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CALCULATION AND VISUALIZATION OF QUANTUM-MECHANICAL TUNNEL EFFECT

Abstract. The article presents calculations and visualization of wave packet tunneling through the potential barrier of various widths done by using the MATLAB software. The graph of distribution of the probability density along barrier width is obtained in two and three dimensions. The article contains materials about quantum-mechanical tunnel effect such as the reflection of the part of the wave packet from the potential barrier and passing through the barrier of the other part. Calculations and visualization of the tunneling process are performed for various widths of the barrier. Figures given in the article show the probability of finding the particle at a certain time, i.e. the square of the absolute value of the state vector$|\psi|^2$. The part of the total number of particles tunnels through barrier, the other part reflects from it. The probability of tunneling increases with decrease of the barrier width. The detailed analysis of the graphs reveals that the wave function exponentially decreases inside the potential barrier therefore the observation of this effect requires a rather small width of the barrier. Students are offered to develop programs for various widths of the potential barrier. Results of experiments are used during the study of the quantum mechanics.

Key words: wave packet, reflected wave, transmitted wave, potential barrier, barrier width, probability.

Nowadays all educational institutions of Kazakhstan are provided with computer hardware and software, interactive boards and internet. Almost all teachers have completed language and computer courses for professional development. Hence the educational institutions have all conditions for using computer training programs and models for performing computer laboratory works. In recent years the new computer system for carrying out mathematical calculations MATLAB is being widely used in many universities and engineering institutions throughout the world [1-7]. Unfortunately, the numerical calculations carried out by students are often done by means of the calculator. Modern computers are frequently used only for presentation of the work. Actually students should be able not only to solve these or other engineering problems, but also do them by using modern methods, that is, using personal computers.

Students of the physics specialties 5B060400 and 5B011000 successfully master the discipline “Computer modeling of physical phenomena” which is the logical continuation of the disciplines “Information technologies in teaching physics” and “Use of electronic textbooks in teaching physics”. The goal of this discipline is to study and learn the MATLAB program language, acquaintance with its huge opportunities for modeling and visualization of physical processes.

In our early works [8-26] we used the MATLAB system for modeling and visualization of physical processes related with mechanics, molecular physics, electromagnetism and quantum physics. This software has enabled us to solve ordinary differential equations (ODE), visualize equipotential lines of charged conductors system, describe the motion of charged particles in electric, magnetic and gravitational fields and etc.

The present article is devoted to calculation and visualization of the quantum-mechanical tunnel effect by using the package of MATLAB applied programs.

Formulation of the problem. Let us consider a well-known example – tunneling of the particle through the potential barrier. Let the particle with mass m to move with speed υ towards the potential barrier of height x (fig.1).

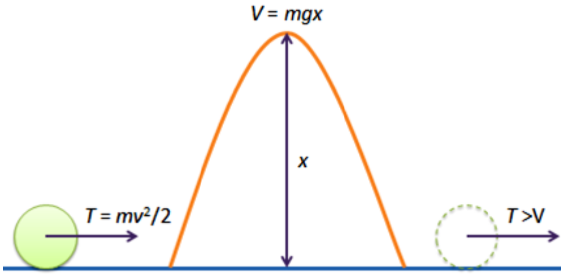

Fig.1 - Tunneling of the particle through the potential barrier

According to the classical mechanics it can surmount this barrier if only its kinetic energy $m\upsilon^2/2$ is greater than the potential energy mgx necessary for surmounting the barrier. But quantum mechanics states that there is a nonzero probability that the particle will surmount the "potential barrier" even its energy is insufficient from the point of view of classical mechanics. It is said that the particle tunnels through the potential barrier.

For calculation of this effect it is necessary to introduce into the Hamiltonian the potential V as a barrier and find how the wave packet will behave itself.

The apparent expression of the time evolution operator is:

$$\tilde{U}(t)=\exp\left(-\frac{i}{h/2\pi}\hat{H}(t)\right) \tag{1}$$

here $\hat{H}$ is the Hamiltonian operator.

In dynamic problems the state vector is usually chosen in the form of the wave packet localized in small area of space. Let's take the state vector at the initial time to be the following function:

$$\psi(x)=\left(\pi d^2\right)^{-1/4}\exp\left(ipx-\frac{x^2}{2d^2}\right) \tag{2}$$

here p is the momentum of the particle, d is the “width” of the wave packet. The mass of the particle and Planck’s constant are taken to be equal to one. The real part of the function is shown in the fig.2.

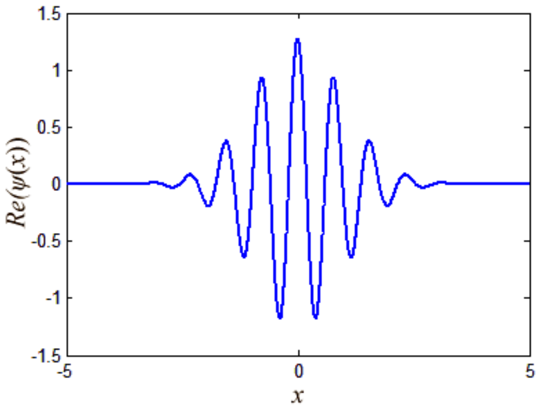

Fig.2 - The wave function at the initial time

This function doesn't depend upon the time. To find the function at the other moment of time it is necessary to act on it with the evolution operator (1).

The dynamics of this action can be observed by using the following Matlab program:

a) barrier's width d = 1;

```
clear % cleaning of the screen
%% Initial data
n = 200; % the number of points (depends upon the power of PC)
% wave packet
p = -4; % packet momentum
d = 1; % barrier's width
x = linspace(-10,10,n);
offset = -7;
wave = ((exp(1i*p*(x-offset))).*(exp(-((x-offset).^2)/(2*d^2))))./((pi*d^2)^1/4);
wave = wave';
%%
x = linspace(-6, 6, n)';
h = (x(2)-x(1));
Dsquared = (diag(ones(1,n-1),1) - 2*diag(ones(1,n)) + diag(ones(1,n-1), -1))/h^2; % the second derivative
V = ((x > 0).*(x<0.5))*60; % potential barrier
%%
H = -Dsquared + diag(V); % Hamiltonian
t = 0.01; % the initial moment of time
figure1 = figure;
axes1 = axes('Parent',figure1);
for i = 1:55 %  the cycle for results output
%%
U = expm(-1i*t*H); % time evolution operator
%%
wave1 = U*wave; % application of the evolution operator to the wave packet
t = t+0.01;
% plot(x, real(wave1),'Color',[1 0 0]) % the real part of  the wave function
plot(x, abs(wave1).^2,'Color',[1 0 0]) % visualization of the probability
hold % resolution of the drawing
plot(x,V) % visualization
ylim(axes1,[-0.5 2]);
hold % resolution of the drawing
pause(0.2); % in dependence upon the power of PC
end
```

The result is shown in the fig.3 (the tunneling picture).

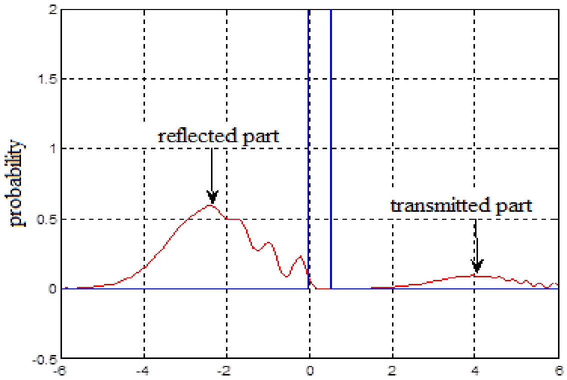

Fig.3 - Tunneling through the potential barrier with the width d =1

b) barrier width *d* = 1;

```
clear % cleaning of the screen
%% Initial data
n = 200; % the number of points (depends upon the power of PC)
% wave packet
p = -4; % packet momentum
>> d=1.25; %  barrier's width
>> x = linspace (-10, 10, n);
offset = -7;
wave = ((exp(1i*p*(x-offset))).*(exp(-((x-offset).^2)/(2*d^2)))))./((pi*d^2)^1/4);
wave = wave';
%%
x = linspace (-6, 6, n)';
h = (x (2)-x(1));
Dsquared = (diag(ones(1,n-1),1) - 2*diag(ones(1,n)) + diag(ones(1,n-1), -1))/h^2; % the second derivative
V = ((x > 0).*(x<0.5))*60; % potential barrier
%%
H = -Dsquared + diag (V); % Hamiltonian
t = 0.01; % the initial moment of time
figure1 = figure;
axes1 = axes ('Parent',figure1);
for i = 1:55 % the cycle for results output
U = expm(-1i*t*H); % time evolution operator
wave1 = U*wave; % application of the evolution operator to the wave packet
t = t+0.01;
% plot(x, real (wave1),'Color',[1 0 0]) % the real part of  the wave function
plot(x, abs (wave1).^2,'Color',[1 0 0]) % visualization of the probability
hold % resolution of the drawing
plot(x,V) % visualization
ylim(axes1,[-0.5 2]);
hold % resolution of the drawing
pause(0.2); % in dependence upon the power of  PC
end
```

The result is shown in the fig.4

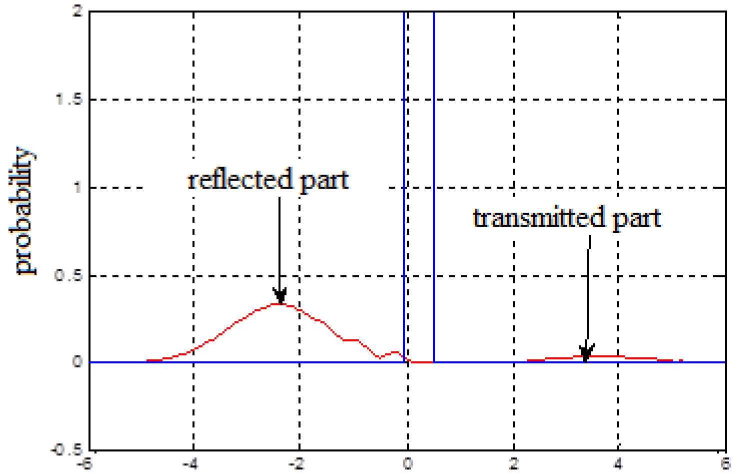

Fig.4 - Tunneling through the potential barrier with the width d =1.25

c) barrier’s width *d*=1.5;

```
% cleaning of the screen
%% Initial data
>>n = 200; % the number of points (depends upon the power of PC)
% wave packet
>>p = -4; % packet momentum
>> d=1.5; % barrier’s width
>> x = linspace (-10, 10, n);
>>offset = -7;
>>wave = ((exp (1i*p*(x-offset))).*(exp(-((x-ffset).^2)/(2*d^2))))./((pi*d^2)^1/4);
>>wave = wave';
%%
>>x = linspace(-6, 6, n)';
>>h = (x(2)-x(1));
>>Dsquared = (diag(ones(1,n-1),1) - 2*diag(ones(1,n)) + diag(ones(1,n-1), -1))/h^2; % the second derivative
V = ((x > 0).*(x<0.5))*60; % potential barrier
%%
>>H = -Dsquared + diag(V); % Hamiltonian
%%
>>t = 0.01; % the initial moment of time
>>figure1 = figure;
>>axes1 = axes('Parent',figure1);
>>for i = 1:55 % the cycle for results output
%%
>>U = expm(-1i*t*H); % time evolution operator
%%
>>wave1 = U*wave; % application of the evolution operator to the wave packet
>>t = t+0.01;
% plot(x, real(wave1),'Color',[1 0 0]) % the real part of  the wave function
>>plot(x, abs(wave1).^2,'Color',[1 0 0]) % visualization of the probability
>>hold % resolution of the drawing
>>plot(x,V) % visualization
>>ylim(axes1,[-0.5 2]);
>>hold % resolution of the drawing
>>pause(0.2); % in dependence upon the power of  PC
>>end
```

The result is shown in the fig.5

The program for visualization of the particle tunneling through potential barrier in three dimensions when *d* =1is given as the following:

```
clear % cleaning of the screen
%% Initial data
>>n = 70; % the number of points (depends upon the power of PC)
% wave packet
>>px = 7; % x –component of the momentum
>>d = 1;
>>x = linspace(-10,10,n);
>>offset = 5;
waveX=((exp(1i*px*(x-offset))).*(exp(-((x-offset).^2)/(2*d^2))))./((pi*d^2)^1/4);
>>waveX = waveX'; % x –component of the wave packet
```

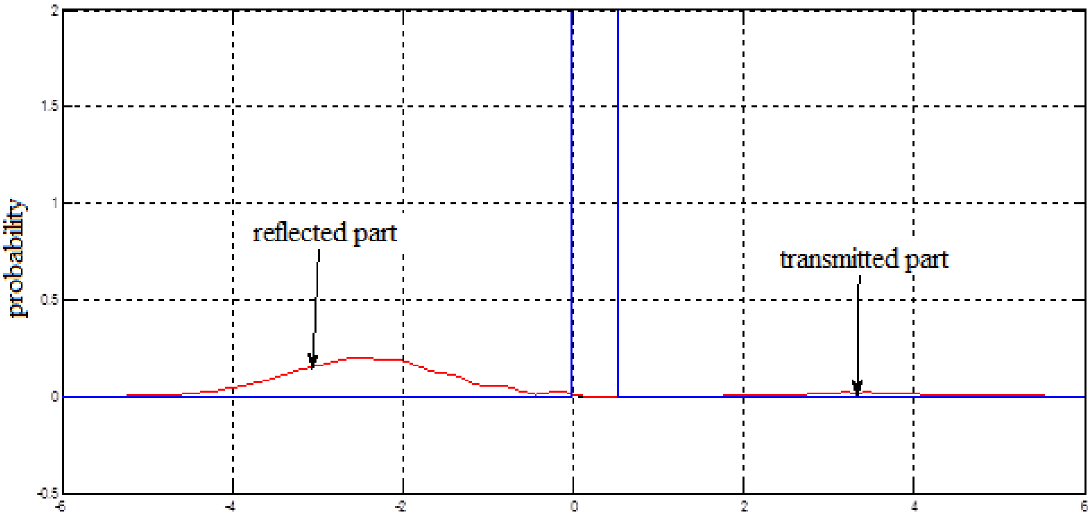

Fig.5 - Tunneling through the potential barrier with the width d =1.5

```
>>py = 0; % y –component of the momentum
>>d = 1;
>>y = linspace(-10,10,n);
>>offset = 0;
waveY=((exp(1i*py*(y-offset))).*(exp(-((y-offset).^2)/(2*d^2)))).((pi*d^2)^1/4);
>>waveY =waveY'; % y –component of the wave packet
>>wave = waveY*waveX'; % two dimensional wave packet
%% components of Hamilton operator
>>h = x(2)-x(1);
Dsquared = (diag(ones(1,n-1),1) - 2*diag(ones(1,n)) + diag(ones(1,n-1), -1))/h^2; %second derivative
>>V = ((x > 0).*(x<0.3))*60; % x-component of the potential barrier
>>Hx = -Dsquared + diag(V); % x-component of Hamiltonian
>>Hy = -Dsquared; % y-component of Hamiltonian
%%
>>t = 0; %the initial moment of time
>>figure1 = figure;
>>axes1 = axes('Parent',figure1);
>>for tt=1:43 % The main cycle of the results output
>>Ux = expm(-1i*t*Hx); % x-component of the time evolution operator
>>Uy = expm(-1i*t*Hy); % y-component of the time evolution operator
%% application of the x-component of the time evolution operator to the wave packet
for i=1:n
>>wave(i,:) = (Ux*wave(i,:)')';
>>end
%% application of the y-component of the time evolution operator to the wave packet
for i=1:n
>>wave(:,i) = Uy*wave(:,i);
>>end
%% drawing the graphs
>> [X,Y] = meshgrid(x,y);
>>mesh(X,Y,abs(wave))
>>zlim(axes1,[0 1.5]);
>>t=t+0.002;
>>pause(0.5); % in dependence upon the power of  PC
>>end
```

The result is shown in the fig.6

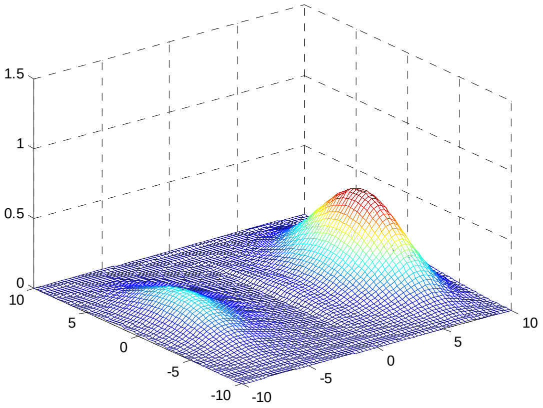

Fig.6 - Tunneling through the potential barrier with the width d =1 in three dimensions

Conclusion

The article presents the program for calculation and visualization of tunneling of a wave packet through a potential barrier with various widths. The graphs of the probability density versus barrier width are drawn in two- and three-dimensions. Brief data from the theory of quantum mechanical tunnel effect states that the one part of the wave packet is reflected from a potential barrier and the other part passes through it. Calculations and visualization of the particle tunneling are given for various width of the barrier. The obtained figures show the squares of absolute values of the state vector, i.e. the probability to find the particle at a given moment of time. The part of the total number of particles tunnels through the barrier, and the other part of them is reflected. The probability of passing through the barrier increases with the decrease of the barrier's width. The detailed analysis of the graphs reveals that the wave function exponentially decreases inside the potential barrier therefore the observation of this effect requires a rather small width of the barrier. Students are offered to develop programs for various widths of the potential barrier. Results of experiments are used during the study of the quantum mechanics.

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MATLAB ЖҮЙЕСІНДЕ «КВАНТТЫҚ МЕХНИКАЛЫҚ ТУННЕЛДІК ЭФЕКТІНІ ЕСЕПТЕУ МЕН БЕЙНЕЛЕУ»

Аннотация. Толқындық пакеттің потенциалдық тосқауылдан туннелденіп өту процесін есептеу мен бейнелеу ұсынылады және ықтималдық тығыздығының тосқауыл ені бойында өзгерісінің екі өлшемдік және үшөлшемдік кеңістікте графиктерін салу ұсынылады. Кваттық-механикалық туннелдік эффектінің қысқаша теориясы берілген: тосқауылға соққан толқындық пакеттің бір бөлігі тосқауылдан шағылады, ал қалған бөлігі тосқауылдан өтеді. Тосқауылдың енінің әртүрлі шамасына байланысты туннелдену есептелген және бейнеленген. Суреттерде күй векторының абсолют шамасының квадраты салынған, яғни берілген уақыттағы бөлшектің табылуының ықтималдығы салынған. Тосқауылға соққан бөлшектердің жалпы санының бір бөлігі туннелденеді де, ал қалған бөлігі тосқуылдан шағылады. Тосқауылдан өту ықтималдығы оның ені кішіреуімен артады. Процесті талдаудан келесіні байқайтынымыз: тосқауыл ішінде толқындық функция экспоненциалды өшеді, сондықтан оны бақылау үшін тосқауылдың енін мүмкіндігінше кішірейту керек. Студенттерге өз бетінше бірнеше тәжірибелер жасау ұсынылады. Тәжірибелер нәтижелері кванттық механиканы меңгеруде қолданылады.

Түйін сөздер. Толқындық пакет, шағылған толқын, өткен толқын, потенциальнық тосқауыл, тосқауыл ені, ықтималдық.

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«РАСЧЕТ И ВИЗУАЛИЗАЦИЯ КВАНТОВОМЕХАНИЧЕСКОГО ТУННЕЛЬНОГО ЭФФЕКТА» В СИСТЕМЕ MATLAB

Аннотация. Предлагается программа расчета и визуализации процесса туннелирования волнового пакета сквозь потенциальный барьер с построением графика эависимости плотности вероятности вдоль ширины барьера в двумерном и трехмерном представлениях. Приводятся краткие сведения из теории квантовомеханического тунннельного эффекта: часть волнового пакета отражается от потенциального барьера, но другая часть проходит его. Приведены расчеты и визуализация туннелирования при различной ширине барьера. На рисунках показаны квадрат абсолютного значения вектора состояния $|\psi|^2$, то есть вероятность обнаружить частицу в данный момент времени. Из общего количества частиц какая-то их часть туннелирует сквозь барьер, а какая-то отражается. Вероятность прохождения увеличивается с уменьшением толщины барьера. Детальный анализ показывает, что волновая функция экспоненциально затухает внутри потенциального барьера, поэтому для наблюдения данного эффекта ширина барьера должна быть достаточно мала. Студентам предлагается самостоятельно поэкспериентировать. Результаты экспериментов используются при изучении и освоении квантовой механики.

Ключевые слова. Волновой пакет, отраженная волна, прошедшая волна, потенциальный баръер, ширина баръера, вероятность.

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