To better understand the energy scale, we should return to the natural units, replacing (we accept centimeter as a unit of length)

$$\beta\to\frac{\beta}{c\hbar}, \quad p\to c\hbar p, \quad q\to c\hbar q \quad (c\hbar\approx 3\cdot 10^{-17}\mathrm{erg}\cdot\mathrm{cm}).$$

For example, in the temperature range under consideration, the values $\beta = 100\,\mathrm{cm}$ and $p\sim q\sim 1\,\mathrm{cm}^{-1}$ (physically, these values are more than enough for the estimates (21) and (22) to be quite correct) correspond to the inverse temperature $\beta\approx 3\cdot 10^{18}\,\mathrm{erg}^{-1}$ and the energy $\langle E\rangle\sim -6\cdot 10^{-17}\mathrm{erg}$, that is, $T\approx 3\cdot 10^{-19}\,\mathrm{erg}$ ($\approx 0.002\,\mathrm{K}$). These estimates show that the model under consideration is quite realistic.

6 Conclusion

In this note, we have described a base technique for working with anticommutatively decomposed Hamiltonians. This means that a Hamiltonian admits the decomposition into several parts consisting of linear combination of pairwise anticommuting Pauli operators. We show by the example of the Trotter-Suzuki algorithm that the efficiency of the known quantum algorithms for quantum Hamiltonian simulation

can be significantly improved if the corresponding Hamiltonian can be anticommutatively decomposed. The key point in our consideration is the use of the Pauli basis, since in this case the exponential of a linear combination of pairwise anticommuting Pauli operators can be expressed explicitly as the sum of two operator terms, where one of them is proportional to the identity, and second is proportional to the linear combination itself. It turns out that this technique is useful also in classical Hamiltonian simulation. Moreover, if the parts of an anticommutatively decomposed Hamiltonian are connected by some simple algebraic relations, then the exponential of the Hamiltonian admits explicit analytical calculation or the derivation of recurrent expressions for the powers of the Hamiltonian; in the simplest cases, these parts commute, or their (anti)commutators are proportional to a basis Pauli operator, or these parts form a closed system of operators with respect to anticommutation, etc. It should be remarked, however, that there is a serious obstacle in using the technique of anticommutatively decomposed Hamiltonians, since we do not have any efficient algorithm for obtaining such a decomposition in the case of a large number of qubits. This problem has been studied [21, 22], for example, within the framework of graph theory; the main difficulty is that anticommutativity is not an equivalence relation, that is, anticommutativity of $\hat{\sigma}_K$ with $\hat{\sigma}_I$ and $\hat{\sigma}_J$ does not imply anticommutativity of $\hat{\sigma}_I$ and $\hat{\sigma}_J$.

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