

Quantum Simulation of the Pauli Particle

Abstract. In this paper we examine whether a quantum computer can efficiently simulate Pauli particle in external magnetic field. We consider Gaussian wave packet in two cases: in uniform magnetic field and in magnetic field with rectangular amplitude. We compare the results obtained from quantum algorithm with the results of classical simulations.

Streszczenie. W niniejszej pracy badamy czy komputer kwantowy może efektywnie symulować cząstkę Pauliego w zewnętrznym polu magnetycznym. Rozważamy pakiet gaussowski w dwóch przypadkach: w jednorodnym polu magnetycznym i w polu o amplitudzie prostokątnej. Porównujemy wyniki otrzymane dla algorytmu kwantowego z rezultatami symulacji klasycznej. **(Symulacja zachowania cząstki Pauliego w zewnętrznym polu magnetycznym)**

Keywords: quantum computations, quantum simulations, Pauli particle
Słowa kluczowe: obliczenia kwantowe, symulacje kwantowe, cząstka Pauliego

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

As is well known, simulations of quantum systems performed using conventional computers are not very effective. This means that for classical computer the memory resources and time required to simulate grow exponentially with 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. Also the number of elementary operations (quantum gates) to be performed on the register as a rule does not grow exponentially.

This work is a continuation of our earlier discussion. In papers [4-5] we investigated the simulations of Schrodinger particle scattered on a rectangular potential. It turned out that quantum algorithm tested by us gives good results. Now, it is natural to investigate the case of particles endowed with spin (Pauli particles) in the presence of an external magnetic field.

Description of the method. Pauli equation - brief reminder

Recall that the Pauli equation is extended Schrodinger equation for particles with spin.¹ It can be written in standard form:

$$(1) \quad i\hbar\partial_t\Psi_a = H_{ab}\Psi_b$$

where a, b are matrix indices. $\Psi_a(x, t)$ is now a vector² with two components:

$$(2) \quad \Psi_a(x, t) = \begin{bmatrix} \Psi_+(x, t) \\ \Psi_-(x, t) \end{bmatrix}$$

where function $\Psi_+(x, t)$ describes the probability amplitude for a spin "upward" while function $\Psi_-(x, t)$ is probability amplitude for spin "downward".³

¹Description of the Pauli particles can be found in standard textbooks of quantum mechanics, for example: [6].

²From a physical point of view it is a spinor. However, we will call it a vector

³We use here the standard representation related with the projection of the spin on the z-axis.

In the presence of an external electromagnetic field (represented by: vector potential $\vec{A}(x)$, scalar potential $\phi(x)$ and magnetic induction $\vec{B}(x)$) Hamilton operator takes the form: (3)

$$H_{ab} = 1/(2m)(\vec{p} - e\vec{A}(x))^2 I_{ab} + e\phi(x)I_{ab} - \mu\vec{B}(x)\vec{\sigma}_{ab}$$

where m is mass, \vec{p} is momentum, e is electric charge and μ is magnetic moment of particle. We also use the unit matrix I_{ab} and Pauli matrices in the standard form: (4)

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

In analogy with the Schrodinger particle, a formal solution of Eq. (1) can be written as follows:

$$(5) \quad \Psi_a(x, t) = \exp(-iH_{ab}t/\hbar)\Psi_b(x, 0)$$

Encoding of the state of particle in the quantum register

In n -qubit quantum register state of the Pauli particle can be encoded in following way: qubits numbered from 0 to $n-2$ are used to encoding sampled positional representation, while the last qubit (with number $n-1$) stores the state of spin of the particle $|q_{n-1}\rangle = |s\rangle$. This means that the state encoded in the register has the form:

$$(6) \quad |\Psi\rangle = \sum_{s=0}^1 \sum_{q_{n-2}=0}^1 \cdots \sum_{q_0=0}^1 a_{s q_{n-2} \dots q_0} |s\rangle |q_{n-2}\rangle \cdots |q_0\rangle$$

where $a_{s q_{n-2} \dots q_0}$ are coefficients that encode sampled $\Psi_+(x)$ and $\Psi_-(x)$ functions in following way:

$$(7) \quad a_{0 q_{n-2} \dots q_0} = \Psi_+(\Delta x k)$$

$$(8) \quad a_{1 q_{n-2} \dots q_0} = \Psi_-(\Delta x k)$$

where Δx is a distance between the spatial samples of wavefunctions Ψ_+ and Ψ_- , while $k = \sum_{i=0}^{n-2} 2^i q_i$ is a number of a sample.

The algorithm simulating time evolution of the system

Inserting Eq. (3) to Eq. (5) and assuming that $\vec{A}(x) = 0$, $\phi(x) = 0$ and $dt \rightarrow 0^4$ we get:

$$(9) \quad \Psi_a(x, t + dt) = \exp(-ip^2 dt^2 / (2m\hbar)) \exp(i\mu\vec{B}(x)\vec{\sigma}_{ab} dt / \hbar) \Psi_b(x, t)$$

⁴For small values of dt we can use approximation $\exp((A+B)dt) \rightarrow \exp(A dt) \exp(B dt)$. Recall that a similar method has been used by us in [4-5]. These types of methods have been introduced in the work of other authors [7-10].

Evolution of state of the particle described by Eq.(9) corresponds to change of state of the quantum register in the following way:

$$(10) \quad |\Psi(t + dt)\rangle = U_{\vec{B}} \mathcal{F}_*^{-1} \exp_*(-ip^2/(2m\hbar)) \mathcal{F}_* |\Psi(t)\rangle$$

where symbols \mathcal{F}_* i \mathcal{F}_*^{-1} denote the quantum Fourier transform and its inverse. Index $*$ near the operators \exp_* , \mathcal{F}_* i \mathcal{F}_*^{-1} means that they do not operate on the entire register but only on qubits from 0 to $n - 2$ (i.e. except the last one).

Eq. (10) describes one time step of the simulation. Scheme of algorithm implementing change of state of the register in accordance with Eq. (10) is shown in Fig. 1. Blocks QFT, FE (implementing free evolution operator $\exp_*(-ip^2/(2m\hbar))$) and RQFT have been shown in [4]. Now we describe the implementation of the $U_{\vec{B}}$ block responsible for interaction of particle with an external magnetic field \vec{B} .

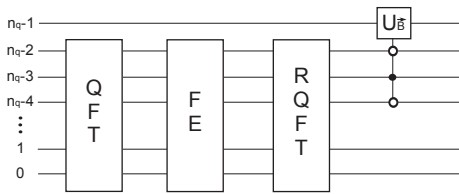


Fig. 1. Scheme of the quantum algorithm simulating the Pauli particle in an external magnetic field

In case of a homogeneous magnetic field unconditional operation $U_{\vec{B}}$ is applied to qubit s . The form of $U_{\vec{B}}$ is given by:

$$(11) \quad U_{\vec{B}} = U_{B_x} U_{B_y} U_{B_z}$$

where operators U_{B_i} have the form:

$$U_{B_x} = \exp(i\theta_x \sigma_x) = \begin{bmatrix} \cos \theta_x & i \sin \theta_x \\ i \sin \theta_x & \cos \theta_x \end{bmatrix},$$

$$U_{B_y} = \exp(i\theta_y \sigma_y) = \begin{bmatrix} \cos \theta_y & \sin \theta_y \\ -\sin \theta_y & \cos \theta_y \end{bmatrix},$$

$$U_{B_z} = \exp(i\theta_z \sigma_z) = \begin{bmatrix} \exp(i\theta_z) & 0 \\ 0 & \exp(-i\theta_z) \end{bmatrix}$$

where $\theta_i = \mu B_i dt / \hbar$.

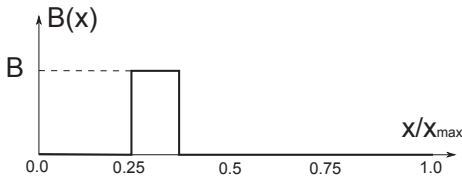


Fig. 2. The magnetic field of rectangular amplitude used to simulation

In case of an inhomogeneous magnetic field (as in Fig. 2) we use a conditional operation (showed in Fig. 1 as the last) given in the form:

$$(12) \quad |s\rangle|0\rangle|1\rangle|0\rangle \rightarrow (U_{\vec{B}}|s\rangle)|0\rangle|1\rangle|0\rangle$$

where $U_{\vec{B}}$ is given by Eq. (11).⁵

⁵Example of implementation of such an operation with using two-input gates can be found in [11].

The simulation results. Comparison with classical algorithm

As an initial state of simulated particle we choose the Gaussian distribution of the form:

$$(13) \quad \Psi(x) = C_n \exp\left(\frac{(x - \langle x \rangle)^2}{4dx^2} + i\langle p \rangle x\right)$$

where $\langle x \rangle$ is expected value of the position, $\langle p \rangle$ is expected value of the momentum, dx is indeterminacy of the position while C_n is a normalization constant.

Simulations for a homogeneous magnetic field

We performed simulations for a quantum register consisting of $n = 9$ qubits with the following parameter values: size of the simulated area $x_{max} = 5\mu m$, initial position of center of the packet $\langle x \rangle = 0.5\mu m$, average kinetic energy of the packet $\langle E \rangle = 4eV$, indeterminacy of position $dx = 0.1\mu m$, mass of particle $m = 9.1 \times 10^{-31} kg$ (mass of electron), time step $dt = 10^{-12} s$. Results are shown in Fig. 3.

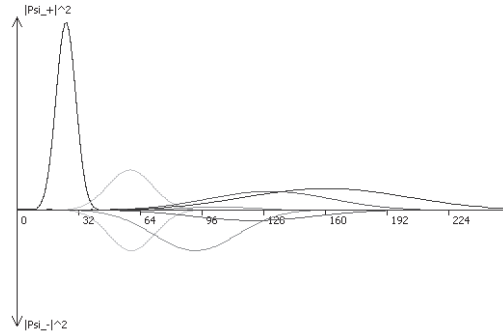


Fig. 3. The simulation results for particle in homogeneous magnetic field $B_y=0.1T$. Lines are successive phases of movement, taken at intervals of 90 time steps ($9 \times 10^{-11} s$)

Recall that in this situation, the position of the particle and its spin evolve independently of each other. The spin precession with a period equal to $T = 2\pi m / (eB_y) = 3.57 \times 10^{-10} s$ occurs.

Simulations for an inhomogeneous magnetic field

In this case, a simulation of quantum register with a capacity of $n = 9$ qubits was also done. We implemented a magnetic field B_y with rectangular amplitude shown in Fig. 2. The simulation was performed for particle with the same initial parameters as in Section 3.1. Results are shown in Fig. 4. For comparison of the results, we have simulated the same case using the classical Cayley method (described in Appendix A). Its results are shown in Fig. 5.

Conclusions

- Comparing the Fig. 4 and Fig. 5, we can conclude the convergence of the results obtained with both methods.
- We simulate the register of small size $n = 9$. It is dictated by hardware constraints. If in future quantum computer a larger register can be used then the effective simulation of such processes in more complex cases will be possible.
- In this paper, we omit the analysis of the process of reading the final data from the register. We have analyzed only if the final state is correct. We have not analyzed what information can be read from it in practice.

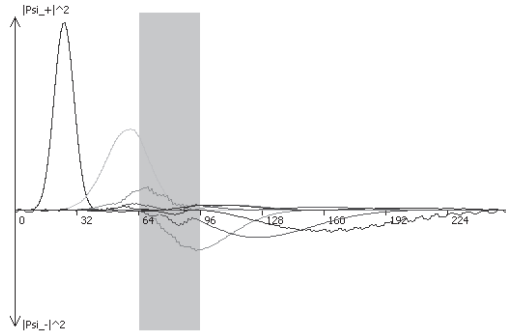


Fig. 4. Results of quantum simulations for particle in inhomogeneous magnetic field with amplitude $B_y=0.2T$. Lines are successive phases of movement, taken at intervals of 90 time steps ($9 \times 10^{-11}s$). Shaded area is the area of occurrence of the magnetic field

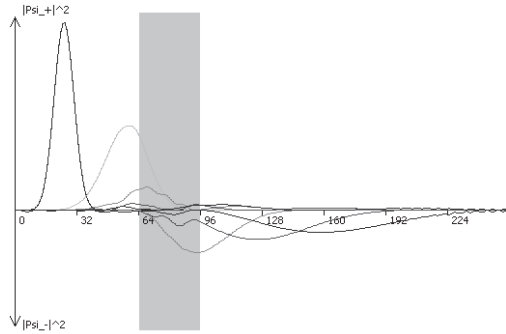


Fig. 5. Results of classical simulations (Cayley method) for particle in inhomogeneous magnetic field with amplitude $B_y=0.2T$. Lines are successive phases of movement, taken at intervals of 90 time steps ($9 \times 10^{-11}s$)

Appendix A. Brief description of the classical algorithm used for comparison

As a comparative method, we used the classical Cayley's method [12]. It is based on Schrodinger equation of motion written in the following form:

$$(14) \quad (1 + \frac{1}{2}i H dt/\hbar)\Psi(t + dt) = (1 - \frac{1}{2}i H dt/\hbar)\Psi(t)$$

where H is the hamiltonian (3) with $p = -i\hbar\partial_x$ and second derivative is carried out by three-point approximation. In such a situation equations for one time step of simulation take the

form:

$$\begin{aligned} -iA\Psi_{n+1}^+(t_2) + CEM_n\Psi_n^+(t_2) - iA\Psi_{n-1}^+(t_2) - iE_{xy n}\Psi_n^-(t_2) &= \\ = iA\Psi_{n+1}^+(t_1) + CEM_n^*\Psi_n^+(t_1) + iA\Psi_{n-1}^+(t_1) + iE_{xy n}\Psi_n^-(t_1) \\ -iA\Psi_{n+1}^-(t_2) + CEP_n\Psi_n^-(t_2) - iA\Psi_{n-1}^-(t_2) - iE_{xy n}\Psi_n^+(t_2) &= \\ = iA\Psi_{n+1}^-(t_1) + CEP_n^*\Psi_n^-(t_1) + iA\Psi_{n-1}^-(t_1) + iE_{xy n}\Psi_n^+(t_1) \end{aligned}$$

where

$$\begin{aligned} t_2 = t_1 + dt, \quad E_{xy n} &= \mu dt/(2\hbar)(B_{x n} + iB_{y n}), \\ A &= \hbar dt/(4m\Delta x^2), \quad E_{z n} = \mu dt/(2\hbar)B_{z n}, \\ CEM_n &= C_n - iE_{z n}, \quad CEP_n = C_n + iE_{z n}, \\ C_n &= 1 + i(2A + V_n dt/(2\hbar)), \end{aligned}$$

while $B_{x n}$, $B_{y n}$ and $B_{z n}$ are sampled values of magnetic field.

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