

Quantum simulation of the tunnel effect

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Abstract. In this paper, we examine whether a quantum computer can efficiently simulate quantum processes such as the tunnel effect. We examine a quantum algorithm that calculates the value of transition and reflection coefficients for the Gaussian wave packet scattered on a rectangular potential. We compare the results obtained in this way with the results of classical simulations and analytical calculations.

Key words: quantum computations, quantum simulations, tunnel effect.

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 [2]. Therefore, it is worth examining the properties of such machines.

Today we know the Shor [3] and Grover [4] algorithms which are faster than their best classical counterparts. Another promising application of the quantum computer is quantum simulations, i.e. computer modelling of the behaviour of physical quantum systems.

As it is well known, simulations of quantum systems performed using conventional computers are not effective. This means that for a classical computer, the memory resources and time required to simulate grow exponentially with the size of the quantum system. In the case of a quantum computer, a situation is different. The relationship between the size of the 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 usually does not grow exponentially.

Among many scientists (not professionally involved in quantum computing) there is a belief that a quantum computer will have a limited application. Indeed, despite the fact that there is a lot of papers on quantum computing, only a few quantum algorithms have proved to produce satisfactory results.

Our main goal is to investigate this problem. In this paper, we examine whether the quantum computer can calculate the probability of reflection R and the probability of transition T for a particle scattered on the rectangular barrier of the potential. We have chosen this task because it has an analytical solution which gives the opportunity to examine the accuracy of the obtained results.

Recall that quantum tunnelling refers to the quantum mechanical phenomenon where a particle tunnels through a barrier that it could not surmount classically (i.e. where the energy of the particle E is lower than the height V_0 of the barrier). This plays an essential role in the physical phenomena occur-

ring in the nucleus (synthesis and decomposition reactions), in semiconductors (negative dynamic resistance of the tunnel diode) or in superconducting structures (Josephson junction). The effect was predicted in the early 20th century, and was accepted as a general physical phenomenon in the middle of the 20th century.

Although the tunnel effect has been known for over a century, it still raises interest among researchers. This is reflected both in the scientific literature [5] and popular science books [6].

In this paper, we examine the process of tunnelling for the Schrödinger particle. The quantum algorithm simulating the Schrödinger particle has been exhaustively described in our earlier work [7]. Its modification for the case of the particle with spin (Pauli particle) has been successfully examined in [8]. It is based on the Quantum Fourier Transform and the procedure of diagonalisation of a time evolution operator. In the next section, we briefly recall its essential elements.

It is worth mentioning that the possibility of using a quantum register to simulate the Schrödinger particle has already been discussed in the literature. For example, papers [9, 10] have examined the quantum lattice-gas model. An algorithm similar to the one proposed in this paper has been tested in papers [11–14] for free particle and for a harmonic oscillator. The possibility of using the parallel computation methods for simulation of a quantum computer was shown in [15]. An introduction to the basic computational models used in quantum information theory can be found in [16].

2. Quantum simulations of the Schrödinger particle

The time evolution of the Schrödinger particle in one-dimensional case takes the form:

$$i\hbar \frac{d}{dt} \Psi(x, t) = (H_0 + V(x)) \Psi(x, t), \quad (1)$$

where $H_0 = p^2/(2m)$ is free Hamiltonian and $V(x)$ is the potential describing interactions with an external force. In our considerations it is the stationary rectangular potential (Fig. 1).

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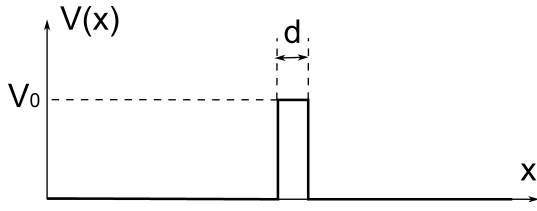


Fig. 1. Rectangular potential with an amplitude V_0 and width d used to examine the tunnel effect

The formal solution of Eq. (1) can be expressed in the following form:

$$\Psi(x, t_1) = \exp(-i(H_0 + V(x))\Delta t/\hbar)\Psi(x, t_0), \quad (2)$$

which describes the evolution of the system from the initial state at time t_0 to the state at time $t_1 = t_0 + \Delta t$.

In our method, the wave function is sampled $\Psi(x) \rightarrow \Psi_n = \Psi(\Delta x n)$ and encoded in the state of the quantum register. Time evolution operator from Eq. (2) is approximated as follows:

$$\begin{aligned} & \exp(-i(H_0 + V(x)) \Delta t/\hbar)\Psi_n(t) \\ &= \exp(-i V(x)\Delta t/\hbar) \\ & \cdot \mathcal{F}^{-1}\{\exp(-i p^2/(2m\hbar))\mathcal{F}\{\Psi_n(t)\}\}, \end{aligned} \quad (3)$$

where \mathcal{F} is Quantum Fourier Transform.

The process of simulation is shown in Fig. 2. In the first block (initial state preparation) Gaussian state (4) is entered to the register (black curve on Fig. 3). Blocks QFT, FE, RQFT and POT implement one time step of simulation (evolution operator from Eq. (3)). Blocks POT and FE implement operators $\exp(-iV(x)\Delta t/\hbar)$ and $\exp(-ip^2/2m\hbar)$ respectively. Block QFT and RQFT implement Quantum Fourier Transform and its inverse¹. In the measurement block state of the oldest qubit is measured. The reflection coefficient R_q is identified with the probability of finding the particle in the left half of the simulated area (corresponding to state $|0\rangle$ of the oldest qubit). Analogously, the transmission coefficient T_q is identified with the probability of finding particle in the right half of the area (corresponding to state $|1\rangle$ of the oldest qubit).

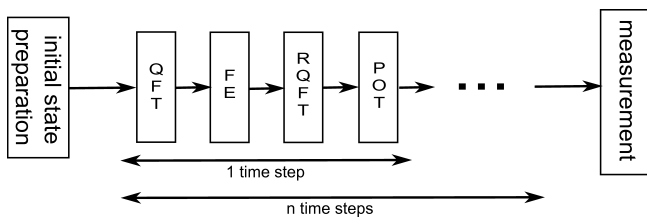


Fig. 2. Scheme of the quantum algorithm

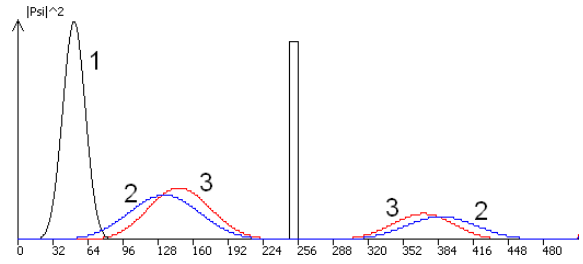


Fig. 3. Sample output of the algorithm. Black line (no. 1) is the initial state of quantum register (Eq. (4)). Blue line (no. 2) is the final state of register after the quantum simulation (before measurement). Red line (no. 3) is a result of the Cayley's simulation. (no. 3, Table 2)

3. The simulation results

The main result of our work is the calculation of the probability of reflection R_q and transmission T_q of the Gaussian packet whose initial state has the form:

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

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

We have analyzed the Gaussian particle with parameters: $m = 9.1 \cdot 10^{-31}$ kg (mass of the electron), kinetic energy (the most probable value): $E_{mp} = 1.0$ eV, standard deviation of the position of the packet: $\Delta x = 1.0$ nm. The size of the simulation area was $x_{max} = 50.0$ nm and initial position of the maximum of the packet (against the left edge of investigated area) $\langle x \rangle = 5.0$ nm. The obtained results for different values of d and V_0 are presented in the Tables 1–3 and Figs. 4, 5.

Table 1

Comparison of the results of quantum simulations (R_q, T_q) with the results of classical simulations (R_k, T_k) and analytical results (R_a, T_a) for $d = x_{max}/16$. In both cases we took $dt = 10^{-16}$ s and $n = 540$ time steps. The register of size $n_q = 9$ qubits has been used, which gives $n_b = 512$ spatial samples

No.	V_0 [eV]	R_a	T_a	R_k	T_k	R_q	T_q
1	0.8	0.3717	0.6283	0.4566	0.5434	0.4186	0.5814
2	1.0	0.6964	0.3036	0.7851	0.2149	0.7441	0.2559
3	1.2	0.9158	0.0841	0.9540	0.0460	0.9331	0.0669
4	1.4	0.9875	0.0125	0.9947	0.0053	0.9854	0.0146
5	1.6	0.9983	0.0017	0.9996	0.0004	0.9906	0.0094

Table 2

Comparison of the results of quantum simulations (R_q, T_q) with the results of classical simulations (R_k, T_k) and analytical results (R_a, T_a) for $d = x_{max}/128$. In both cases, we took $dt = 10^{-16}$ s and $n = 540$ time steps. The register of size $n_q = 9$ qubits has been used

No.	V_0 [eV]	R_a	T_a	R_k	T_k	R_q	T_q
1	0.8	0.3340	0.6660	0.3612	0.6388	0.3455	0.6545
2	1.0	0.4996	0.5004	0.5268	0.4732	0.5119	0.4881
3	1.2	0.6452	0.3547	0.6669	0.3331	0.6560	0.3440
4	1.4	0.7572	0.2428	0.7717	0.2283	0.7654	0.2346
5	1.6	0.8360	0.1634	0.8448	0.1553	0.8420	0.1580
6	1.8	0.8899	0.1101	0.8940	0.1060	0.8934	0.1066

¹Implementation of QFT, FE, RQFT and POT block on a two-qubit logical gates are presented in [7].

Table 3

Comparison of the results of quantum simulations (R_q, T_q) with the analytical results (R_a, T_a) for $d = x_{\max}/16$. Two times smaller time step ($dt = 5 * 10^{-17}$ s and $n=1080$ time steps) and two times greater spatial sampling density (size of register: $n_q = 10$ and $n_b = 1024$ spatial samples) than in the case of Table 1 has been used

No.	V_0 [eV]	R_a	T_a	R_q	T_q
1	0.8	0.3717	0.6283	0.4135	0.5865
2	1.0	0.6964	0.3036	0.7395	0.2605
3	1.2	0.9158	0.0841	0.9302	0.0698
4	1.4	0.9875	0.0125	0.9829	0.0171
5	1.6	0.9983	0.0017	0.9879	0.0121

For comparison, the transition and reflection coefficients calculated by other methods have also been included in the tables. These are: the analytical method (described in Appendix A) and the method based on classical simulations (described in Appendix B). Values calculated analytically (using the Eqs. (16)–(17)) have been named R_a and T_a while the values calculated using the classical simulation are denoted by R_k, T_k .

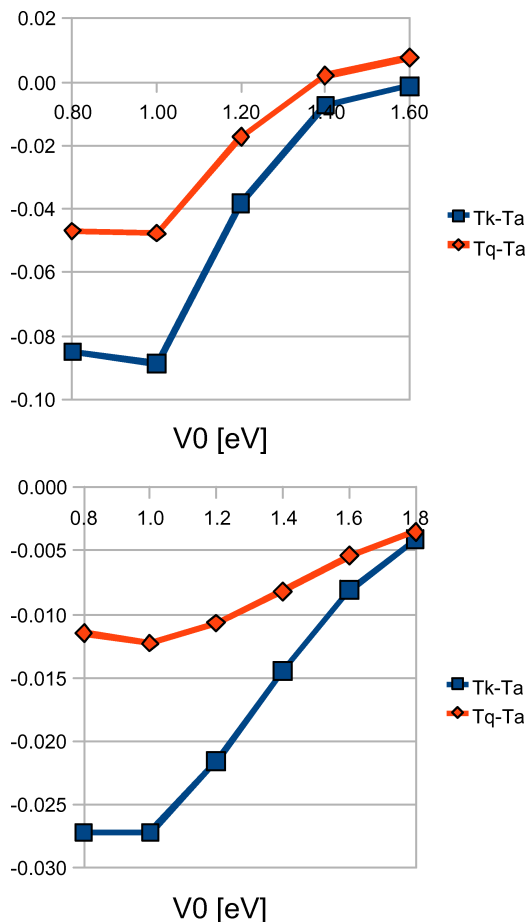


Fig. 4. Absolute error for the transition coefficient T as a function of V_0 . Top plot for results from Table 1, bottom plot for results from Table 2. Red line: for quantum simulation, blue line: for classical simulation

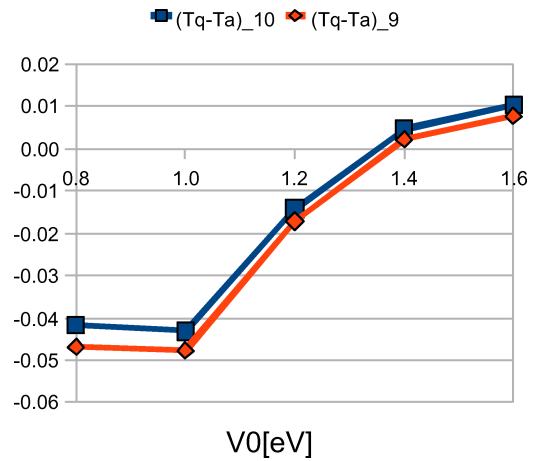


Fig. 5. Absolute error for the transition coefficients T as a function of V_0 . Red line for simulation with $n_q = 9$ (Table 1), blue line for simulation with $n_q = 10$ (Table 3)

4. Conclusions

- After comparing the results from Table 1 and Table 2, we can conclude that at the same spatial resolution the accuracy of quantum and classical algorithms is similar. In addition, we noticed (based on the results which are not presented in this paper) that the quantum algorithm is more stable.
- Even a small quantum register ($n_q = 9$) has proved to give reliable results.
- The main advantage of the quantum algorithm is that it requires a smaller amount of logic gates at each step. For one time step in the register of n_q qubits length ($N = 2^{n_q}$ spatial samples) we need only $3/2n_q^2 + 5/2n_q + 19$ quantum logic gates. It gives time complexity equal to $\mathcal{O}(\log^2 N)$. In comparison, the classical (Cayley's) algorithm provide time complexity no better than $\mathcal{O}(N \log N)$. This is due to the fact that system of N linear equations must be solved at each time step of simulation.
- The main (well known) disadvantage of a quantum algorithm is the problem with reading the results. Recall that quantum algorithm, by its very nature, is a probabilistic algorithm. We cannot read the results R_q and T_q in terms of symbolically encoded numbers but in terms of probabilities that the register reaches a certain state. In order to read these probabilities, the algorithm and the act of measurement must be repeated many times as a random process. This results from the fact that it is impossible to clone the quantum state.
- In our work, we did not analyse of the process of initial data entry in the register ("initial state preparation" block from Fig. 2). This issue is examined in next work [17].
- We do not review here the factors affecting the accuracy of the results such as accuracy of quantum gates realization or noise in the register (decoherence). The analysis of these problems is left for future research.

Appendix A. Analytical formulas for the reflection and transition coefficients

The problem of calculation of the transition and reflection coefficients for particles in plane wave state can be found in many textbooks on quantum mechanics (e.g. [18]). Here, we present only a sketch of that derivation.

In order to find $R(k)$ and $T(k)$ coefficients for particle with momentum k , time-independent Schrödinger equation $H\Psi(x) = E\Psi(x)$ should be solved. In the case of the rectangular potential, for $E < V_0$, specific solution takes the form:

$$\begin{aligned} \Psi(x, k) = & \theta(-x - a)(\exp(ikx) + R(k) \exp(-ikx)) \\ & + \theta(x + a)\theta(-x + a)(A(k) \exp(-\beta x) \\ & + B(k) \exp(\beta x)) + \\ & + \theta(x - a)T(k) \exp(ikx), \end{aligned} \quad (5)$$

where $k = \sqrt{2Em}\hbar^{-1}$ and $\beta = \sqrt{2(V_0 - E)m}\hbar^{-1}$. For $E > V_0$ Eq. (5) remains valid if we make the substitution $\beta \rightarrow ik'$ where $k' = \sqrt{2(E - V_0)m}\hbar^{-1}$.

Coefficients $R(k)$ and $T(k)$ are calculated from the continuity conditions:

$$\Psi(x, k)|_{x \rightarrow -a^-} = \Psi(x, k)|_{x \rightarrow -a^+}, \quad (6)$$

$$\partial_x \Psi(x, k)|_{x \rightarrow -a^-} = \partial_x \Psi(x, k)|_{x \rightarrow -a^+}, \quad (7)$$

$$\Psi(x, k)|_{x \rightarrow +a^-} = \Psi(x, k)|_{x \rightarrow +a^+}, \quad (8)$$

$$\partial_x \Psi(x, k)|_{x \rightarrow +a^-} = \partial_x \Psi(x, k)|_{x \rightarrow +a^+}, \quad (9)$$

where $+a$ and $-a$ are the position of the left and right edge of the barrier potential respectively.

For $E < V_0$ we obtain:

$$|T(k)|^2 = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta d)}, \quad (10)$$

$$|R(k)|^2 = \frac{\frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta d)}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta d)}, \quad (11)$$

while for $E > V_0$:

$$|T(k)|^2 = \frac{1}{1 + \frac{V_0^2}{4E(E - V_0)} \sin^2(k'd)}, \quad (12)$$

$$|R(k)|^2 = \frac{\frac{V_0^2}{4E(E - V_0)} \sin^2(k'd)}{1 + \frac{V_0^2}{4E(E - V_0)} \sin^2(k'd)}. \quad (13)$$

These formulas can be written together:

$$|T(k)|^2 = \theta(k_0 - k) |T_-|^2 + \theta(k - k_0) |T_+|^2, \quad (14)$$

$$|R(k)|^2 = \theta(k_0 - k) |R_-|^2 + \theta(k - k_0) |R_+|^2, \quad (15)$$

where $|T_-|^2$ is given by Eq. (10), $|R_-|^2$ is given by Eq. (11), $|T_+|^2$ is given by Eq. (12), $|R_+|^2$ is given by Eq. (13) and $k_0 = \sqrt{2V_0m}\hbar^{-1}$.

The probability of transition T_a of Gaussian wave packet is given by:

$$T_a = \int_{-\infty}^{\infty} dk |a(k)|^2 |T(k)|^2 \quad (16)$$

while the probability of reflection R_a is equal to:

$$R_a = \int_{-\infty}^{\infty} dk |a(k)|^2 |R(k)|^2 \quad (17)$$

where $a(k)$ is a Fourier transform of initial state (4) of the particle.

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

As a comparative method, we used the classical Cayley's method [19]. It is based on the Schrödinger equation of motion written in the following form:

$$(1 + 1/2i H dt/\hbar)\Psi(t + dt) = (1 - 1/2i H dt/\hbar)\Psi(t), \quad (18)$$

where $H = p^2/2m + V$ is the Hamiltonian of the particle with $p = -i\hbar\partial_x$ and the second derivative is carried out by a three-point approximation. In such a situation, the equation for one time step of simulation takes the following form:

$$\begin{aligned} -iA\Psi_{n+1}(t_2) + C_n\Psi_n(t_2) - iA\Psi_{n-1}(t_2) \\ = iA\Psi_{n+1}(t_1) + C_n^*\Psi_n(t_1) + iA\Psi_{n-1}(t_1), \end{aligned} \quad (19)$$

where

$$t_2 = t_1 + dt,$$

$$A = \hbar dt/(4m\Delta x^2),$$

$$C_n = 1 + i(2A + V_n dt)/(2\hbar)$$

while V_n are sampled values of the potential.

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