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Simulation of the excited state decay in the quantum register

Abstract. *This paper investigates whether a quantum computer can efficiently simulate an exponential decay of probability of finding a quantum system in an excited state. An algorithm is presented for simulating the time evolution of such a system, implemented on standard two-input gates. The paper examines the properties of the proposed algorithm and then compares the obtained results with theoretical predictions.*

Streszczenie. *W artykule badamy czy komputer kwantowy potrafi efektywnie symulować eksponencjalny zanik prawdopodobieństwa przebywania układu kwantowego w stanie wzbudzonym. Głównym rezultatem pracy jest algorytm, który umożliwia symulację czasową tego typu układów zaimplementowany na standardowych dwówejściowych bramkach. Badamy tutaj własności proponowanego algorytmu i porównujemy go z przewidywaniami teoretycznymi.* ***(Symulacja rozpadu stanu wzbudzonego w rejestrze kwantowym)***

Keywords: quantum computations, quantum simulations, excited state decay
Słowa kluczowe: obliczenia kwantowe, symulacje kwantowe, rozpad stanu wzbudzonego

In the near future, quantum calculations can make a major contribution to the development of informatics [1]. Although practical implementations of quantum computer have not been built yet, its existence seems to be possible. Therefore, it is worth examining the properties of such machines.

Today we know Shor [2] and Grover [3] algorithms which are of lower computational complexity than their best classical counterparts. Another promising application of quantum computer are quantum simulations [4, 5, 6], i.e. the computer modeling of behavior of physical quantum systems. It gives the possibility of effective modeling quantum processes, which is not possible using classical computers [7]. Quantum computers can simulate a wide variety of quantum systems, including fermionic lattice models [8, 9], quantum chemistry [10, 11], and quantum field theories [12].

As is well known, simulations of quantum systems performed using conventional computers are not effective. This means that for classical computer the memory resources and time required to simulate grow exponentially with the size of quantum system. In the case of a quantum computer, the situation is different. The relationship between the size of quantum computer (register) and the size of the simulated quantum system is linear. Therefore, a very important task is to find the appropriate algorithms that can properly simulate complex quantum systems and non-trivial interactions between them. This is a difficult issue, because most of the interesting quantum systems is feasible in infinitely-dimensional Hilbert spaces. In such situations, we can use the technique of sampling the wave function and build an algorithm based on Quantum Fourier Transform. This case was tested in [13, 14, 15, 16], which examined the free particle and the harmonic oscillator. The main limitation of this coding method of the particle state is that it does not enable implementing an arbitrary potential $V(x)$. It allows only a few special cases such as the $V(x) \sim x^2$ potential. In our previous works we have shown that also rectangular potentials (like thresholds and wells) can be simulated using this method. This provides the ability to examine other interesting processes, such as the tunnel effect [17] and scatering of Pauli[18] and Dirac[19] particle.

In this work, we deal with other type of problem. As is well known, in a typical process occurring in nature, the excited states of quantum systems (like chemical particles or atoms) are unstable. A system undergoes a transition to the ground state and gets rid of the excess of energy by emission of a photon. The loss of probability of finding the system in an excited state has an exponential character. Since this is a common phenomenon, it seems interesting to investigate how to simulate it in a simple manner in the quantum register. Unfortunately, the processes of this type usually occur as a result of interaction with quantum fields (such as electromagnetic field), which are systems with an infinite number of degrees of freedom. In this paper, we propose an algorithm which replaces the quantum field receiving energy from an excited state with a system with a finite number of base states. The algorithm presented can be efficiently simulated in a small (12-16-qubit) quantum register and can be used as a component part of a bigger algorithm simulating more complex processes.

Theoretical approach to the problem of unstable quantum systems decay can be found in [20]. Other works focus on the simulation of excited states decay. In particular, models based on cavity QED are tested. For example, processes such as: beta decay of helium atom [21] and decay of two-level atom in crystal [22] are examined. In contrast to the cited works, we examine the problem on purely algorithmic grounds, using abstract model of quantum gates. We abstract completely from specified physical implementation.

In order to simulate a quantum register, we used a simple environment written in C language for a single processor. However, there is possibility of using parallel computation methods for the simulation of a quantum computer [23]. Moreover, some quantum algorithms can also be studied using neural networks and machine learning models [24].

Description of the simulated system

Let us consider a complex quantum system AB, which is composed of two parts A and B (Fig. 1). Subsystem A has two energy levels: level $|0\rangle_A$ with energy equal to zero (the ground state) and level $|1\rangle_A$ with energy E (the excited state). Subsystem B has a spectrum of energy consisting of $n+1$ levels, where n is a sufficiently large odd number. Level $|0\rangle_B$ is the ground state with energy equal to zero. Other n excited levels have energies given by the following formula:

$$E_{Bi} = E + \Delta\left(i - \frac{n+1}{2}\right) \qquad \text{for } i = 1, \ldots, n. \tag{1}$$

Parameter Δ is a gap between neighboring levels. Excited levels form a structure similar to the band. The center of this band ($\frac{n+1}{2}$ level) has energy equal to the energy of the excited state of subsystem A.

The following operator is chosen as the Hamiltonian of interaction between subsystems A and B:

$$\hat{H}_{int} = \sum_{i=1}^{n} (g_i \hat{a}^\dagger \hat{b}_i + g_i^* \hat{a} \hat{b}_i^\dagger), \tag{2}$$

where $\hat{a}$ is an operator decreasing energy of subsystem A

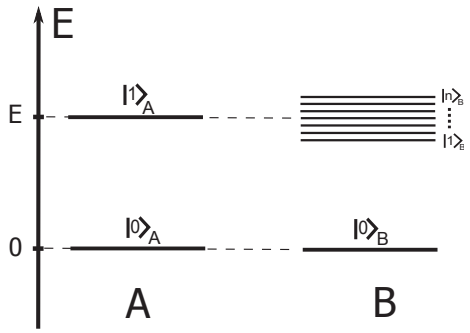

Fig. 1. Energy levels of A and B subsystems (in the absence of interactions)

and $\hat{b}_i$ are operators decreasing energies of subsystem B from i-th the excited state $|i\rangle_B$ to the ground state $|0\rangle_B$. Complex parameter g_i is a coupling constant. The form of the Hamiltonian (2) means that in addition to the resonant transition (i.e. the transition between states $|0, \frac{n+1}{2}\rangle \leftrightarrow |1, 0\rangle$) many other transitions near resonance are also allowed (i.e. transitions between states $|0, i\rangle \leftrightarrow |1, 0\rangle$).

The total Hamiltonian of the system AB has the form:

$$\hat{H} = E\,\hat{a}^\dagger\hat{a} + \sum_{i=1}^{n} E_{Bi}\,\hat{b}_i^\dagger\hat{b}_i + \hat{H}_{int}. \tag{3}$$

We are interested in examining the Schrödinger evolution of such a system for an initial state given in the form: $|\psi_{AB}(0)\rangle = |1, 0\rangle$. Thus, let us calculate the probability of finding subsystem A in an excited state as a function of time. This probability is given by the following formula:

$$P_{10}(t) = |\langle 0, 1|\psi_{AB}(t)\rangle|^2. \tag{4}$$

Let us introduce an additional constant parameter $\tilde{g}$ which is independent of Δ and n and fulfills the following relation:

$$g_i = \sqrt{\Delta}\tilde{g}. \tag{5}$$

It has been proved (see e.g. [25]) that for $n \to \infty$, $\Delta \to 0$ and $\tilde{g} = \text{const}$ searched distribution of probability (4) tends to the exponential distribution in the form:

$$P_{10}(t) = \exp\left(-\frac{2\pi}{\hbar}|\tilde{g}|^2 t\right). \tag{6}$$

If $n \to \infty$, then the number of possible channels of transition from state $|1, 0\rangle$ to states $|0, i\rangle$ becomes infinitely large. Hence, in order to obtain a finite time of transition, parameters g_i associated with these channels must be scaled according to the formula (5).

The aim is to obtain a result close to Eq. (6) for finite values of n and Δ in the quantum register. For this purpose, another simplification is made. Instead of simulating a single system B with n excited states, we simulate n two-levels B_i systems that have a single excited state with energy given by the formula (1). The interaction Hamiltonian between B_i and A subsystems is i-th component of the sum from the Hamiltonian (3). This manipulation increases the number of qubits necessary for the simulation, but it simplifies the implementation of the algorithm on the quantum gates.

The algorithm simulating time evolution of the system

The algorithm is implemented in a n_q-qubit register. In the first qubit, the state of subsystem A is stored. In states $|0\rangle$ and $|1\rangle$, the ground state and the excited state are encoded, respectively. In other $n_q - 1$ qubits, the states of subsystems B_i are stored. Analogously, states $|0\rangle_i$ and $|1\rangle_i$ are the ground state and the excited state of free Hamiltonian of systems B_i, respectively. The scheme of the algorithm is shown in Fig. 2. It is based on the time evolution operator $\hat{U}(\mathrm{d}t)$, which is given by:

$$\hat{U}(\mathrm{d}t) = \exp\left(-\mathrm{i}\hbar^{-1}\hat{H}\mathrm{d}t\right), \tag{7}$$

where dt is the time step.

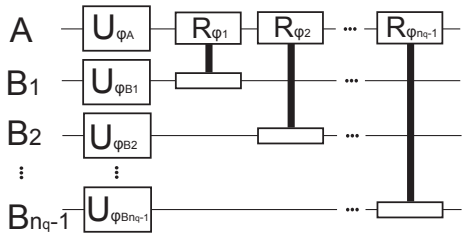

Fig. 2. The implementation of the algorithm. Blocks R_ϕ are shown in Fig. 3.

Gates $U_{\phi A}$ and $U_{\phi B_i}$ are phase-shift gates, which operate according to the scheme:

$$|0\rangle \to |0\rangle, \qquad |1\rangle \to \exp(-i\phi)|1\rangle, \tag{8}$$

where: $\phi_A = E\hbar^{-1}dt$, $\phi_{Bi} = E_{Bi}\hbar^{-1}dt$. Gates U_ϕ implement the free evolution of the system (the first two components from Eq. (3)). Implementation of two qubits interacting R_{ϕ_i} modules are shown in Fig. 3. Each of the modules implements the successive sum component from Eq. (2).

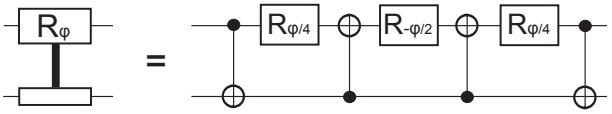

Fig. 3. The implementation of the interacting module. In addition to the one-input R_ϕ gates (described in the text), standard CNOT gates (denoted by $\bigoplus$) have also been used.

One-input R_ϕ gates from Fig. 3 operate as follows:

$$|0\rangle \to \cos\phi\,|0\rangle + \sin\phi\,|1\rangle, \tag{9}$$

$$|1\rangle \to \cos\phi\,|1\rangle - \sin\phi\,|0\rangle, \tag{10}$$

where $\phi = |g_i|dt/\hbar$. Parameters g_i are assumed to be independent of i. We calculate them using Eq. (5).

The simulation results

This part of the paper examines the implementation of the algorithm using ideal quantum gates. As an initial state of the simulated system we choose state in the form: $|1, 0, \ldots 0\rangle$ i.e. the excited state of A and ground states of B_i. The results of the simulation are shown in Figs 4-7. In Figs 4-6 solid (black) lines show theoretical results given by Eq. (6), whereas doted lines denote the results of the simulation (for $n_q = 4$(violet), 8(green), 12(blue) and 16(yellow) qubits). All these figures have been made for $E = 1.6 \cdot 10^{-19}$J, $\tilde{g} = 5 \cdot 10^{-11}\mathrm{J}^{1/2}$, $dt = 10^{-17}$s and for $200 \cdot 20$ time steps.

Conclusions

- From the above discussion, it can be seen that even for $n_q = 16$ qubits it is possible to obtain satisfying results.
- In the cases examined in this study, the best value obtained for Δ was $\Delta = 10^{-20}$J (in Fig. 5). Generally, high values of the Δ parameter seem better. However, for too large a value of Δ the subsystem A returns to the excited state at the end of the simulation (Fig. 6).

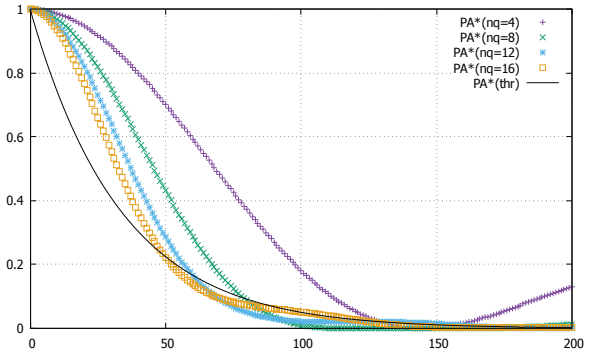

Fig. 4. The probability of finding system A in an excited state as a function of time, for $\Delta = 0.5 \cdot 10^{-20}$J.

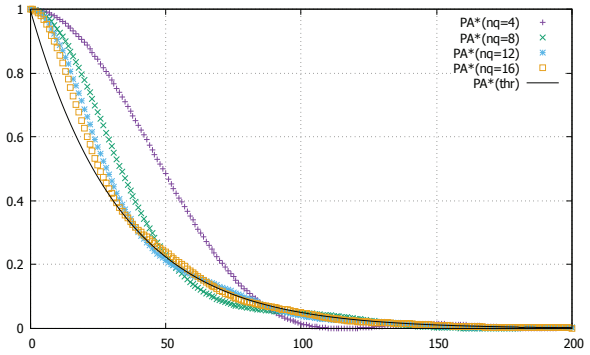

Fig. 5. The probability of finding system A in an excited state as a function of time, for $\Delta = 1 \cdot 10^{-20}$J.

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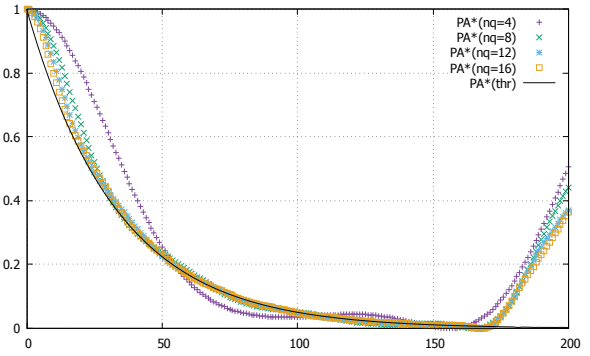

Fig. 6. The probability of finding system A in an excited state as a function of time, for $\Delta = 2 \cdot 10^{-20}$J.

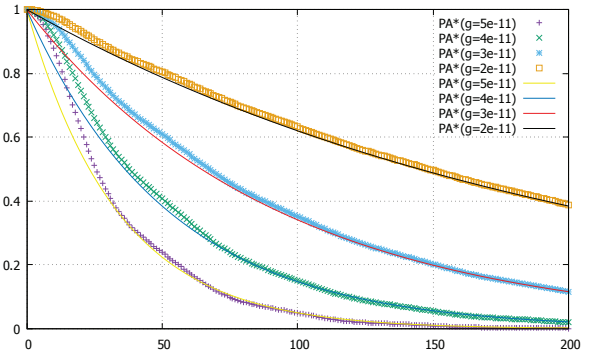

Fig. 7. The probability of finding system A in an excited state as a function of time, for $\tilde{g} = 2 \cdot 10^{-11}\text{J}^{1/2}, 3 \cdot 10^{-11}\text{J}^{1/2}, 4 \cdot 10^{-11}\text{J}^{1/2}$ and $5 \cdot 10^{-11}\text{J}^{1/2}$. Solid lines show theoretical results given by Eq. (6), wheras doted lines denote the results of the simulation. All curves have been made for $n_q = 16$, $E = 1.6 \cdot 10^{-19}$J, $\Delta = 10^{-20}$J, $dt = 10^{-17}$s and for $200 \cdot 20$ time steps.

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