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Simulation of Quantum Resonance in the Quantum Register

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Abstract. *In this paper, we examine whether a quantum computer can efficiently simulate resonant interaction between a pair of two-level quantum systems. We present an algorithm for simulating time evolution of such a system, implemented on standard two-input gates. We study the influence of accuracy of gates and decoherence on the quality of results.*
Keywords: *quantum computations, quantum simulations, quantum resonance.*

1. Introduction

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 Grower [3] algorithms which are faster than their best classical counterparts. Another promising application of quantum computer are quantum simulations, i.e. the computer modeling of behavior of physical quantum systems.

This work is a continuation of our earlier discussion. In papers [4, 5], we investigated the simulations of Schrödinger particle scattered on a rectangular potential.

In papers [6, 7], we investigated the case of Pauli and Dirac particle respectively. In this paper, we present an algorithm for simulating a pair of two-level quantum systems, which interact with each other. The Hamiltonian of interaction is chosen, such that it enables an exchange of energy between subsystems and leads to resonance.

In the literature, the problem of resonance in the context of quantum calculations often arises. However, in contrast to our considerations, the possibility of using NMR resonance to the quantum computation is tested (e.g. [8]). The problem of physical implementation of a quantum register is excluded from the present discussion. We are primarily interested in issues of quantum algorithmics.

The possibility of using a quantum register to simulate quantum systems has already been discussed in the literature ([9, 10]). The possibility of using parallel computation methods for the simulation of a quantum computer was shown in [11].

2. Quantum resonance - brief reminder

Let us consider a complex quantum system AB which is composed of two parts A and B. Both A and B are quantum systems with two base states. The system A is described by free Hamiltonian $\hat{H}_A$ which has two stationary states $|0\rangle_A$ and $|1\rangle_A$ with energies (eigenvalues) E_{A0} and E_{A1}, respectively. Analogously we assume that the system B is described by free Hamiltonian $\hat{H}_B$ with eigenstates $|0\rangle_B$ and $|1\rangle_B$ and energies equal to E_{B0} and E_{B1}, respectively. These states are shown in Fig. 1.

The free Hamiltonian of system AB (i.e. describing the lack of interaction between subsystems A and B) takes the form:

$$\hat{H}_0 = E_{A0}\hat{a}\hat{a}^\dagger + E_{A1}\hat{a}^\dagger\hat{a} + E_{B0}\hat{b}\hat{b}^\dagger + E_{B1}\hat{b}^\dagger\hat{b}, \tag{1}$$

where $\hat{a}$, $\hat{a}^\dagger$, $\hat{b}$ and $\hat{b}^\dagger$ are operators decreasing and increasing the energy defined as follows:

$$\begin{aligned} &\hat{a}|1\rangle_A = |0\rangle_A, \qquad \hat{a}|0\rangle_A = 0, \qquad \hat{a}^\dagger|0\rangle_A = |1\rangle_A, \qquad \hat{a}^\dagger|1\rangle_A = 0, \\ &\hat{b}|1\rangle_B = |0\rangle_B, \qquad \hat{b}|0\rangle_B = 0, \qquad \hat{b}^\dagger|0\rangle_B = |1\rangle_B, \qquad \hat{b}^\dagger|1\rangle_B = 0. \end{aligned}$$

As the Hamiltonian of interaction, we choose an operator in the form:

$$\hat{H}_{int} = g\hat{a}^\dagger\hat{b} + g^*\hat{a}\hat{b}^\dagger \tag{2}$$

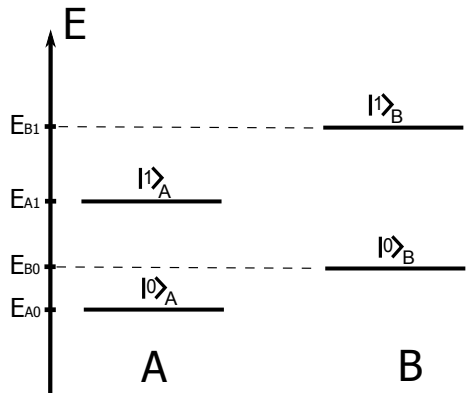

Figure 1: Energy levels of systems A and B in the case of absence of interaction

where g is a coupling constant. The Hamiltonian (2) causes transitions between states in the form: $|0,1\rangle \leftrightarrow |1,0\rangle$ and provides the ability to exchange energy between subsystems A and B.

Total Hamiltonian of the system AB has the form:

$$\hat{H} = \hat{H}_0 + \hat{H}_{int}. \tag{3}$$

3. The algorithm simulating time evolution of the system

The main purpose of this study is to introduce and examine an algorithm for simulating the interaction between two subsystems described by the Hamiltonian (3). We implement the algorithm in a two-qubit register. Stationary states of systems A and B correspond to base states ($|0\rangle$ and $|1\rangle$) of qubits.

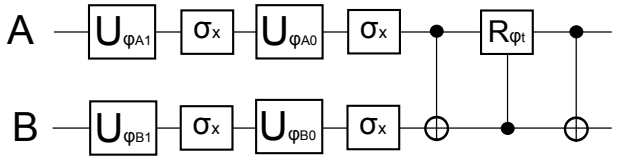

Figure 2: The scheme of the algorithm

The scheme of the algorithm is shown in Fig. 2. Gates $U_{\phi Ai}$, $U_{\phi Bi}$ and σ_x (NOT gate) implement the simulation of free evolution of subsystems A and B. The last three gates in Fig. 2 simulate the interaction described by the Hamiltonian (2). Gates $U_{\phi Ai}$ and $U_{\phi Bi}$ operate according to the scheme:

$$|0\rangle \to |0\rangle, \qquad |1\rangle \to e^{-i\phi}|1\rangle, \tag{4}$$

where: $\phi_{Ai} = E_{Ai}\hbar^{-1}dt$, $\phi_{Bi} = E_{Bi}\hbar^{-1}dt$ and dt is time step. Implementation of the controlled gate $R_{\phi i}$ is shown in Fig. 3. It works correctly only for $g = |g|\exp(\pm i\pi/2)$.

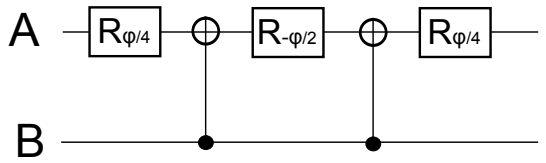

Figure 3: The implementation of controlled $R_{\phi i}$ gate

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

$$|0\rangle \to \cos\phi\,|0\rangle + \sin\phi\,|1\rangle, \tag{5}$$

$$|1\rangle \to \cos\phi\,|1\rangle - \sin\phi\,|0\rangle, \tag{6}$$

where $\phi = |g|dt/\hbar$.

4. The simulation results

4.1. Ideal simulation

In this part of the paper we examine implementation of the algorithm with use ideal quantum gates. As an initial state of the simulated system we choose state in the form: $|\psi\rangle = |0\rangle_A|1\rangle_B$. Parameters of the system we choose as follows: $E_{A0} = 1.6{\cdot}10^{-19}$J, $E_{A1} = 3.2{\cdot}10^{-19}$J, $E_{B0} = 1.6{\cdot}10^{-19}$J, $E_{B2} = \text{var}$, $|g| = 3.2{\cdot}10^{-20}$J and $\arg g = \pi/2$. Time step of the simulation is $dt = 2 \cdot 10^{-17}$s.

The results of simulation are shown in Fig. 4. The comparative results, presented in Fig. 4 in the form of solid lines, have been obtained from Eqs (25) and (26) (see the Appendix).

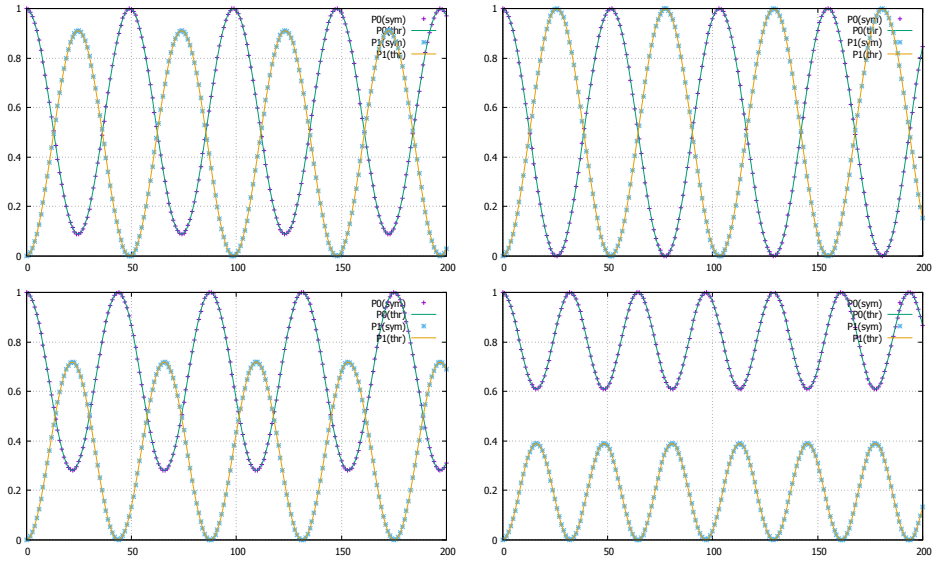

Figure 4: Probabilities of finding A and B systems in excited state ($|1\rangle_A$ and $|1\rangle_B$, respectively) as functions of number of time sample. Successive plots are made for energy E_2 equal to $3.0 \cdot 10^{-19}$J, $3.2 \cdot 10^{-19}$J (resonance), $3.6 \cdot 10^{-19}$J and $4.0 \cdot 10^{-19}$J, respectively. The dotted lines shows the results of the simulation. Solids lines represent comparative theoretical results. Plots for system A are shown as the yellow solid line and the line denoted by "x". Plots for system B are shown as the blue solid line and the line denoted by "+".

4.2. Simulation with the use of imperfect gates

In this case, we examine the algorithm implemented with the use of imperfect R_ϕ and U_ϕ gates. We assume that in each step of the simulation a phase error appears and phase ϕ has a uniform distribution in $(\phi_{ex} - 0.5 \cdot \phi_M, \phi_{ex} + 0.5 \cdot \phi_M)$ range, where ϕ_{ex} is an exact value of ϕ and ϕ_M is an error rate.

We perform the simulation for the same initial state and for the same parameters of the system as in the previous case (from section 3.1). We choose energy $E_2 = 3.0 \cdot 10^{-19}$J (it is first case from Fig. 4). We change only time step dt to 10^{-17}s. The results of simulation are shown in Fig. 5. Solid lines represent theoretical results obtained from Eqs (25) and (26).

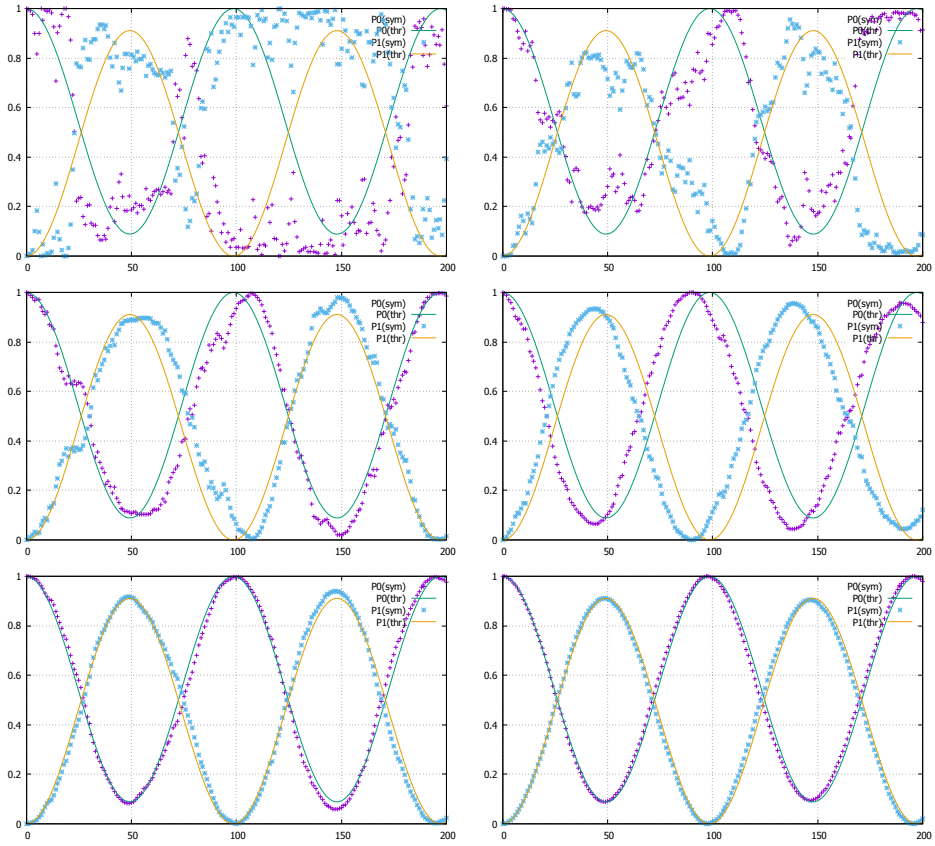

Figure 5: The simulation of the first case (from Fig. 4) for $dt = 10^{-17}s$ with the use of imperfect R_ϕ and U_ϕ gates. Successive plots are made for $\phi_M = 0.1, 0.05, 0.02, 0.01, 0.005, 0.002$, respectively.

4.3. Simulation with decoherence

In this case, we assume that each qubit of the register interacts independently with the environment. Therefore, matrix elements of the state operator of the qubit q_i evolve according to the scheme:

$$|0\rangle\langle 0| \to |0\rangle\langle 0|, \qquad |0\rangle\langle 1| \to (1-d)|0\rangle\langle 1|,$$
$$|1\rangle\langle 1| \to |1\rangle\langle 1|, \qquad |1\rangle\langle 0| \to (1-d)|1\rangle\langle 0|.$$

The results of simulation for different values of parameter d are shown in Fig. 6.

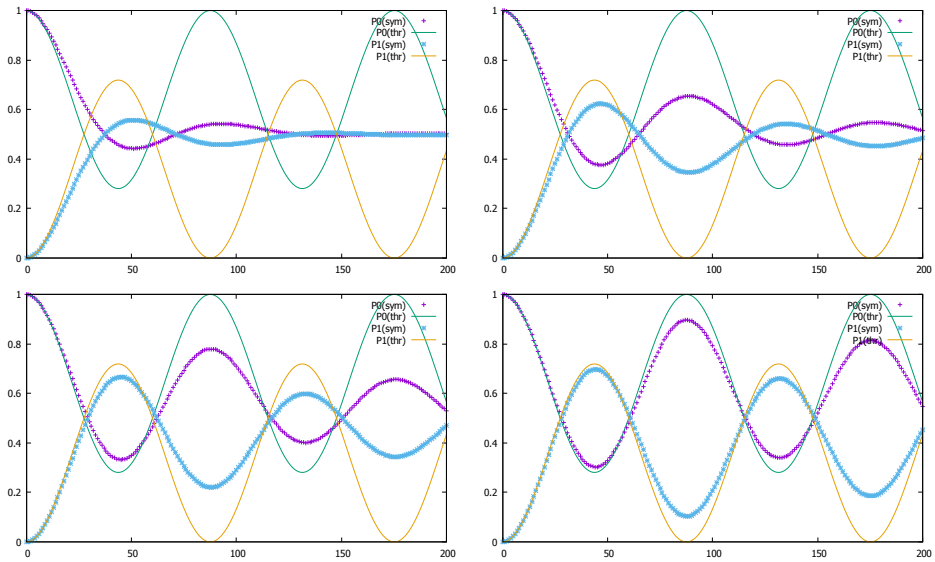

Figure 6: The simulation of the case $E_2 = 2.8 \cdot 10^{-19}$J for $dt = 10^{-17}s$ with decoherence. Succesive plots are made for $d = 0.002, 0.001, 0.0005, 0.0002$, respectively.

5. Conclusions

- The algorithm presented in this work simulates a simple process between two qubits. However, it can become a part of simulation of more complex process.
- The results of the ideal simulation (section 3.1) overlap with the results of theoretical analysis.
- In the case of simulation using imperfect gates (section 3.2), we obtain satisfactory results for ϕ_M approximately equal to 0.01.
- In the case of the simulation with decoherence (section 3.3), we obtain satisfactory results for $d = 2 \cdot 10^{-4}$ per each time step. In future research we are

going to investigate whether these results may be improved using quantum error correction methods.

6. Appendix

Our main task is solving the Schrödinger equation for the system AB. For this purpose, the Hamiltonian (3) diagonalization procedure is applied. First, we introduce auxiliary notation:

$$\Delta_A = E_{A1} - E_{A0}, \tag{7}$$

$$\Delta_B = E_{B1} - E_{B0}, \tag{8}$$

$$E_0 = E_{A0} + E_{B0}. \tag{9}$$

Next, we calculate eigenvalues of the Hamiltonian (3):

$$\lambda_1 = E_0, \quad \lambda_2 = \frac{1}{2}(\Delta_A + \Delta_B - \sqrt{\Delta}) + E_0, \tag{10}$$

$$\lambda_3 = \frac{1}{2}(\Delta_A + \Delta_B + \sqrt{\Delta}) + E_0, \quad \lambda_4 = E_0 + \Delta_A + \Delta_B, \tag{11}$$

where $\Delta = (\Delta_B - \Delta_A)^2 + 4|g|^2$.
Eigenvectors of the Hamiltonian (3) are given by:

$$|w_1\rangle = |0,0\rangle, \tag{12}$$

$$|w_2\rangle = C_m^{-1}[(\Delta_B - \Delta_A - \sqrt{\Delta})|0,1\rangle + 2g|1,0\rangle], \tag{13}$$

$$|w_3\rangle = C_p^{-1}[(\Delta_B - \Delta_A + \sqrt{\Delta})|0,1\rangle + 2g|1,0\rangle], \tag{14}$$

$$|w_4\rangle = |1,1\rangle, \tag{15}$$

where

$$C_m = \sqrt{4|g|^2 + (\Delta_B - \Delta_A - \sqrt{\Delta})^2} = \sqrt{2\sqrt{\Delta}(\sqrt{\Delta} - \Delta_B + \Delta_A)}, \tag{16}$$

$$C_p = \sqrt{4|g|^2 + (\Delta_B - \Delta_A + \sqrt{\Delta})^2} = \sqrt{2\sqrt{\Delta}(\sqrt{\Delta} + \Delta_B - \Delta_A)}. \tag{17}$$

The diagonalizing matrix has the following form:

$$U_{diag} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & C_m^{-1}(\Delta_B - \Delta_A - \sqrt{\Delta}) & C_p^{-1}(\Delta_B - \Delta_A + \sqrt{\Delta}) & 0 \\ 0 & 2C_m^{-1}g & 2C_p^{-1}g & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{18}$$

We obtain the time evolution operator in the form:

$$U(t) = \exp(-iHt/\hbar) = U_{diag}\exp(-iH_{diag}t/\hbar)U_{diag}^{\dagger} = \\ = \begin{pmatrix} \exp(-iE_0t/\hbar) & 0 & 0 & 0 \\ 0 & u_{22} & u_{23} & 0 \\ 0 & u_{32} & u_{33} & 0 \\ 0 & 0 & 0 & \exp(-i(E_0+\Delta_A+\Delta_B)t/\hbar) \end{pmatrix} \tag{19}$$

where

$$u_{22} = \exp\Big(-\frac{it}{2\hbar}(\Delta_A+\Delta_B+2E_0)\Big)\Big(\cos\Big(\frac{t\sqrt{\Delta}}{2\hbar}\Big) - i\frac{\Delta_B-\Delta_A}{\sqrt{\Delta}}\sin\Big(\frac{t\sqrt{\Delta}}{2\hbar}\Big)\Big), \tag{20}$$

$$u_{23} = -\frac{2ig}{\sqrt{\Delta}}\exp\Big(-\frac{it}{2\hbar}(\Delta_A+\Delta_B+2E_0)\Big)\sin\Big(\frac{t\sqrt{\Delta}}{2\hbar}\Big), \tag{21}$$

$$u_{32} = -\frac{2ig^*}{\sqrt{\Delta}}\exp\Big(-\frac{it}{2\hbar}(\Delta_A+\Delta_B+2E_0)\Big)\sin\Big(\frac{t\sqrt{\Delta}}{2\hbar}\Big), \tag{22}$$

$$u_{33} = \exp\Big(-\frac{it}{2\hbar}(\Delta_A+\Delta_B+2E_0)\Big)\Big(\cos\Big(\frac{t\sqrt{\Delta}}{2\hbar}\Big) + i\frac{\Delta_B-\Delta_A}{\sqrt{\Delta}}\sin\Big(\frac{t\sqrt{\Delta}}{2\hbar}\Big)\Big). \tag{23}$$

If we choose the initial state of the system as $|\psi(0)\rangle = |0,1\rangle$, the time evolution of the system takes the following form:

$$|\psi(t)\rangle = u_{22}(t)|0,1\rangle + u_{23}(t)|1,0\rangle. \tag{24}$$

The probability of finding system AB in the state $|0,1\rangle$ as a function of time t can be written as follows:

$$p_0(t) = |\langle 0,1|\psi(t)\rangle|^2 = |u_{22}|^2 = 1 - \frac{4|g|^2}{\Delta}\sin^2\Big(\frac{\sqrt{\Delta}t}{2\hbar}\Big). \tag{25}$$

The probability of finding system AB in the state $|1,0\rangle$ is equal to:

$$p_1(t) = |\langle 1,0|\psi(t)\rangle|^2 = |u_{23}|^2 = \frac{4|g|^2}{\Delta}\sin^2\Big(\frac{\sqrt{\Delta}t}{2\hbar}\Big). \tag{26}$$

In the resonance (when $\Delta_A = \Delta_B$) we have:

$$p_0(t) = \cos^2\Big(\frac{\sqrt{\Delta}t}{2\hbar}\Big), \tag{27}$$

$$p_1(t) = \sin^2\Big(\frac{\sqrt{\Delta}t}{2\hbar}\Big). \tag{28}$$

The condition for the proximity of the resonance can be written as follows: $4|g|^2\Delta^{-1} \rightarrow 1$ or $(\Delta_B - \Delta_A)^2 \ll 4|g|^2$.

References

[1] Feynman, R., Internat. J. Theor. Phys., Vol. 21, 1982, pp. 467–488.

[2] Shor, P. W., Proc 35th Ann. Symp. Found. Comp. Sci., IEEE Comp.Soc. Pr., Vol. 124, 1994.

[3] Grover, L. K., *From Schrödinger equation to the quantum search algorithm*, Am. J. Phys., Vol. 69, 2001, pp. 769–777.

[4] Ostrowski, M., *Quantum simulation of particle scattered by a rectangular potential*, Journ. of Applied Comp. Sci., Vol. 20, No. 2, 2012.

[5] Ostrowski, M., *Quantum Simulation of the Tunnel Effect*, Bulletin of the Polish Academy of Sciences Technical Sciences, Vol. 63, No. 2, 2015, pp. 379–383.

[6] Ostrowski, M., *Quantum simulaton of the Pauli Particle*, Przeglad Elektrotechniczny, ISSN 0033-2097, Vol. 89, No. 7, 2013.

[7] Ostrowski, M., *Quantum simulation of the Dirac Particle*, Open Systems & Information Dynamics, Vol. 22, No. 1, 2015, pp. 1550002.

[8] Warren, W. S., *The usefulness of NMR quantum computing*, Science, Vol. 277, No. 5332, 1997, pp. 1688–168.

[9] Zalka, C., *Efficient simulation of quantum system by quantum computers*, Fortschr. Phys., Vol. 46, 1998, pp. 877–879.

[10] Strini, G., *Error sensitivity of a quantum simulator I: a first example*, Fortschr. Phys., Vol. 50, 2002, pp. 171–183.

[11] Sawerwain, M. and Pilecki, J., *Parallel implementation of a quantum computing simulator*, Journal of Applied Computer Science, Vol. 14, No. 2, 2006.