

Time Dependent Tunneling in One Dimensional Quantum Mechanics

Final Report

O.O. Oncel*

Department of Physics, Bilkent University, 06800 Ankara, Turkey

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The project aims to investigate time dependent tunneling of a quantum mechanical particle across a simple potential barrier with numerical techniques. Rectangular potential barrier and an electron is chosen which is represented by a Gaussian wavefunction form. Transmission and reflection coefficients for the barrier are calculated for $E < V_0$, $E > V_0$ and $E = V_0$ conditions. Conditions for numerical implementation discussed. Fourier space transformations and time dependence addition explained. Using Riemann Sum, numerical integration is done on MATLAB and resulting wavefunctions for gaussian wave packet and its tunneling are obtained as motion pictures. Atomic units are used for easy manipulation. Wave packets with zero average momentum are observed to be not changing average position in time. Very high momentum values increase transmission rate whereas very high potentials lowers the transmission. And lastly, the calculations are carried on a ring and quantization of wavenumbers for ring are found to be $k = 2\pi n/L$ where L is circumference and n is an integer. Scattering and transmission matrices are constructed for barrier potential on ring. MATLAB codes are provided in the appendix. (Advisor: Assoc. Prof. Tugrul Hakioglu)

I. INTRODUCTION

Tunneling is a purely quantum mechanical effect which has no counterpart in classical mechanics. Classically it is impossible for a particle with energy E to pass through a potential region V if $E < V$. Conversely in quantum mechanics such a particle has nonzero probability of passing through this potential. Also $E > V$ case has nonzero probability of scattering back off the potential, which, again cannot be explained by classical physics.[1] This nonclassical and conceptually difficult phenomenon creates a broad range of applications such as STM[2] and new approaches in physics[3].

Here our problem is a rather simplified version of this large branch. We have a finite, rectangular, time independent potential barrier with potential V_0 . We will send an electron in the form of a time dependent Gaussian wave packet incident from the left of the barrier. Gaussian will move towards the barrier with time, and tunneling takes place according to energy, wave function, transmission and reflection coefficients. This numerical study is made with MATLAB.

After having a firm understanding of Gaussian tunneling problem, we moved to ring problem where periodic boundary conditions appear. The effect of periodic boundary conditions investigated firstly on free particle, then in the presence of a potential barrier. Scattering and transfer matrices are derived and formed.

II. THEORY

II. I Units

In this study I have used atomic units. Though it is more common to use Angstrom units in quantum me-

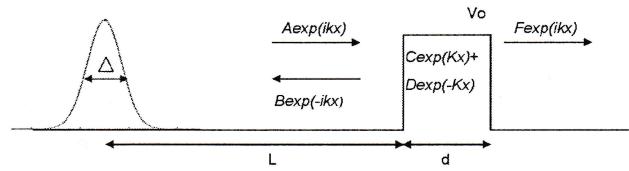


FIG. 1: Tunneling Scheme of the problem. L is the distance from the center of the Gaussian to the barrier start. d is the barrier width which is $2a$ in our problem($-a, a$). Only F labeled transmission wave occupies right of the tunnel since we assume incident from the left($G=0$). V_0 is the barrier potential.

chanical studies atomic units have great advantage in simplification of constants. The cost is you deviate from 'daily life' units and intuitive thinking of dimensions becomes very hard.

The beauty of atomic units is that many constants we use frequently becomes equal to 1: $a_0 = e = \hbar = m_e = 1$. Let us show the dimensional units[9]:

Length unit: a_0 (0.528 Å) - Bohr

Energy unit: E_h (27.287 eV) - Hartree

Time unit: τ_0 (2.41×10^{-17} s)

Some conversion values are given in parentheses for better understanding. Our k values are now have the units of $Bohr^{-1}$.

II. II Transmission and Reflection Coefficients

ψ_I is the incident from left. ψ_B is the barrier region wave function and ψ_T is the transmitten wave function.

II. III Fourier Space Transformations and Time Evolution

$$\psi_I = Ae^{ikx} + Be^{-ikx} \quad (-\infty < x < -a) \quad (1)$$

$$\psi_B = Ce^{Kx} + De^{-Kx} \quad (-a < x < a) \quad (2)$$

$$\psi_T = Fe^{ikx} \quad (a < x < +\infty) \quad (3)$$

Where;

$$k = \sqrt{2mE}/\hbar \quad (4)$$

$$K = \sqrt{2m(E - V_0)}/\hbar \quad (5)$$

Transmission(T) and reflection(R) coefficients gives the amount of transmitted and reflected parts of incident wave respectively. They differ for three cases $E < V_0$, $E > V_0$ and $E = V_0$. Continuity condition for ψ and its derivative at boundary points must be satisfied. By this token[4];

For $E < V_0$

$$T_{E < V_0} = \frac{F}{A} = \frac{e^{-2ika} \frac{2ik}{K}}{\frac{2ik}{K} \cosh(2Ka) - (1 - \frac{k^2}{K^2}) \sinh(2Ka)} \quad (6)$$

$$R_{E < V_0} = \frac{B}{A} = \frac{e^{-2ika} \sinh(2Ka) (1 + \frac{k^2}{K^2})}{\frac{2ik}{K} \cosh(2Ka) - (1 - \frac{k^2}{K^2}) \sinh(2Ka)} \quad (7)$$

For $E = V_0$

$$T_{E=V_0} = \frac{F}{A} = \frac{e^{-2ika}}{1 - iak} \quad (8)$$

$$R_{E=V_0} = \frac{B}{A} = \frac{e^{-2ika} (-iak)}{1 - iak} \quad (9)$$

For $E > V_0$

$$T_{E > V_0} = \frac{F}{A} = \frac{e^{-2ika} \frac{2k}{p}}{\frac{2k}{p} \cos(2pa) - (1 + \frac{k^2}{K^2}) i \sin(2pa)} \quad (10)$$

$$R_{E > V_0} = \frac{B}{A} = \frac{e^{-2ika} (i \sin(2pa)) (1 - \frac{k^2}{p^2})}{\frac{2k}{p} \cos(2pa) - (1 + \frac{k^2}{K^2}) i \sin(2pa)} \quad (11)$$

Coefficients are dependent on energy, hence momentum. We can't use these with $\psi(x, 0)$ but $\phi(k, 0)$ is appropriate. This is a call for space transformation which can be done by fourier transformations. Given our initial $\psi(x, 0)$ we can move to $\phi(k, 0)$ which will also be a Gaussian since fourier transformation of a Gaussian is again a gaussian distribution in transformed space[1]. For our normalized initial Gaussian wave packet

$$\psi(x, 0) = e^{ik_0(x-x_0)} \frac{e^{-(x-x_0)^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}} [5] \quad (12)$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x, 0) e^{-ikx} dx = \phi_I(k, 0) \quad (13)$$

To find $\phi_I(k, 0)$, integrating (13) with (12) plugged in;

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ik_0(x-x_0)} \frac{e^{-(x-x_0)^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}} e^{-ikx} dx = \phi_I(k, 0) \quad (14)$$

$x' = x - x_0$. So, $x = x' + x_0$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ik_0(x')} \frac{e^{-(x')^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}} e^{-ik(x'+x_0)} dx = \phi_I(k, 0) \quad (15)$$

$$\frac{1}{\sqrt{2\pi}} \frac{e^{-ik(x_0)}}{(\pi\Delta^2)^{1/4}} \int_{-\infty}^{+\infty} e^{i(k_0-k)x'} e^{-(x')^2/2\Delta^2} dx = \phi_I(k, 0) \quad (16)$$

$$C = \frac{1}{\sqrt{2\pi}} \frac{e^{-ik(x_0)}}{(\pi\Delta^2)^{1/4}} \quad (17)$$

Let $\alpha = i(k_0 - k)$ and $\beta = 1/2\Delta^2$ So, integral becomes;

$$C \int_{-\infty}^{+\infty} e^{\alpha x'} e^{-\beta(x')^2} dx = \phi_I(k, 0) \quad (18)$$

$$C \int_{-\infty}^{+\infty} e^{-(\beta(x')^2 - \alpha x')} dx = \phi_I(k, 0) \quad (19)$$

We need to manipulate exponential part so as to give complete square, than we will be able to evaluate integral in terms of familiar gaussian integral.

$$(\beta(x') - ?)^2 = \beta(x')^2 - 2\sqrt{\beta}x' + ?^2 \quad (20)$$

$$-2\sqrt{\beta}x' = -\alpha x' \quad (21)$$

$$? = \alpha/2\sqrt{\beta} \quad (22)$$

$$\gamma^2 = \alpha^2/4\beta$$

to be added(23)So, our integral is now;

$$Ce^{-\frac{\alpha^2}{4\beta}} \int_{-\infty}^{+\infty} e^{-\beta((x') - \frac{\alpha}{2\beta})} dx = \phi_I(k, 0) \quad (24)$$

Note that, $x' = x - x_0$ $dx' = dx - dx_0$ so $dx' = dx$

$$Ce^{-\frac{\alpha^2}{4\beta}} \sqrt{\frac{\pi}{\beta}} = \phi_I(k, 0) \quad (25)$$

Plugging in α and β back;

$$Ce^{-\frac{(k-k_0)^2 \Delta^2}{2}} \sqrt{2\Delta^2\pi} = \phi_I(k, 0) \quad (26)$$

simplifying, we have found;

$$\phi_I(k, 0) = \left(\frac{\Delta^2}{\pi}\right)^{1/4} e^{-(k-k_0)^2 \Delta^2/2} e^{ikx_0} \quad (27)$$

Above equation gives a gaussian distribution in momentum space, corresponding to our initial gaussian in position space.

Now T and R can work for us to determine potential barrier effects in k-space, for corresponding region' T and R:

$$\phi_R = \phi_I * R \quad (28)$$

$$\phi_T = \phi_I * T \quad (29)$$

Now we can define ψ_R and ψ_T in addition to ψ_I . Let's also add time evolution to these wave functions. Time evolution for stationary state wave functions can be made by just adding multiplication factor of $e^{-iE_k t}$.

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi_I(k, 0) e^{i(kx - E_k t)} dk = \psi_I(x, t) \quad (30)$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi_R e^{-i(kx + E_k t)} dk = \psi_R(x, t) \quad (31)$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi_T e^{i(kx - E_k t)} dk = \psi_T(x, t) \quad (32)$$

Making time evolution in k-space is meaningful. Since momentum is a constant of motion[6] it preserves the normalization in future times.

In principle we are done with the problem since $\psi(x, t)$ is found. But from another point of view we have just arrived to the beginning of solving process. Above integrals need to be evaluated numerically. The technique we will try to employ is finite integration by discretizing continuous variables x and t, hence creating grid points (x, t) to define discrete ψ .

III. NUMERICAL STUDY

III. I MATLAB Code

The code[?] is essentially consist of four parts. In the first part I defined initial values and functions. Second part calculates transmission and reflection coefficients for corresponding k values. Third part, which is the main engine of procedure, calculates $\psi(x, t)$ with discrete integration. Last part creates a movie for visualization of tunneling problem.

III. II Initial Conditions and Limitations

For a successful computational output, we have to consider some ratios and approximations so that problem can be observed correctly[7]:

(1) $L \gg a$: Because Gaussian should initially stand at the left to the barrier so that we can investigate propagation and tunneling with passing time.

(2) $\Delta \ll L$: This condition ensures that Gaussian is localized enough.

(3) Comparable V_0 : A very high potential with respect to E will decrease transmission rate and may prevent us from observing transmission explicitly. On the other hand, very little potential may create negligible amount of reflection.

(4) Above criterias are heavily depend on choice of x_0 and k_0 .

In addition to these theoretical criterions I have experimented with code for additional fitting. My code, which runs many loops, is a computationally expensive one and need further refinements. That's why selecting discrete steps to little(for ex. 0.05) increases loops to be turned and data to be stored such that my computer often runs out of memory. Though I have increased virtual memory it was still insufficient. So I am forced to increase discretization interval, which brings higher distortion in higher time values. Time values are selected in order to cover accurate intervals.

Another thing to concern is normalization. Since we are working on finite domains, normalization cannot hold perfectly. I have taken very large x and t domains specifically to check whether my gaussian wave packet is normalized or not. Results were positive. The problem with normalization is, when small x interval is chosen, probability density escapes out of sight after sometime since it propagates. And taking very small time domains(small enough to preserve normalization) may not be enough for us to observe complete action we wish to investigate. To solve this dilemma, I have first worked on normalization of function I would like to use. After being sure that what I got is a normalized function, I have used it in larger time domains with comparably small x inter-

vals where it seems unnormalized to our snapshot but it actually behaves as a normalized function.

Let us now choose a appropriate set of conditions:

- (1) $L >> a$: $L=7$ Bohr and $a=1$ Bohr.
- (2) $\Delta \ll L$: Our Δ is $\Delta = 0.8$

(3) and (4) Comparable V_0 and choice of x_0 and k_0 . k distribution is from -10.005 to 10.005 . An average momentum $k_0=1$. And a comparable value, V_0 is set to 1.3

Time, momentum and position steps are chosen as $dt = dk = dx = 0.1$

III. III Transmission & Reflection Coefficients Matrix Representation

Transmission(T) and reflection(R) coefficients differ for three cases $E < V_0$, $E > V_0$ and $E = V_0$. I have defined two general ($1 \times k_n$) arrays T and R where k_n stand for n^{th} component of k array which runs from -10.005 to 10.005 with $dk = 0.1$. Hence, for each k , corresponding energy compared with V_0 and n^{th} column of matrix chooses and reads from previously defined transmission and reflection equations for $E < V_0$, $E > V_0$ and $E = V_0$. So that, every k value will encounter its specific T and R conditions.

III. IV Numerical Integral

The integrals we need to evaluate numerically are (31) and (32).

These equations can be generalized under the form of

$$C \int_a^b f(k) dk = I(k)$$

Where C contains every multiplicative factor not including k . This integral can be discretized by using Riemann Sum[10]:

$$\sum_{i=1}^n f(G_i)(k_{i+1} - k_i)$$

Where $f(G_i)$ is the value of f at i^{th} point and $k_{i+1} - k_i = \Delta_k$ discrete spacing unit.

In the code, I have first assigned values to x and t . k is now only *variable* to computer. At this point the Riemann Sum is evaluated. And this process generalized to repeat for all x and t values by using *for* loops. In other words, we first take a discrete time value say t_1 , at t_1 we assign x_1 to x value. And take integral over all k . Then moving to $x_2=x_1+dx$, we again sum over all k integral. When all position domain is defined for specific

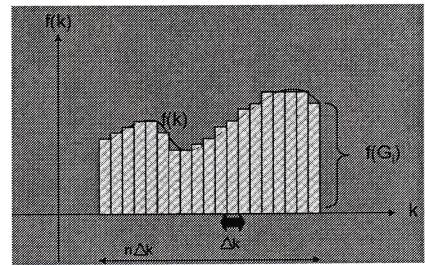


FIG. 2: Riemann Sum Scheme

time, we now move to next time value, say $t_2=t_1+dt$ and repeat all process. If we are to observe this on a 3D mesh, it will look like filling space slice by slice.

III. V Visualization

Visualization of quantum mechanical phenomena is of central importance for understanding. It is not an easy job to intuitively simulate quantum mechanics problems in mind since they are not among our daily life experience. Our perception domain of dimensions allows us to experience with particle nature of matter rather than its wave form. In this part previously calculated wavefunction of electron is transformed into a movie. This is succeeded by MATLAB's *movie* function, which constructs a movie over specified domain by showing 2D plots after each other. The method is same as constructing a video from a collection of photographs where specified domain is time.

To plot the tunneling of the wave function, I have divided position axis into two parts. This method is taken from K. Chu's code[11]. Before the barrier start, and after the barrier start. $\psi_T(x, t)$ is defined on second region. On the other hand there raises a problem in defining reflected wave. Because $\psi_I(x, t)$ and $\psi_R(x, t)$ are expected to interact and crumble. The superposition of these two waves are revealed in a combined function named $\psi_B(x, t)$, and its position interval is first region.

Important Note: Barrier height in plots does not resemble any value or quantity, it is placed in favor of visualization and always equal to half of maximum y value.

IV. RESULTS AND DISCUSSIONS FOR 1D GAUSSIAN TUNNELING

IV. I Procedure

We will start with a gaussian wavepacket, and observe its propagation in space. Then we will send this gaussian wavepacket to a barrier as an incident wave from left. We will investigate how changing parameters (V_0, d) effect transmission and reflection processes.

IV. II Gaussian Wavepacket

Gaussian wave packet propagation in space with time is observed as expected. Two cases are investigated here. In the first one our average $k k_0=0$, hence x_0 does not move in time. On the other hand, I set $k_0=1$, in the latter case, and observed the travelling wave.

IV. III Tunneling

In the previous report our initial picture in mind was;

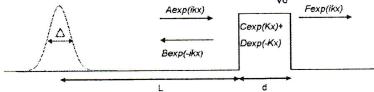


FIG. 3: Tunneling Scheme of the problem.

Let us now see how it looks in our computer program

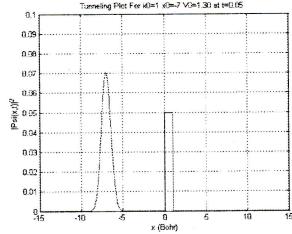


FIG. 4: Computer version of our initial problem setup.

Fitting the picture in our mind to our screen, we can now watch our gaussian tunneling: The gaussian first approaches the barrier(Fig 7.Slide 2). Highest momentum components encounter barrier first, since they have highest velocities. These components have also the highest energies and produce the highest transmission rate(Fig 7.Slide 3 and 4). As wave travels, energy of momentum components interacting with barrier decreases, hence transmission rate starts to decrease from its peak and reflected wave density sharpens near barrier(Fig 7.Slide 5 and 6). In the next figure(Fig 8), we are now close to end of action. Transmitted portion formed a plane wave itself and continues to right, and crumbled reflected wave continues to be fed by lowest energy components of ψ_I and lastly fades out.

Let us now investigate what happens when V_0 is very high compared to k_0 (Fig 9), as an educated guess, we expect very low transmission and very high reflection.

We were right! Packet begins to interact with barrier about $t=2$ again, since we do not manipulated wavepacket's properties. Change applied to barrier and eventually different results revealed themselves: The transmission rate at $t=2.5$ (Fig 9.Slide 4) is almost negli-

gible compared to $V_0=1.3$ case. On the other hand, we have a sharply peaked reflected wave.

Another game can be played by leaving potential same and changing momentum distribution of wavepacket(Fig 10). Increasing k_0 from 1 to 5, conversely to previous case with enhanced potential barrier, we now give power to the wave packet and hence expect a great rate of transmission. First notice that wavefunction travels faster than any previous waves, because of high momentum components wave is almost out of sight just at $t=2$. And clearly reflection was very small compared to almost total transmission.

V. A DIFFERENT GEOMETRY: QUANTUM RING SYSTEM

We will now move to periodic system from our open boundaries. We will achieve this by closing the path on to itself, hence imprisoning the wavefunctions into a ring. The quantum ring system is important especially for our purposes, because it is easy to work with magnetic forces in circular symmetry.

VI. THEORY OF TUNNELING ON QUANTUM RING

VI. I Quantization on Ring

Take a ring of radius r and circumference $L = 2\pi r$. For any point on this ring we have the periodic boundary condition of

$$\Psi(x) = A e^{ikx} + B e^{-ikx} \quad (33)$$

$$\Psi(x + L) = A e^{ikx} e^{ikL} + B e^{-ikx} e^{-ikL} \quad (34)$$

$$\Psi(x + L) = \Psi(x) \quad (35)$$

No boundary condition for derivative required because above conditions apply for *any* point on the ring. Let us fetch the quantization information for wavenumbers

$$A e^{ikx} + B e^{-ikx} = A e^{ikx} e^{ikL} + B e^{-ikx} e^{-ikL} \quad (36)$$

$e^{-+ikL} = 1$ for boundary conditions to be satisfied.

$$kL = 2\pi n \quad (37)$$

$$k_n = \frac{2\pi n}{L} \quad (38)$$

VI. II Tunneling Problem on Quantum Ring

Thinking in terms of the axis as the radial axis of ring, we can place our potential barrier centered at $x = 0$ and occupying the space between $-a$ to a . We have two functions namely, to the left of the potential and to the right of the potential

$$\Psi_L(x) = A_n e^{ik(x+a)} + B_n e^{-ik(x+a)} \quad (39)$$

$$\Psi_R(x) = F_n e^{ik(x-a)} + G_n e^{-ik(x-a)} \quad (40)$$

Applying boundary conditions on the barrier edge

$$\Psi_L(-(L-2a)) = \Psi_R(a) \quad (41)$$

$$\Psi'_L(-(L-2a)) = \Psi'_R(a) \quad (42)$$

This time we must include the derivative in the boundary conditions because barrier edge points are special points. The two boundary conditions give

$$A_n e^{-ik(L-a)} + B_n e^{ik(L-a)} = F_n + G_n \quad (43)$$

$$A_n e^{-ik(L-a)} - B_n e^{ik(L-a)} = F_n - G_n \quad (44)$$

The components to the left and the components to the right are related via Transfer Matrix(T)

$$\begin{pmatrix} F_n \\ G_n \end{pmatrix} = (T) \begin{pmatrix} A \\ B \end{pmatrix}$$

We can also write F_n and G_n in terms of A and B. From (11) and (12)

$$F_n = A_n e^{-ik(L-a)} \quad (45)$$

$$G_n = B_n e^{ik(L-a)} \quad (46)$$

So;

$$\begin{pmatrix} e^{-ik(L-a)} & 0 \\ 0 & e^{ik(L-a)} \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix} = \begin{pmatrix} F_n \\ G_n \end{pmatrix}$$

Hence;

$$\begin{pmatrix} e^{-ik(L-a)} & 0 \\ 0 & e^{ik(L-a)} \end{pmatrix} \begin{pmatrix} A_n \\ B_n \end{pmatrix} = (T) \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

In order to have a nontrivial solution, determinant of

$$\begin{vmatrix} T_{11} - e^{-ik(L-a)} & T_{12} - 0 \\ T_{21} - 0 & T_{22} - e^{ik(L-a)} \end{vmatrix}$$

must be equal to zero. In order to solve above determinant, we need to find out the components of T matrix related to the our previously found Transfer and Reflection coefficients.

VI. III Scattering Matrix and Transfer Matrix

We will first construct the scattering matrix. Than move to transfer matrix from it. Scattering matrix is a 2x2 matrix which gives the outgoing amplitudes in terms of incoming ones.

$$B = S_{11}A + S_{12}G \quad (47)$$

$$F = S_{21}A + S_{22}G \quad (48)$$

In the case of incident from left, G=0 and

$$S_{11} = B/A = R_l \quad (49)$$

$$S_{21} = F/A = T_l \quad (50)$$

And in the case of incident from right, A=0 and

$$S_{22} = F/G = R_r \quad (51)$$

$$S_{12} = B/G = T_r \quad (52)$$

If we now relate S matrix to transfer matrix, our job will be done. Transfer matrix is a 2x2 matrix, which relates the components to the left of the barrier to the components to the right of the barrier

$$T_{11}A + T_{12}B = F \quad (53)$$

$$T_{21}A + T_{22}B = G \quad (54)$$

Introducing S matrix into T matrix;

$$T_{21}A + T_{22}B = \frac{B - S_{11}A}{S_{12}} \quad (55)$$

$$T_{21} = -\frac{S_{11}}{S_{12}} \quad (56)$$

$$T_{22} = -\frac{1}{S_{12}} \quad (57)$$

$$T_{11}A + T_{12}B = S_{21}A + S_{22}[B/S_{12} - S_{11}A/S_{12}] \quad (58)$$

$$T_{11} = S_{21} - S_{11}S_{22}/S_{12} \quad (59)$$

$$T_{12} = \frac{S_{22}}{S_{12}} \quad (60)$$

Defined all terms related to transmission and reflection coefficients we can now make some estimates. One can easily see that for very high k values, T matrix elements will get close to 1 since: $S_{11} \rightarrow 0$ and $S_{21} \rightarrow 1$ so $T_{11} \rightarrow 1$, $S_{12} \rightarrow 1$ so $T_{22} \rightarrow -1$, $S_{11} \rightarrow 0$ so $T_{21} \rightarrow 1$, $S_{22} \rightarrow 0$ so $T_{12} \rightarrow 0$. hence the determinant term becomes a unit matrix minus the exponential matrix. This matrix will converge to $k = 2\pi n/(L-a)$ which at the $L \rightarrow \infty$ limit converges to (38). The idea makes perfect physical sense: The more high valued k's, the more system overcomes potential so in the far approximation it behaves as if only subject to periodic ring boundary conditions.

VII. FUTURE WORKS

I have tried to obtain roots for above determinant via symbolic computation tools of MATLAB. But an error occurred and running out of time problem is still unsolved. Though I included this simple MATLAB file as the last file in the appendix. Some topics in the proposed project abstract is not completed. This is due to lack of time and tiring process of coding and debugging codes which takes times up to a month. Introduction of magnetic field to ring problem and making the system time dependent is left for future study. We will continue to complete this study in 2008-2009 spring semester. Progress can be tracked from project website[4].

ACKNOWLEDGEMENTS

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- * Electronic address: ooncel@ug.bilkent.edu.tr
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```

clear all;
clc

% Propagation of a Gaussian Wavepacket
% Author: Omer Ogul Oncel
% Dept. of Physics, Faculty of Science, Bilkent University, Ankara, Turkey
% Questions and Comments: ooncel@ug.bilkent.edu.tr
% v1.1 - 17.Jan.2009

x_start= -15.005; % x lower limit
x_finish=15.005; % x upper limit

t_start= -6.505; % t lower limit
t_finish=6.500; % t upper limit

k_start= -10.005; % k lower limit
k_finish=10.005; % k upper limit

dk=0.1; % increment step of k
dt=0.1; % increment step of t
dx=0.1; % increment step of x

x=[x_start:dx:x_finish]; % matrix containing x values
t=[t_start:dt:t_finish]; % matrix containing x values
k=[k_start:dk:k_finish]; % matrix containing x values

h_bar=1; % h bar
m=1; % electron mass

```