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Hamiltonian simulation in the Pauli basis of multi-qubit clusters for condensed matter physics

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Abstract. We propose an efficient method for Hamiltonian simulation of multi-qubit quantum systems with special types of interaction. In our approach, the Hamiltonian of a n-qubit system should be represented as a linear combination of the standard Pauli basis operators, and then decomposed into a sum of partial Hamiltonians, which are, in general, not Pauli operators and satisfy some anticommutation relations. For three types of Hamiltonians, which are invariant with respect to permutations of qubits, the effectiveness of the main algorithm in the three-qubit cluster model is shown by calculating the operator exponentials for these Hamiltonians in an explicit analytical form. We also calculate the density operator, partition function, entropy, and free energy of the cluster weakly coupled to a thermal environment. In our model, the cluster is in the Gibbs state in the temperature interval $0.1-2$K, which corresponds to the operating range of modern quantum processors. It follows from our analysis that the thermodynamic properties of such systems strongly depend on the type of internal interaction of qubits in the cluster.

Key words and phrases: Hamiltonian simulation, cluster of qubits, operator exponential, thermal environment, Gibbs state, thermodynamic properties

1. Introduction

In recent decades, effective mathematical methods and computational algorithms have been developed to simulate the dynamics of quantum systems and their thermodynamic properties on classical computers. It is believed that classical modeling of quantum systems, at least in quantum computation and chemical physics [1, 2], is potentially the shortest path to substantive quantum algorithms. In quantum information and condensed matter physics, the Hamiltonian simulation is one of the most important problems [3–5]. This problem can be mathematically formulated as the task of computing, exactly

or approximately, the operator exponential $\exp\left(\tau\hat{H}\right)$ for a Hamiltonian of the form $\hat{H} = \sum \hat{H}_k$, where each summand is assumed to be a Hermitian operator [6, 7]. Usually the simulating Hamiltonian has a simpler form in comparison with the Hamiltonian of a real quantum system, but they both have the same specific features; in particular, their spectra should be close to each other.

In this paper we propose a method for computing the operator exponentials based on the decomposition of a simulating Hamiltonian into a linear combination of n-qubit Pauli operators to reduce the complexity of the computations. The method is suitable for Hamiltonians of a certain type, which, nevertheless, represent a wide class of quantum systems in condensed matter physics. Note that we will understand the problem of Hamiltonian simulation in a wide sense. Namely, if the parameter τ is purely imaginary, say $\tau = -it$, then the operator exponential describes the unitary time evolution of a closed quantum system. On the other hand, the exponential $\exp\left(-\beta\hat{H}\right)/Z$ is the density operator of a quantum subsystem weakly interacting with a thermal environment having the inverse temperature β. We will consider only time-independent Hamiltonians.

The paper is organized as follows. Sec. 2 contains some mathematical preliminaries, in particular necessary definitions and properties of the Pauli basis. Sec. 3 is devoted to the description of our method and the corresponding algorithm. In Sec. 4 we consider a cluster consisting of three qubits, three model Hamiltonians for different types of interaction, and compute the corresponding exponentials and spectra. Sec. 5 deals with the same cluster interacting with a thermal environment. In the last two sections, our goal is twofold: first, we want to demonstrate the proposed method with a specific example (which admits fully analytical calculations), and second, to present a prototype of some realistic models for clusters that include a three-qubit interaction.

Throughout the paper, we use the natural system of units with $c = 1$, $\hbar = 1$, and $k_B = 1$, so that energy and temperature are measured in units of inverse length.

2. Pauli basis

Let $\mathcal{H}$ be a one-qubit Hilbert space and $\mathcal{H}_n = \mathcal{H}^{\otimes n}$ be the corresponding 2^n-dimensional Hilbert space for a quantum system of n distinguishable qubits. Let $L(\mathcal{H}_n) = \mathcal{H}_n \otimes \mathcal{H}_n^\dagger$ be the space of linear operators acting on $\mathcal{H}_n$ and $\mathcal{H}_n^\dagger$ by the left and right contractions respectively. It is obvious that $L(\mathcal{H}_n)$ is a Hilbert space with respect to the Hilbert-Schmidt inner product, $\langle \hat{A}, \hat{B}\rangle = \operatorname{tr}(\hat{A}^\dagger \hat{B})$, $\hat{A}, \hat{B} \in L(\mathcal{H}_n)$, and obviously $\dim_{\mathbb{C}} L(\mathcal{H}_n) = 4^n$. The identity operator, $\hat{\sigma}_0 = |0\rangle\langle 0| + |1\rangle\langle 1|$, and the three Pauli operators

$$\hat{\sigma}_1 = |0\rangle\langle 1| + |1\rangle\langle 0|, \quad \hat{\sigma}_2 = -i\,|0\rangle\langle 1| + i\,|1\rangle\langle 0|, \quad \hat{\sigma}_3 = |0\rangle\langle 0| - |1\rangle\langle 1|$$

form the Pauli basis in $L(\mathcal{H})$. Recall that

$$\begin{gathered} \operatorname{tr}\hat{\sigma}_k = 0, \quad \hat{\sigma}_k^2 = \hat{\sigma}_0, \\ \{\hat{\sigma}_k, \hat{\sigma}_l\} = 0, \quad [\hat{\sigma}_k, \hat{\sigma}_l] = 2i\operatorname{sign}(\pi)\hat{\sigma}_m, \quad (klm) = \pi(123), \end{gathered} \tag{1}$$

where $\pi(123)$ is a permutation of $\{1,2,3\}$, $k,l,m \in \{1,2,3\}$; $[\,,]$ and $\{\,,\}$ denote the commutator and anticommutator respectively.

The *Pauli basis* in $L(\mathcal{H}_n)$ is defined by

$$\left\{\hat{\sigma}_{k_1\ldots k_n}\right\}_{k_1,\ldots,k_n\in\{0,1,2,3\}}, \quad \hat{\sigma}_{k_1\ldots k_n} = \hat{\sigma}_{k_1}\otimes\ldots\otimes\hat{\sigma}_{k_n}, \tag{2}$$

where $\hat{\sigma}_{0\ldots0}$ is the identity operator. It is obvious that the Pauli basis consists of 4^n elements. We will use compact notations like $\hat{\sigma}_K = \hat{\sigma}_{k_1\ldots k_n}$, denoting the string $k_1\ldots k_n$, $k_1,\ldots,k_n \in \{0,1,2,3\}$, by the corresponding decimal representation K, $0 \leqslant K \leqslant 4^n-1$. Note that all the operators $\hat{\sigma}_K$ are Hermitian and unitary at the same time. In addition, one can easily check the useful relations

$$\hat{\sigma}_K^2 = \hat{\sigma}_{0\ldots0}, \quad \left\{\operatorname{tr}\hat{\sigma}_K\right\}_{K\neq0} = 0, \quad \operatorname{tr}\hat{\sigma}_{0\ldots0} = 2^n. \tag{3}$$

In what follows, we often use the symbol $\hat{I}$ to denote $\hat{\sigma}_{0\ldots0}$, if its meaning is clear from the context.

The following proposition is a direct consequence of relations (1): *any two operators of the Pauli basis, say $\hat{\sigma}_K$ and $\hat{\sigma}_L$, either commute or anticommute, that is*,

$$\textit{either}\ \ [\hat{\sigma}_K,\hat{\sigma}_L] = 0\ \ \textit{or}\ \ \ \{\hat{\sigma}_K,\hat{\sigma}_L\} = 0. \tag{4}$$

The strings $K = k_1\ldots k_n$ and $L = l_1\ldots l_n$ completely define the corresponding Pauli operators $\hat{\sigma}_K$ and $\hat{\sigma}_L$. Let p be the number of pairs (k_α, l_α), where $k_\alpha \in K$ and $l_\alpha \in L$, such that $k_\alpha \neq 0$, $l_\alpha \neq 0$, and $k_\alpha \neq l_\alpha$, $\alpha = 1,2,\ldots,n$. *If p is even (odd), then the operators commute (respectively, anticommute).* The proof of this statement is elementary.

The statement (4), which can be rewritten in the form $\hat{\sigma}_L\hat{\sigma}_K\hat{\sigma}_L = \pm\hat{\sigma}_K$, play a key role in implementation of our algorithm presented in the next section. Note also that Hamiltonians and density operators, being Hermitian, are written as linear combinations of the Pauli basis operators with *real* coefficients.

3. Decompositions of Hamiltonians in the Pauli basis

The simplest version of the Lie–Trotter–Suzuki decomposition has the form

$$e^{\tau H} = (e^{\tau H_1/m}e^{\tau H_2/m}\ldots e^{\tau H_r/m})^m + O(\tau^2 r^2/m).$$

In practice, one usually uses an enhanced formula of forth order, which gives an error of order $O(\tau^5 r^5/m^4)$, however, in any case, the operator exponentials in the product must be calculated with very high accuracy. Note that if these exponentials can be represented analytically in a simple closed form, it may be possible to reduce the exponential complexity to polynomial.

In Hamiltonian simulation, the first step as always is to divide, in some "maximal" way, the original Hamiltonian into pairwise commuting Hermitian parts, so that the total operator exponential will be found as the product of the exponentials of these partial Hamiltonians. Let $\hat{H}$ be such a partial

Hamiltonian. In what follows, we require that it can be represented as the sum

$$\hat{H} = \sum_{k=1}^{K} a_k \hat{H}_k, \quad a_k \in \mathbb{R}, \tag{5}$$

where the operators $\hat{H}_k$ are Hermitian and satisfy the conditions

$$\{\hat{H}_k, \hat{H}_l\}_{k \leqslant l} = b_m \hat{H}_m, \quad b_m \in \mathbb{R}, \quad k, l, m \in \{1, 2, \dots, K\}. \tag{6}$$

In addition, we assume that $K \ll 4^n$, since otherwise this decomposition does not have any meaningful sense. In formula (6), the integer-valued function $m = m(k, l)$ completely defines the anticommutation relations. Therefore, from a purely computational point of view, our algorithm reduces to an iterative procedure for this function and finite summation operations. Indeed, the next step obviously consists in computing the powers of $\hat{H}$. The second power is

$$\hat{H}^2 = \sum_{k \leqslant l} a_k a_l b_{m(k,l)} \hat{H}_{m(k,l)},$$

so that, after collecting similar terms, we obtain the decomposition of the form (5) with other coefficients, say c_k. Then the third power (and analogously the fourth one) of $\hat{H}$ has the form

$$\hat{H}^3 = \sum_{k \leqslant l} a_k c_l b_{m(k,l)} \hat{H}_{m(k,l)}.$$

It is important that the series of coefficients at the powers of the operator can often be summarized into a simple closed expression.

The proposed algorithm starts with the decomposition of the Hamiltonian in accordance with the expressions (5) and (6). Here the conditions (6) seem to be very strong. However, first, they are automatically satisfied for any set of anticommuting Pauli basis operators and, therefore, are of great significance in applications. Second, the model Hamiltonian of a quantum system often has a high degree of symmetry. It takes place, for example, under the quite weak assumption that there exists some sufficiently large permutation group, acting on qubits, such that the Hamiltonian is invariant with respect to this action. In the latter case, the conditions (6) usually hold and, moreover, the terms in the decomposition (5) have a number of common eigenvectors. And third, for Ising-type Hamiltonians, the corresponding lattice, as a rule, can be partitioned in some suitable way into local subsets for which the conditions (6) hold.

In conclusion of this section, we consider a special but very important version of the conditions (6) when

$$\hat{H}_k^2 = \hat{I}, \quad \{\hat{H}_k, \hat{H}_l\}_{k \neq l} = 0, \quad k, l = 1, 2, \dots, \tag{7}$$

where we formally add the identity operator $\hat{I} = \hat{H}_0$ to the set $\{\hat{H}_k\}_{k=1}^K$ to keep it closed under the anticommutation operation. In this case, an elementary calculation gives the following relations for the powers of $\hat{H}$:

$$\hat{H}^{2k+1} = a^{2k}\hat{H}, \quad \hat{H}^{2k} = a^{2k}\hat{I}, \quad k = 1, 2, \dots, \quad a = \left(\sum_{k=1}^{K} a_k^2\right)^{1/2}.$$

From the power series expansion, the exponential of the Hamiltonian (5), in its turn, can now be obtained in a simple closed form:

$$\exp\left(\tau\hat{H}\right) = \hat{I} + \tau\hat{H} + \frac{\tau^2}{2!}\hat{H}^2 + \frac{\tau^3}{3!}\hat{H}^3 + \frac{\tau^4}{4!}\hat{H}^4 + \dots =$$

$$= \left(\hat{I} + \frac{a^2\tau^2}{2!}\hat{I} + \frac{a^4\tau^4}{4!}\hat{I} + \dots\right) + \left(\frac{a\tau}{a}\hat{H} + \frac{a^3\tau^3}{a3!}\hat{H} + \dots\right) =$$

$$= \operatorname{ch}(a\tau)\hat{I} + \frac{\operatorname{sh}(a\tau)}{a}\hat{H}. \quad (8)$$

It is appropriate to clarify the significance of the obtained formula by the fact that the relations (7) are automatically fulfilled if the decomposition (5) contains only anticommuting Pauli operators. Note also that there is one more important special case when, in addition to the conditions (6), the operators $\hat{H}_k$ commute pairwise, $[\hat{H}_k, \hat{H}_l] = 0$ (the next section deals with just such a case). Then the exponential $\exp\left(\tau\hat{H}\right)$ is the product of exponentials $\exp\left(\tau a_k \hat{H}_k\right)$ of partial Hamiltonians, and each exponential can be calculated using a simple version of the basic algorithm and naturally represented as a linear combination of the operators $\hat{H}_k$. Then the product should be expanded into a linear combination of all the same operators.

4. Three-qubit model Hamiltonians

In the literature, there are many examples of few-qubits (usually two- and three-qubits) systems with various model Hamiltonians (see e.g. [8] and the references therein). In this section, we consider a three-qubit cluster and three model Hamiltonians describing different types of internal interaction between the qubits. The most important distinctive feature of these Hamiltonians is the presence of three-qubit interactions. In order to perform all calculations in an analytical form and thereby provide an illustrative example of using our algorithm, the Hamiltonians are chosen to be invariant under permutations of qubits. Namely, we define two Hamiltonians (the third one is $\hat{H}_1 + \hat{H}_2$) by the relations

$$\hat{H}_1 = \frac{1}{12}\left(\hat{F}_1 + \hat{F}_2 + \hat{F}_3 + 3\hat{S}\right), \quad \hat{H}_2 = \frac{1}{12}\left(\hat{G}_1 + \hat{G}_2 + \hat{G}_3 + 3\hat{I}\right). \quad (9)$$

where $\hat{S} = -\hat{\sigma}_{333}$, and

$$\hat{F}_1 = \hat{\sigma}_{113} + \hat{\sigma}_{131} + \hat{\sigma}_{311}, \quad \hat{F}_2 = \hat{\sigma}_{223} + \hat{\sigma}_{232} + \hat{\sigma}_{322}, \quad \hat{F}_3 = \hat{\sigma}_{003} + \hat{\sigma}_{030} + \hat{\sigma}_{300},$$

$\hat{G}_1 = \hat{\sigma}_{022}+\hat{\sigma}_{202}+\hat{\sigma}_{220}, \quad \hat{G}_2 = \hat{\sigma}_{011}+\hat{\sigma}_{101}+\hat{\sigma}_{110}, \quad \hat{G}_3 = -\hat{\sigma}_{033}-\hat{\sigma}_{303}-\hat{\sigma}_{330}.$

Given the symmetry, one can easily obtain the relations

$$\{\hat{F}_i, \hat{S}\} = 2\hat{G}_i, \quad \{\hat{G}_i, \hat{S}\} = 2\hat{F}_i, \quad i = 1, 2, 3,$$

$$\{\hat{F}_i, \hat{F}_j\} = 2\hat{G}_k, \quad \{\hat{G}_i, \hat{G}_j\} = 2\hat{G}_k, \quad \{\hat{F}_i, \hat{G}_j\} = 2\hat{F}_k, \quad i \neq j \neq k,$$

$$\{\hat{F}_1, \hat{G}_1\} = 6\hat{S} + 4\hat{F}_1, \quad \{\hat{F}_2, \hat{G}_2\} = 6\hat{S} + 4\hat{F}_2, \quad \{\hat{F}_3, \hat{G}_3\} = 6\hat{S} - 4\hat{F}_3.$$

The squares of the operators are $\hat{S}^2 = \hat{I}$ and

$$\hat{F}_1^2 = \hat{G}_1^2 = 3\hat{I} + 2\hat{G}_1, \quad \hat{F}_2^2 = \hat{G}_2^2 = 3\hat{I} + 2\hat{G}_2, \quad \hat{F}_3^2 = \hat{G}_3^2 = 3\hat{I} - 2\hat{G}_3.$$

Using these relations, we find that the Hamiltonians $\hat{H}_1$ and $\hat{H}_2$ commute, $[\hat{H}_1, \hat{H}_2] = 0$, and

$$\{\hat{H}_1, \hat{H}_2\} = 2\hat{H}_1, \quad \hat{H}_1^2 = \hat{H}_2^2 = \hat{H}_2, \tag{10}$$

so that

$$\hat{H}_1^3 = \hat{H}_1, \;\; \hat{H}_1^4 = \hat{H}_2, \;\; \hat{H}_1^5 = \hat{H}_1, \ldots, \quad \hat{H}_2^3 = \hat{H}_2, \quad \hat{H}_2^4 = \hat{H}_2, \ldots.$$

Finally, using the above relations and the Taylor series expansion of the operator exponential, we obtain

$$\exp\left(\tau\hat{H}_1\right) = \hat{I} + \tau\hat{H}_1 + \frac{\tau^2}{2}\hat{H}_1^2 + \frac{\tau^3}{3!}\hat{H}_1^3 + \frac{\tau^4}{4!}\hat{H}_1^4 + \frac{\tau^5}{5!}\hat{H}_1^5 + \cdots =$$

$$= \hat{I} + \left(\tau + \frac{\tau^3}{3!} + \frac{\tau^5}{5!} + \cdots\right)\hat{H}_1 - \hat{H}_2 + \left(1 + \frac{\tau^2}{2} + \frac{\tau^4}{4!} + \cdots\right)\hat{H}_2 =$$

$$= \hat{I} + \mathrm{sh}\tau\hat{H}_1 + (\mathrm{ch}\tau - 1)\hat{H}_2, \tag{11}$$

and analogously,

$$\exp\left(\tau\hat{H}_2\right) = \hat{I} + (\mathrm{e}^\tau - 1)\hat{H}_2. \tag{12}$$

We will also consider the Hamiltonian

$$\hat{H} = \hat{H}_1 + \hat{H}_2, \tag{13}$$

for which the corresponding exponential is

$$\exp\left(\tau\hat{H}\right) = \hat{I} + \mathrm{e}^\tau\mathrm{sh}\tau\hat{H}_1 + \mathrm{e}^\tau\,(\mathrm{ch}\tau - 1)\hat{H}_2. \tag{14}$$

The Hamiltonians (9) and (13) have the same eigenvectors, but of course their eigenvalues must be different. We also have the following consequence of the symmetry of $\hat{H}_1$, $\hat{H}_2$, and $\hat{H}$: if a state is invariant under all permutations

of qubits, then it is obviously the eigenvector of these Hamiltonians. This implies that the states

$$S_0 = |000\rangle\,, \quad S_1 = |111\rangle\,,$$
$$W = \frac{|001\rangle + |010\rangle + |100\rangle}{\sqrt{3}}, \quad \widetilde{W} = \frac{|011\rangle + |101\rangle + |110\rangle}{\sqrt{3}},$$

are eigenvectors for them, where W is one of the two inequivalent classes of completely entangled states, and $\widetilde{W}$ is the "false", W-state. Other four eigenvectors can be chosen as

$$V_1 = \frac{2\,|001\rangle - |010\rangle - |100\rangle}{\sqrt{6}}, \quad V_2 = \frac{|010\rangle - |100\rangle}{\sqrt{2}},$$
$$V_3 = \frac{2\,|011\rangle - |101\rangle - |110\rangle}{\sqrt{6}}, \quad V_4 = \frac{|101\rangle - |110\rangle}{\sqrt{2}}.$$

These eight eigenvectors make up an orthonormal basis in the Hilbert space $\mathcal{H}^{\otimes 3}$. The Hamiltonians (9) and (13) have strongly degenerate spectra. By introducing the notations $[S] = \{S_0, S_1\}$ and $[V] = \{V_1, V_2, V_3, V_4\}$, we can write down these spectra as

$$\mathrm{Spec}\,\hat{H}_1 = \{\,(-1, \widetilde{W}),\, (0, [S], [V]),\, (1, W)\}, \tag{15}$$

$$\mathrm{Spec}\,\hat{H}_2 = \{(0, [S], [V]),\, (1, W, \widetilde{W})\}, \tag{16}$$

$$\mathrm{Spec}\,\hat{H} = \{(0, [S], [V], \widetilde{W}),\, (2, W)\}, \tag{17}$$

where the real numbers in round parentheses denote the corresponding eigenvalues.

5. Three-qubit cluster in a thermal environment

Model Hamiltonians provide wide possibilities for approximate simulation of real quantum systems in condensed matter physics. This section is devoted to a toy model of a material consisting of three-qubit clusters with strong intracluster quantum coherence and a weak (thermal) intercluster interaction. Such models of clusters in the presence of a thermal environment were considered earlier for two-qubit clusters [9] and three and four-qubit clusters [10–12] with simpler but less symmetric Hamiltonians. We will use the Hamiltonians that were studied in the previous section.

In general, the total Hamiltonian of a subsystem and a thermal environment (bath), weakly coupled with each other, is given by the sum

$$\hat{H} = \hat{H}_s + \hat{H}_b + \hat{H}_{int}.$$

In this connection, there arises a subtle issue whether the density operator of the subsystem, $\rho(t)$, given in an arbitrary initial state $\rho(0)$, will come to an equilibrium (Gibbs) state over long time. For Hamiltonians with nondegenerated spectrum, von Neumann proves this statement rigorously in his

pioneer paper [13] (see also [14, 15]). However, it is shown in [16] that the requirement of non-degeneracy can be ruled out; in this case, the subsystem will reside close to a fixed equilibrium state most of the time. Also, there are no theoretical or experimental examples of degenerate subsystems with non-equilibrium long time dynamics in the literature. On the other hand, the degeneracy is a consequence of the high symmetry of the subsystem's Hamiltonian, but in realistic situations, perturbations violate the degeneracy of energy level [17]. Our consideration will be based on the following assumption: if the intensity of the interaction (in the sense of the usual operator norm of $\hat{H}_{int}$) between the subsystem and the environment is much less than the temperature $1/\beta$, and the internal interaction (determined by H_s) of qubits in the subsystem is greater than $1/\beta$, then the subsystem will be in a state being very close to the Gibbs state $\hat{\rho} = \exp\bigl(-\beta\hat{H}_s\bigr)/Z$.

At this stage, we have to introduce a dimensional factor into the Hamiltonians (9) and (13) by replacing $\hat{H} \to \omega\hat{H}$ or, equivalently, by setting $\tau = -\beta\omega$, where $[\omega] = L^{-1}$; in other words, the coefficient $1/12$ in (9) will be replaced by $\omega/12$. According to formulae (15)–(17), the eigenvalues of the Hamiltonians $\hat{H}_1$, $\hat{H}_2$, and $\hat{H}$ are $\{-\omega, 0, \omega\}$, $\{0, \omega\}$, and $\{0, 2\omega\}$, respectively. For the interaction $\hat{H}_1$, the ground state of the system is non-degenerated, as well as the exited state for $\hat{H}$, while both the states for the Hamiltonian $\hat{H}_2$ are degenerated. From the expressions (11), (12), and (14), one can find the corresponding partition functions $Z = \operatorname{tr}\exp\bigl(-\beta\hat{H}\bigr)$ and density operators $\hat{\rho} = \exp\bigl(-\beta\hat{H}\bigr)/Z$. Taking into account that $\operatorname{tr}\hat{H}_1 = 0$ and $\operatorname{tr}\hat{H}_2 = 2\omega$, we obtain

$$
\begin{gathered}
Z_1 = 6 + 2\operatorname{ch}(\omega\beta), \quad Z_2 = 6 + 2\mathrm{e}^{-\omega\beta}, \quad Z = 9 - 2\mathrm{e}^{-\omega\beta} + \mathrm{e}^{-2\omega\beta}, \\
\hat{\rho}_1 = \frac{1}{Z_1}\left[\hat{I} - \frac{\operatorname{sh}(\omega\beta)}{\omega}\hat{H}_1 + \frac{\operatorname{ch}(\omega\beta) - 1}{\omega}\hat{H}_2\right], \\
\hat{\rho}_2 = \frac{1}{Z_2}\left[\hat{I} + \frac{\mathrm{e}^{-\omega\beta} - 1}{\omega}\,\hat{H}_2\right],
\end{gathered}
\tag{18}
$$

$$
\hat{\rho} = \frac{1}{Z}\left[\hat{I} - \frac{\mathrm{e}^{-\omega\beta}\operatorname{sh}(\omega\beta)}{\omega}\hat{H}_1 + \frac{\mathrm{e}^{-\omega\beta}(\operatorname{ch}(\omega\beta) - 1)}{\omega}\,\hat{H}_2\right]. \tag{19}
$$

We see that the partition function Z_1 diverges in the low temperature limit. In a real system, the divergence will be compensated by the sharp dominance of the Hamiltonian H_{int} in comparison with the temperature. In fact, the condition of weak coupling between the cluster and its thermal environment is violated for all the three types of interaction in the region $\beta \gg 1$. Therefore, there are no equilibrium states despite of good definiteness of the density operators: for $\beta \to \infty$, we have (with the same error $O(\mathrm{e}^{-\omega\beta})$)

$$
\hat{\rho}_1 = \frac{\hat{H}_2 - \hat{H}_1}{2\omega}, \quad \hat{\rho}_2 = \frac{\hat{I}}{6} - \frac{\hat{H}_2}{6\omega}, \quad \hat{\rho} = \frac{\hat{I}}{9} + \frac{\hat{H}_2 - \hat{H}_1}{18\omega}.
$$

The divergence of Z_1 is reflected in the fact that $\hat{\rho}_1$ is a pure state in the zero temperature limit, $\hat{\rho}_1^2 = \hat{\rho}_1$, so that it cannot represent any Gibbs state. An analogous picture takes place at high temperatures. In this case, the internal interaction between qubits becomes of the order of $1/\beta$ or less than it, so that the cluster again cannot be considered in isolation from the entire system. In the region $\beta \ll 1$ where quantum effects no longer dominate, we have the usual semiclassical behavior (in particular, all eigenstates are almost equally probable)

$$\hat{\rho} = \hat{\rho}_1 = \frac{\hat{I} - \beta\hat{H}_1}{8} + O(\beta^2), \quad \hat{\rho}_2 = \frac{4 + \omega\beta}{32}\hat{I} - \frac{\beta}{8}\hat{H}_2 + O(\beta^2), \quad \beta \to 0.$$

Using the well-known expressions for the average energy, von Neumann entropy, and free energy,

$$\mathcal{E} = \operatorname{tr}(\hat{\rho}\hat{H}) = -\partial_\beta \ln Z, \quad S = \ln Z + \beta\mathcal{E}, \quad \mathcal{F} = \mathcal{E} - TS = -\frac{1}{\beta}\ln Z, \quad (20)$$

we have plotted in figures 1 and 2, respectively, the entropies and free energies for the three states under considerations. Recall that the transition from natural units to ordinary units consists in the replacements

$$\beta \to \frac{\beta}{c\hbar}, \quad \omega \to c\hbar\omega.$$

Thus the value $\beta = 1$ corresponds to the inverse temperature $1/T \approx 3 \cdot 10^{16}\,\mathrm{erg}^{-1}$, that is, $T \approx 3 \cdot 10^{-17}\,\mathrm{erg} \approx 0.2\,\mathrm{K}$. Note that the usual working inverse temperatures of qubits, realized, for example, in the form of quantum dots or superconducting artificial atoms, are in the interval $0.2 \leqslant \beta \leqslant 2$.

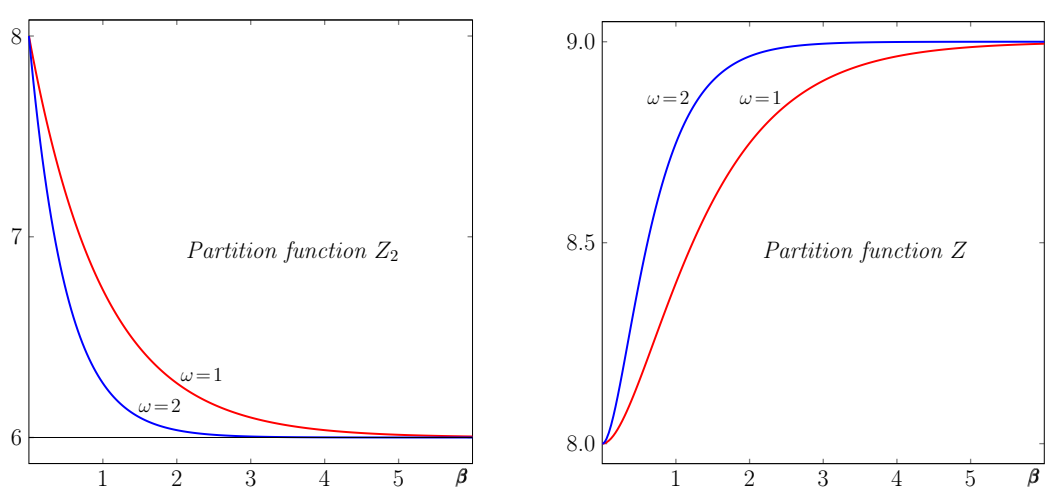

Figure 1. In the low temperature region, $\lim\limits_{\omega\to\infty} Z_2 = 6$ and $\lim\limits_{\omega\to\infty} Z = 9$, in contrast to the partition function Z_1, which diverges

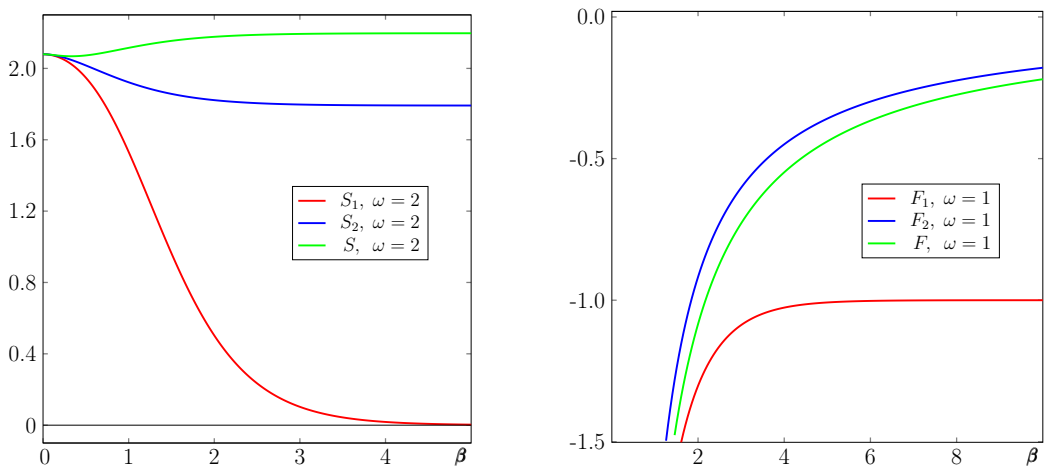

Figure 2. Entropy $S(\beta)$ (left panel) and free energy $F(\beta)$ (right panel) for the states (18) and (19). In the low temperature limit $\beta \to \infty$, we have, with an error $O(\mathrm{e}^{-2\omega\beta})$, the expansions $F_1 = -\omega - (6/\beta)\mathrm{e}^{-\omega\beta}$, $F_2 = -(\ln 6)/\beta - \mathrm{e}^{-\omega\beta}/(3\beta)$, $F = -(\ln 9)/\beta + 2\mathrm{e}^{-\omega\beta}/(9\beta)$. In the high temperature limit $\beta \to 0$, we have $F_1 \sim F_2 \sim F \sim -3(\ln 2)/\beta$

6. Conclusions

We have presented a simple method for simulating multi-qubit clusters having Hamiltonians of a special form, but nevertheless covering a wide range of quantum systems in condensed matter physics. It is assumed that the Hamiltonian of a quantum system can be represented as a linear combination of some set of partial Hamiltonians, so that their anticommutators up to a factor are themselves elements of this set. Another feature of our approach is the use of the Pauli basis, in which all calculations have the simplest form. To demonstrate the effectiveness of the main algorithm, we considered a cluster of three qubits and three model Hamiltonians representing various types of interactions that are symmetric under permutations of qubits and therefore make possible a fully analytical treatment.

Our algorithm was used to find the density operator, partition function, entropy, and free energy of such a cluster, weakly coupled to a thermal environment, for the Hamiltonians under consideration. In our model, the cluster is in a Gibbs state in the temperature interval 0.1−2 K, that is, in the operating range of modern quantum processors. Our analysis showed that the thermodynamic properties of such a system strongly depend on the type of internal interaction of qubits in the cluster.

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Моделирование в базисе Паули гамильтонианов многокубитных кластеров физики конденсированного состояния

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Аннотация. Предлагается эффективный метод математического моделирования гамильтонианов многокубитных квантовых систем с взаимодействием специального вида. В нашем подходе гамильтониан системы n кубитов должен быть представлен линейной комбинацией в стандартном базисе Паули, а затем разложен в сумму частичных гамильтонианов, которые, вообще говоря, не являются операторами Паули и удовлетворяют некоторым антикоммутационным соотношениям. Для трёх типов гамильтонианов, инвариантных относительно перестановок кубитов, эффективность основного алгоритма в модели трёхкубитного кластера показана посредством вычисления операторных экспонент этих гамильтонианов в явном аналитическом виде. Кроме того, вычислен оператор плотности состояния, статистическая сумма, энтропия и свободная энергия для кластера, слабо связанного с термостатом. В нашей модели кластер находится в состоянии Гиббса в интервале температур 0,1—2 K, что соответствует рабочему диапазону современных квантовых процессоров. Из нашего анализа следует, что термодинамические свойства такой системы сильно зависят от типа внутреннего взаимодействия кубитов в кластере.

Ключевые слова: моделирование квантовых гамильтонианов, кластер кубитов, операторная экспонента, термостат, состояние Гиббса, термодинамические свойства