

Problem Set 3
Physics 480 / Fall 1999
Professor Klaus Schulten

Problem 1: Wave Packet in 1-Dimensional Box

Using **Mathematica** evaluate the time-dependence of a Gaussian wave packet moving in a 1-dimensional box as illustrated in class. Follow the computational procedure presented in class employing the propagator $\phi(x, t|x_o, t_o)$. Explore the behaviour of wave packets in two ways: (i) choose a wave packet of widths half as wide as the box and vary its energy around the value E_2 , i.e., choose k_0 values $k_o = \sqrt{2mE}/\hbar$ varying E in the interval $[E_2 - 1.5\hbar^2\pi^2/8ma^2, E_2 + 2.5\hbar^2\pi^2/8ma^2]$; (ii) choose $k_o = \sqrt{2mE_2}/\hbar$ fixed and decrease the width of the wave packet from a to $a/10$ in steps of $a/10$. Monitor in each case the interference patterns apparent in plots of $|\psi(x, t)|^2$ and describe them.

Problem 2: Particle in Two-Dimensional Box

A quantum mechanical particle of mass m moves in the (x, y) -plane in a box centered around the origin with impenetrable walls at $x = \pm a$ and $y = \pm a$. Determine the wave functions and associated energies of the stationary states. The wave functions should reflect the full symmetry of the system and should be categorized according to the complete set of symmetry classes.

Problem 3: Triangular Quantum Billiard

A quantum mechanical particle moves in the (x, y) -plane in a triangular billiard whose boundary forms an equilateral triangle with side length L . The boundary of impenetrable walls is defined through the three vertices of the triangle at points $(0, 0)$, $(L/2, \sqrt{3}L/2)$, and $(-L/2, \sqrt{3}L/2)$.

(a) Show that the following two wave functions describe stationary states of the billiard:

$$\begin{aligned} \psi_{mn}^{(1)}(x, y) = & \cos\left[(2m-n)\frac{2\pi}{3L}x\right] \sin\left(n\frac{2\pi}{\sqrt{3}L}y\right) \\ & - \cos\left[(2n-m)\frac{2\pi}{3L}x\right] \sin\left(m\frac{2\pi}{\sqrt{3}L}y\right) \\ & + \cos\left[-(m+n)\frac{2\pi}{3L}x\right] \sin\left[(m-n)\frac{2\pi}{\sqrt{3}L}y\right] \end{aligned} \quad (1)$$

$$\begin{aligned}
\psi_{mn}^{(2)}(x, y) &= \sin\left[(2m-n)\frac{2\pi}{3L}x\right] \sin\left(n\frac{2\pi}{\sqrt{3}L}y\right) \\
&- \sin\left[(2n-m)\frac{2\pi}{3L}x\right] \sin\left(m\frac{2\pi}{\sqrt{3}L}y\right) \\
&+ \sin\left[-(m+n)\frac{2\pi}{3L}x\right] \sin\left[(m-n)\frac{2\pi}{\sqrt{3}L}y\right] \quad (2)
\end{aligned}$$

For this purpose proceed as follows: (i) show that the solutions satisfy the Schrödinger equation inside the billiard; (ii) define for the point P at (x, y) new (overcomplete!) variables ρ_1, ρ_2, ρ_3 that measure the distance of P to the three sides of the triangle

$$\rho_1 = \frac{\sqrt{3}}{2}L - y \quad (3)$$

$$\rho_2 = \frac{\sqrt{3}}{2}x + \frac{y}{2} \quad (4)$$

$$\rho_3 = -\frac{\sqrt{3}}{2}x + \frac{y}{2} \quad (5)$$

and express the wave functions in terms of functions of ρ_1, ρ_2, ρ_3 to demonstrate that the functions (1, 2) obey the proper boundary conditions.

(b) Plot the wave functions $\psi_{mn}^{(1)}(x, y), \psi_{mn}^{(2)}(x, y)$ for representative choices of n, m (i) along the sides of the billiard (to check the boundary condition) and (ii) in the (x, y) -plane.

(c) Identify all symmetry relationships of the stationary states. Show that all stationary states are described by

$$m = 1, 2, 3, \dots, \quad n = 1, 2, 3, \dots, \quad m \geq 2n. \quad (6)$$

(d) State the energies associated with the stationary states described above.

Problem 4: Tunneling Through a δ -Barrier

Consider the stationary states

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) - \frac{\hbar^2 k^2}{2m}\right] \phi_k(x) = 0 \quad (7)$$

describing scattering of one-dimensional particles impinging from the left on a potential $U(x) = U_o\delta(x), U_o > 0$.

(a) Show that the derivative of the stationary states $\phi_k(x)$, i.e., $\phi'_k(x)$, have a discontinuity at $x = 0$. Determine the magnitude of the discontinuity, i.e., determine $\lim_{\epsilon \rightarrow 0} (\phi'_k(\epsilon) - \phi'_k(-\epsilon))$.

(b) Determine the transmission coefficient $T = |j_{>}/j_{in}|$ and the reflection coefficient $R = |j_{<}/j_{in}|$ as a function of U_o and of the energy E of the incoming particles.

(c) Carry out the same calculation (stationary states and transmission, reflection coefficients for particles coming from $x \rightarrow -\infty$) for the potential $U(x) = U_o\delta(x) + U_o\delta(x - a)$, $U_o > 0$.

(d) Plot the resulting transmission coefficient T as a function of energy for various U_o

(e) Plot the stationary states determined in (c) for the energy of the first two minima and maxima of $T(E)$.

(f) Discuss the results in (d) and (e), in particular, relate the stationary states corresponding to the maxima of $T(E)$ to the stationary states of a particle in a one-dimensional box of size a .

Problem 5: Scattering by a Square Barrel Potential

Consider the scattering of particles by a square barrel described by the potential ($U_o > 0$, $\delta > 0$)

$$U(x) = \begin{cases} 0 & x \leq -a - \delta \\ U_o & -a - \delta < x < -a \\ 0 & -a \leq x \leq a \\ U_o & a < x < a + \delta \\ 0 & a + \delta \leq x \end{cases} \quad (8)$$

Potentials of this type can be experimentally realized with high precision in semiconductors. In the form of *Quantum-Well Devices* they have some interesting applications in *nano-technology*, i.e., manufacturing of silicon chips at 10Å resolution, due to electron tunneling and resonance effects at such small length scales. As demonstrated below, the probability that an incident electron will tunnel through a square barrel exhibits sharp resonances as a function of the electron energy and the barrier parameters. In this problem we will understand how these resonances can be explained in terms of *quasi-stationary* states in the barrel¹.

We will assume a barrel with dimensions close to the ones occurring in semiconductor devices., e.g., $U_o = 0.5eV$, $a = 25 \text{ \AA}$, $\delta = 20 \text{ \AA}$. For the effective electron mass we employ $m = 9.1 \times 10^{-32} \text{ kg}$. The effective electron mass replaces the real mass of the electron to account for the proper relationship between wave length and kinetic energy for an electron moving in a semiconductor. In the following calculations we suggest that you employ the

¹For details see L. Esaki, *The Evolution of Semiconductor Quantum Structures in Reduced Dimensionality*, Proc. 3rd Int. Symp. Foundations of Quantum Mechanics, Tokyo, 1989, pp. 369-382)

following units: length / 10 \AA , mass/ $9.1 \times 10^{-32} \text{ kg}$, energy / 1 eV , and time $7.54 \times 10^{-16} \text{ s}$. In these units holds $\hbar = 0.87$. Investigate the following to square barrel potentials in the stated units:

1. $a = 2$, $\delta = 0.3$, $U_o = 2.5$ (these parameters are not quite realistic, but show certain effects better);
2. $a = 2$, $\delta = 2.5$, $U_o = 0.5$ (these parameters correspond to quantum well devices).

A *Mathematica* notebook will be provided which allows you to determine and visualize the transmission coefficient and the stationary state wave functions describing scattering impinging on the square barrel from the left. For optional investigations a notebook will be provided also for scattering of wave packets at a square barrel potential. This notebook demonstrates in how far the stationary states studied in this problem set reflect the scattering behaviour of wave packets as well. Since stationary states with infinite wave trains are very idealistic, a demonstration of wave packet scattering, which models the realistic motion of electrons much better, might be desirable to you.

(a) Familiarize yourself with the notebook and state the steps involved in determining the stationary states for potential (8).

(i) State the form of the wave function $\psi(x, k)$ in each of the five regions I_j $I_1 = \{x, x \leq -a - \delta\}$, $I_2 = \{x, -a - \delta < x \leq -a\}$, $I_3 = \{x, -a < x \leq a\}$, $I_4 = \{x, a < x \leq a + \delta\}$, $I_5 = \{x, x > a + \delta\}$. Use the wave function in the form close to that employed in the notebook.

(ii) State the continuity conditions at the boundaries between the different regions I_j .

(iii) State the transmission coefficient T for the stationary states defined through

$$T = |j_{trans} / j_{in}| \quad (9)$$

where j_{in} is the flux of the right running wave to the left of the square barrel, j_{refl} is the left running wave to the left of the square barrel, and j_{trans} is the flux of the right running wave to the right of the square barrel.

(b1) Employ now the notebook to determine and plot the transmission coefficient as a function of the wave-vector k of the incoming wave. Plot also the amplitude of the wave e^{ikx} in region I_3 .

(b2) Employ now the notebook to determine and plot the wave function $\psi(x; k)$ for k -values which correspond to all maxima and minima of the transmission coefficient in the chosen range of k -values.

The following calculations are aimed at understanding two aspects of the k -dependence of the transmission coefficient: (1) the position of the maxima, (2) the width of the "resonances".

(c) Determine the stationary state k -values and energies for the square barrel potential in the limit $d \rightarrow \infty$. State the equations determining these values and execute the note book to determine the respective value. Compare the resulting k -values with the resonances shown by the transmission coefficient.

The problem set needs to be handed in by Thursday, October 7.
The web page of Physics 480 is at
<http://www.ks.uiuc.edu/Services/Class/PHYS480/>

Barrel Potential

Turn off warnings about spellings:

```
In[1]:= *)
Off[General::spell,General::spell1]
(*
```

Choice of parameters : here we employ the following units, chosen to be numerically convenient in a range of parameters which correspond to electronic quantum well devices length in units of 10 Å mass in units of the effective mass of an electron = 9.1 10⁽⁻³²⁾ kg energy in units of 1 eV. In these units the Planck constant is $\hbar = 0.87$. Here is a possible choice

```
In[2]:= a = 2; d = 0.3; U0 = 2.5; m = 1; hbar = 0.87;
k0 = Sqrt[2 m U0]/hbar;
```

Another interesting, and actually more realistic choice is a = 2, d = 2.5, U0 = 0.5, m=1. Please try this one as well. You can explore at your pleasure.

Definition of the wave functions and statement of continuity conditions:

```
In[3]:= PhiI := Exp[I #2 #1] + r Exp[-I #2 #1] &;
PhiII := u1 Exp[I Sqrt[#2^2-k0^2] #1] +
v1 Exp[-I Sqrt[#2^2-k0^2] #1] &;
PhiIII:= u2 Exp[I #2 #1] + v2 Exp[-I #2 #1]
&;
PhiIV := u3 Exp[I Sqrt[#2^2-k0^2] #1] +
v3 Exp[-I Sqrt[#2^2-k0^2] #1] &;
PhiV := t Exp[I #2 #1] &;

coefficients[k_] := NSolve[{
PhiI[-a-d,k] == PhiII[-a-d,k],
PhiII[-a,k] == PhiIII[-a,k],
PhiIII[a,k] == PhiIV[a,k],
PhiIV[a+d,k] == PhiV[a+d,k],
D[PhiI[x,k],x] == D[PhiII[x,k],x] /. x->-a-d,
D[PhiII[x,k],x] == D[PhiIII[x,k],x] /. x->-a,
D[PhiIII[x,k],x] == D[PhiIV[x,k],x] /. x->a,
D[PhiIV[x,k],x] == D[PhiV[x,k],x] /. x->a+d },
{r,u1,u2,u3,v1,v2,v3,t}][[1]];
```

Define a function equal to the transmission coefficient describing scattering through the barrel:

```
In[4]:= T[k_] := Abs[t/.coefficients[k]]^2
```

Plot the transmission coefficient:

```
In[5]:= Timing[
Plot[T[k],{k,0.1,1.3 k0},
AxesLabel->{"k","T"},
PlotLabel->"Transmission Coefficient"]
]
```

Evaluate the amplitude of the wave function inside the barrel to see how much of the barrel states couple to the incoming plane wave $\text{Exp}[I k x]$:

```
In[6]:= III[k_]:=Abs[ u2/.coefficients[k]]^2
```

Plot the magmitude of the barrel wave function as a function of k

```
In[7]:= Timing[
Plot[III[k],{k,0.1,1.3 k0},
  AxesLabel->{"k","T"},
  PlotLabel->"Density in Barrel"]
]
```

Define the wave function stretching over all five regions I - V for a specified k value. Look at the two figures above [of T[k] and III(k)] to decide which k values might be particularly interesting. To determine k values in the plots precisely click on the plots and then move the mouse to desired places in the plots while holding down the command (on my NeXT, might be slightly different on the machine of your choice) : watch the tow entries in the bottom left corner of this notebook window; while you move the mouse through the figure the two entries change.

```
In[8]:= k=1.2943;
cond=coefficients[k];
Phi[x_]:=Which[x<=-a-d,PhiI[x,k]/.cond,
  x<=-a,PhiIII[x,k]/.cond,
  x<=a,PhiIIII[x,k]/.cond,
  x<a+d,PhiIV[x,k]/.cond,
  True,PhiV[x,k]/.cond];
```

Plot of the probability density corresponding to Phi[x]:

```
In[9]:= Timing[
Plot[Abs[Phi[x]]^2,{x,7/2*(-a-d),3/2*(a+d)},
  PlotRange->All,
  Ticks->{{{-a-d,"-a-d"},{-a,"-a"},{0,"0"}},
  {a,"a"},{a+d,"a+d"}},Automatic]
]
```

The following statements carry out some calculations which identify the maxima and the width of the resonances in T[k] and III[k] as defined above. First we define some functions which are needed to construct stationary states of the following systems

f0[k, n] used to determine the nth stationary state of a square well (a barrel with $d \rightarrow \text{infinity}$) f1[k, n] used to determine the maxima of the resonances shown by T[k] and III[k] obtained by searching for solutions of a square well particle with logarithmic derivative = - k at $x = a + d$ assuming a real and symmetric (even, odd) state f2[k,n] used to determine the width of the maxima of the resonances shown by T[k] and III[k] obtained by searching for solutions of a square well particle with derivatives = -0 at $x = a + d$ assuming a real and symmetric (even, odd) state

```

In[10]:= f0[k_,n_] := ArcTan[ Sqrt[(k0 a /k)^2-1]] + n Pi
/ 2 - k;
f1[k_,n_] := (
kappa = Sqrt[(k0 a)^2 - k^2];
kappad = kappa (d / a);
e1=Exp[kappad];
e2=1/e1;
ratio = (kappa + k)/(kappa - k);
ArcTan[ (kappa / k) (ratio e1 - e2)/(ratio e1 + e2)
] + n Pi / 2 - k
);
dka[k_]:= (
kappa = Sqrt[(k0 a)^2 - k^2];
kappad = kappa (d / a);
Exp[-2 kappad]
);
f2[k_,n_] := ArcTan[ Tanh[(d/a) Sqrt[(k0 a)^2 - k^2]]Sqrt[(k0
a/k)^2-1] ] + n Pi / 2 - k;

```

Evaluate and print now the k-values and energies corresponding to the stationary states of a square well with the three different boundary conditions mentioned above. The statements below carry out a Do-loop to evaluate stationary states for as energy are expected to fall below the barrier of the square barrel potential.

```

In[11]:= n0 = N[Floor[2 k0 a/ Pi]];
Do [(
kstart = 0.5;
ka = k/. FindRoot[ f0[k,n] == 0, {k, kstart}];
e = hbar^2 ka^2/ ( 2 m a^2);
Print[{n, ka/a, e}, " pure square well case"];
kass = k/. FindRoot[ f1[k,n] == 0, {k, kstart}];
ess = hbar^2 kass^2/ ( 2 m a^2);
Print[{n, kass/a, ess}, " square well with deriv =
-k at x=a+d"];
kas = k/. FindRoot[ f2[k,n] == 0, {k, kstart}];
es = hbar^2 kas^2/ ( 2 m a^2);
Print[{n, kas/a, es}, " square well with deriv =
0 at x=a+d"]
), {n, 0, n0-1, 1}]

```