Solution to Problem Set 3, Problem 5
Physics 480 / Fall 1999
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Problem 5: Barrel Potential

(b.i)

$$\begin{aligned}
k &= \sqrt{\tfrac{2mE}{\hbar^2}} \\
k_o &= \sqrt{\tfrac{2m(U_0-E)}{\hbar^2}} \\
\theta_I &= Ie^{ikx} + Re^{-ikx} \\
\theta_{II} &= u_1 e^{k_o x} + v_1 e^{-k_o x} \\
\theta_{III} &= u_2 e^{ikx} + v_2 e^{-ikx} \\
\theta_{IV} &= u_3 e^{k_o x} + v_3 e^{-k_o x} \\
\theta_V &= Te^{ikx} \text{ for transmission only}
\end{aligned}$$

(b.ii)

At the right and left sides of the boundaries we have continuity in the wavefunction $\theta_{left} = \theta_{right}$ and in its derivative $\theta'_{left} = \theta'_{right}$

$$\begin{aligned}
&Ae^{ik(-a-\delta)} + re^{-ik(-a-\delta)} = u_1 e^{k_o(-a-\delta)} + v_1 e^{-k_o(-a-\delta)} \\
&ik\left(Ae^{ik(-a-\delta)} - re^{-ik(-a-\delta)}\right) = k_o\left(u_1 e^{k_o(-a-\delta)} - v_1 e^{-k_o(-a-\delta)}\right) \\
&u_1 e^{k_o(-a)} + v_1 e^{-k_o(-a)} = u_2 e^{ik(-a)} + v_2 e^{-ik(-a)} \\
&k\left(u_1 e^{k(-a)} - v_1 e^{-k(-a)}\right) = ik\left(u_2 e^{ik(-a)} - v_2 e^{-ik(-a)}\right) \\
&u_2 e^{ik(a)} + v_2 e^{-ik(a)} = u_3 e^{k_o(a)} + v_3 e^{-k_o(a)} \\
&ik\left(u_2 e^{ik(a)} - v_2 e^{-ik(a)}\right) = k\left(u_3 e^{k_o(a)} - v_3 e^{-k_o(a)}\right) \\
&u_3 e^{k_o(a+\delta)} + v_3 e^{-k_o(a+\delta)} = te^{ik(a+\delta)} \\
&k_o\left(u_3 e^{k_o(a+\delta)} - v_3 e^{-k_o(a+\delta)}\right) = ikte^{ik(a+\delta)}
\end{aligned}$$

(b.iii) We obtain all the coefficients from the command: **amplitudes = Solve[conditions, r,u1,u2,u3,v1,v2,v3,t];** where the conditions are those defined in part (ii)

Part (b)(iv) We obtain the reflection coefficient by evaluating the results of part (iii) for the coefficient r. It is done by: {**Rb[k,ae,ade,V0e] = N[r/.amplitudes/.qfunct/.a−** > **ae, ad−** > **ade, V0−** > **V0e]**; } where we have inserted the results from *amplitudes* and other specific parameters of the potential. The resulting expression is fairly long and can be obtained from the notebook. Similarly for the transmission coefficient **t** with the command: {**Rb[k,ae,ade,V0e] = N[t/.amplitudes/.qfunct/.a−** > **ae, ad−** > **ade, V0−** > **V0e]**; } i.e. **r** replaced by **t**. **Part (d)**

$$\hbar\left[\frac{\psi_j^{n+1} - \psi_j^n}{\Delta t}\right] = -\frac{\hbar^2}{2m}\left[\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta x)^2}\right] + v(x_j)\psi_j^{n+1}$$

Taylor expand terms

$$\begin{aligned}
\psi_j^{n+1} - \psi_j^n &= \left(\psi_j^n + \tfrac{\partial\psi}{\partial t}\Delta t + \tfrac{1}{2}\tfrac{\partial^2\psi}{\partial t^2}\Delta t^2 + \ldots\right) - \psi_j^n \\
&= \tfrac{\partial\psi}{\partial t}\Delta t + \tfrac{1}{2}\tfrac{\partial^2\psi}{\partial t^2}\Delta t^2 + \ldots \\
\psi_{j+1}^{n+1} - 2\psi_j^{n+1} &+ \psi_{j-1}^{n+1} = \left(\psi_j^n + \tfrac{\partial\psi}{\partial x}\Delta x + \tfrac{1}{2}\tfrac{\partial^2\psi}{\partial x^2}(\Delta x)^2 + \ldots\right) \\
&-2\psi_j^n \\
&+\left(\psi_j^n + \tfrac{\partial\psi}{\partial x}(-\Delta x) + \tfrac{1}{2}\tfrac{\partial^2\psi}{\partial x^2}(-\Delta x)^2 + \ldots\right) \\
&= \tfrac{\partial^2\psi}{\partial x^2}(\Delta x)^2 + \ldots
\end{aligned}$$

Take $\Delta t \to 0$ and $\Delta x \to 0$ limits

$$\lim_{\Delta t \to 0} \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left(\frac{\partial \psi}{\partial t} \Delta t + \frac{1}{2} \frac{\partial^2 \psi}{\partial t^2} \Delta t^2 + \ldots \right) = \frac{\partial \psi}{\partial t}$$

$$\lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0}} \frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta x)^2} = \frac{1}{(\Delta x)^2} \left(\frac{\partial^2 \psi}{\partial x^2} (\Delta x)^2 + \ldots \right) = \frac{\partial^2 \psi}{\partial x^2}$$

In the limit, Eq. (a) becomes

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + v(x)\psi$$

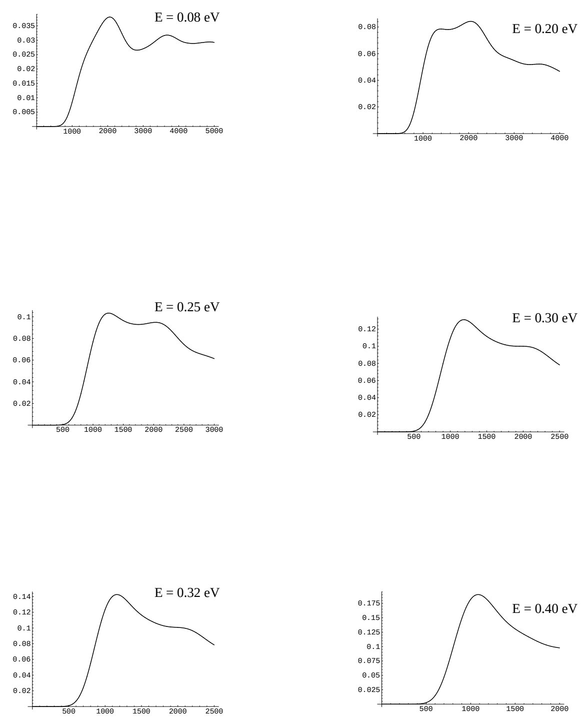


Figure 1: Total probability that the electron can be found inside the barrel vs. time

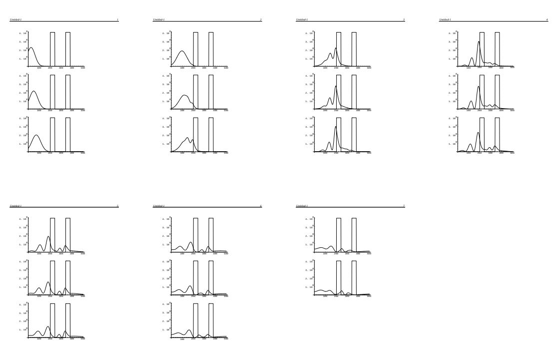


Figure 2: Absolute square $| \psi_j^n |^2$ of the wave function as a function of position x_j for twenty successive times t_n.

`Mathematica` **notebook**

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

Wave Coefficients

We first define the wave functions in the five regions,...

In[2]:=
```
*)
PhiI[x_]        := i  Exp[I k x]        + r Exp[-I k x] ;
PhiII[x_]        := u1 Exp[I q[k] x] + v1 Exp[-I q[k] x] ;
PhiIII[x_]        := u2 Exp[I k x]        + v2 Exp[-I k x] ;
PhiIV[x_]        := u3 Exp[I q[k] x] + v3 Exp[-I q[k] x] ;
PhiV[x_]        := t  Exp[I k x] ;
(*
```

... write down the conditions at the boundaries (ad = a+d)...

In[3]:=
```
*)
conditions = {
PhiI[-ad] == PhiII[-ad],
PhiII[-a] == PhiIII[-a],
PhiIII[a] == PhiIV[a],
PhiIV[ad] == PhiV[ad],
D[PhiI[x],x]   == D[PhiII[x],x]  /. x->-ad,
D[PhiII[x],x]  == D[PhiIII[x],x] /. x->-a,
D[PhiIII[x],x] == D[PhiIV[x],x]  /. x->a,
D[PhiIV[x],x]  == D[PhiV[x],x]   /. x->ad };
(*
```

... and let the Mathematica find the solutions

In[4]:=
```
*)
i = 1;
Timing[amplitudes =
Solve[conditions, {r,u1,u2,u3,v1,v2,v3,t}];]
(*
```

Out[4]=
```
{44.6 Second, Null}
```

In[5]:=
```
*)
qfunct = {q[k] -> Sqrt[k*k - V0]};
(*
```

Reflected Wave Coefficient

Here we obtain the reflection coefficient as a function of k and the barrel parameters

In[6]:=
```
*)
Timing[ Rb[k_,ae_,ade_,V0e_] =
N[r /. amplitudes /. qfunct  /.{a->ae, ad->ade, V0->V0e}];]
(*
```

Out[6]=
```
{1.44 Second, Null}
```

We get a more handy solution by plugging in some values of a barrel; we then plot the new function

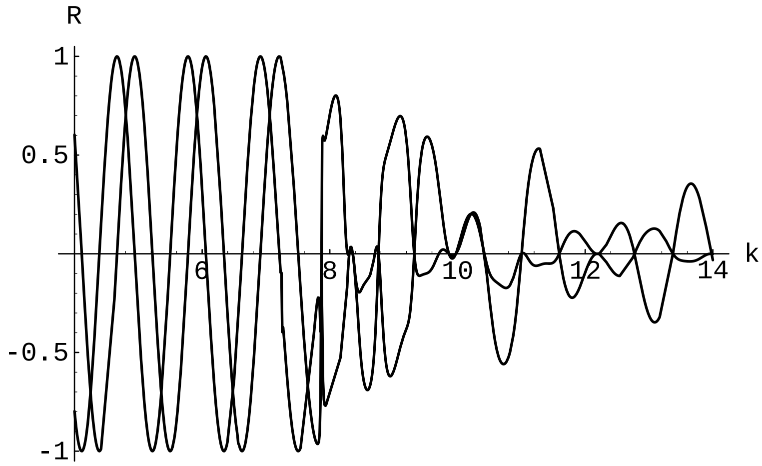
In[7]:=
```
Timing[R[k_] = Rb[k,2,3,60][[1]];]
```

Out[7]=
```
{0.733333 Second, Null}
```

In[8]:=
```
Timing[{Re[R[10]],Im[R[10]]}]
```

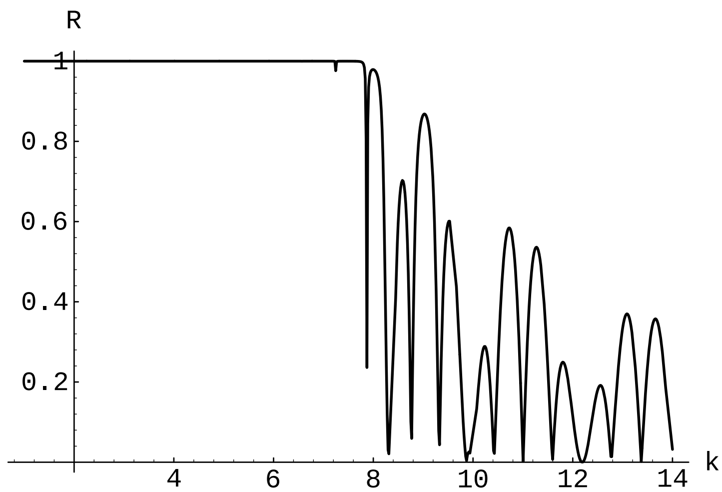
Out[8]=
```
{0.783333 Second, {0.0239463, 0.013467}}
```

In[9]:=
```
Timing[ Plot[{Re[R[k]],Im[R[k]]},{k,4,14},
PlotRange -> All,AxesLabel -> {"k","R"}]  ]
```



Out[9]= `{301.417 Second, -Graphics-}`

In[10]:=
```
Timing[Plot[Abs[R[k]],{k,1,14},PlotRange -> All,
AxesLabel -> {"k","R"}]  ]
```



Out[10]= `{236.333 Second, -Graphics-}`

Transmitted Wave Coefficient

... same procedure for the transmission coefficient...

In[11]:=
```
*)
Timing[ Tb[k_,ae_,ade_,V0e_] = N[ t /. amplitudes /. qfunct /.
{a -> ae, ad-> ade, V0 -> V0e} ];    ]
(*
```

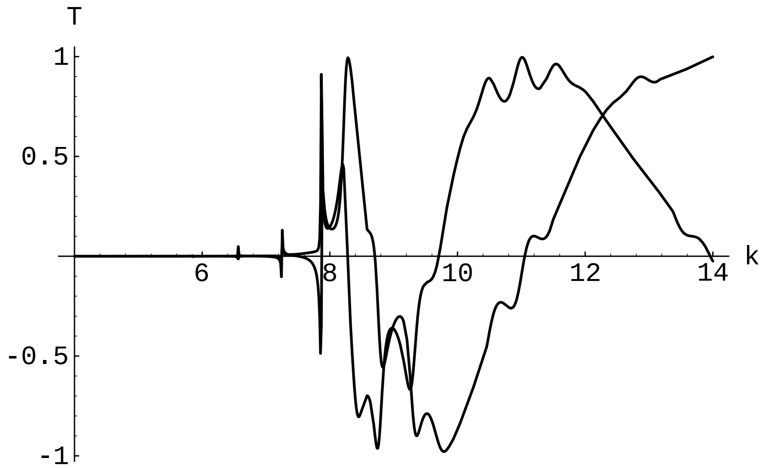
Out[11]= `{0.39 Second, Null}`

After specifying the function T[k] for one particular wave geometry...

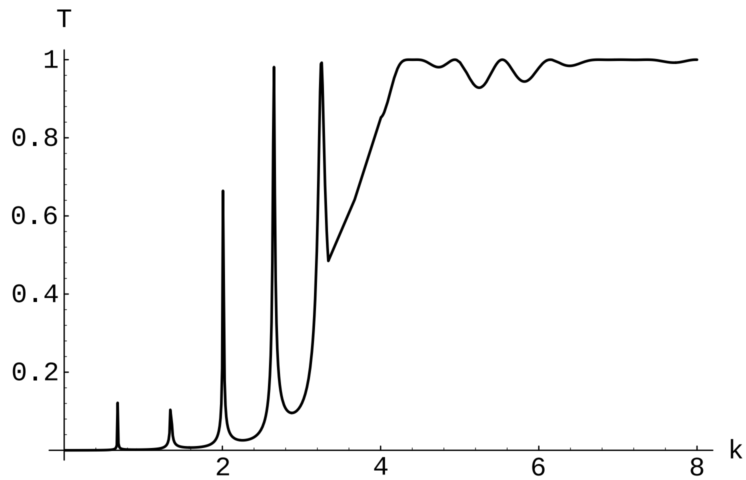
In[12]:=
```
T[k_] = Tb[k,2,3,10][[1]];
```

... we can plot it:

In[13]:=
```
Plot[{Re[T[k]],Im[T[k]]},{k,4,14},PlotRange -> All,AxesLabel -> {"k","T"}]
```



In[14]:=
```
Timing[Plot[Abs[T[k]],{k,0.01,8},PlotRange -> All,
AxesLabel -> {"k","T"}]  ]
```



Out[14]= `{47.1667 Second, -Graphics-}`

Intermediate Wave Coefficients

... and the same procedure again for the intermediate coefficients.

In[15]:=
```
*)
U1a[k_] :=  u1 /. amplitudes /. qfunct
U2a[k_] :=  u2 /. amplitudes /. qfunct
U3a[k_] :=  u3 /. amplitudes /. qfunct
V1a[k_] :=  v1 /. amplitudes /. qfunct
V2a[k_] :=  v2 /. amplitudes /. qfunct
V3a[k_] :=  v3 /. amplitudes /. qfunct

(*
```

In[16]:=
```
*)
U1b[k_,ae_,ade_,V0e_] = N[U1a[k]  /. {a -> ae, ad-> ade, V0 -> V0e}];
U2b[k_,ae_,ade_,V0e_] = N[U2a[k]  /. {a -> ae, ad-> ade, V0 -> V0e}];
U3b[k_,ae_,ade_,V0e_] = N[U3a[k]  /. {a -> ae, ad-> ade, V0 -> V0e}];
V1b[k_,ae_,ade_,V0e_] = N[V1a[k]  /. {a -> ae, ad-> ade, V0 -> V0e}];
V2b[k_,ae_,ade_,V0e_] = N[V2a[k]  /. {a -> ae, ad-> ade, V0 -> V0e}];
V3b[k_,ae_,ade_,V0e_] = N[V3a[k]  /. {a -> ae, ad-> ade, V0 -> V0e}];

(*
```

EigenStates

Definition of the Eigenstates, composed of different exponentials in the five regions:

In[17]:=
```
*)
PhiIeigen[x_]         := i  Exp[I keigen x]          + reigen  Exp[-I keigen x]
PhiIIeigen[x_]         := u1eigen Exp[I qeigen x]      + v1eigen Exp[-I qeigen x]
PhiIIIeigen[x_]         := u2eigen Exp[I keigen x]    + v2eigen Exp[-I keigen x]
PhiIVeigen[x_]         := u3eigen Exp[I qeigen x]      + v3eigen Exp[-I qeigen x]
PhiVeigen[x_]         := teigen  Exp[I keigen x]

Phieigen[x_,a_,d_] := Which[x<-a-d, PhiIeigen[x],
 x <-a, PhiIIeigen[x],
 x < a, PhiIIIeigen[x],
 x <a+d, PhiIVeigen[x],
x >a+d     , PhiVeigen[x]]
(*
```

Plugging in Values for the Potential

We can use procedure BarrelSetup to plug the barrel parameters into the equations for the wave coefficients. Basically, invoking BarrelSetup teaches the computer how to calculate the eigenstates for a certain Barrel Geometry.

In[18]:=
```
*)
BarrelSetup[aplugin_,dplugin_,Vplugin_] := (
Clear[R,T,U1,U2,U3,V1,V2,V3];
R[k_] = Rb[k,aplugin,aplugin+dplugin,Vplugin][[1]];
T[k_] = Tb[k,aplugin,aplugin+dplugin,Vplugin][[1]];

U1[k_] = U1b[k,aplugin,aplugin+dplugin,Vplugin][[1]];
U2[k_] = U2b[k,aplugin,aplugin+dplugin,Vplugin][[1]];
U3[k_] = U3b[k,aplugin,aplugin+dplugin,Vplugin][[1]];
V1[k_] = V1b[k,aplugin,aplugin+dplugin,Vplugin][[1]];
V2[k_] = V2b[k,aplugin,aplugin+dplugin,Vplugin][[1]];
V3[k_] = V3b[k,aplugin,aplugin+dplugin,Vplugin][[1]]; );
(*
```

In[19]:=

In[20]:=
```
*)
Timing[BarrelSetup[2,1,10]]
(*
```

Out[20]=
```
{3.28 Second, Null}
```

Plotting the Eigenstates

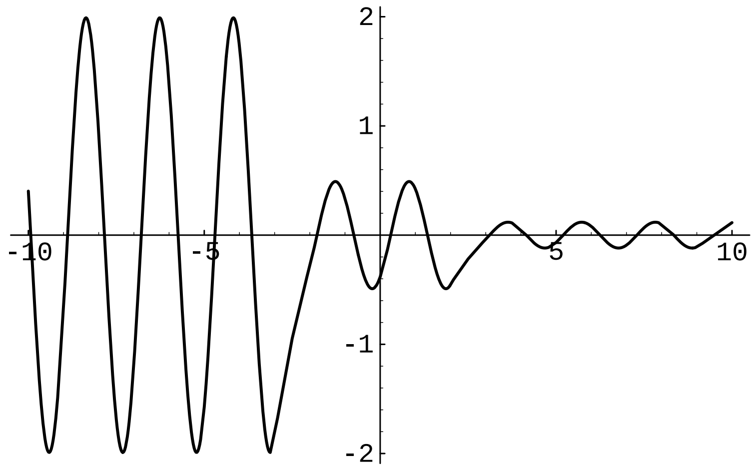
This routine plots the Eigenstates of the barrel potential

In[21]:=
```
*)
EigenPlot[k_,a_,d_,V_,xmin_,xmax_] := (
keigen = k;
qeigen = Sqrt[k^2-V];
reigen = R[k];
teigen = T[k];
u1eigen = U1[k];
u2eigen = U2[k];
u3eigen = U3[k];
v1eigen = V1[k];
v2eigen = V2[k];
v3eigen = V3[k];
Plot[Re[Phieigen[x,a,d]],{x,xmin,xmax},PlotRange->{-2,2}]);
(*
```

If we want to plot the eigenstates, we first have to specify the barrel geometry using BarrelSetup.

In[22]:= `BarrelSetup[2,1,10]`

In[23]:= `Timing[EigenPlot[3,2,1,10,-10,10]]`



Out[23]= `{5.1 Second, -Graphics-}`

The following command will produce a nice movie of the Eigenstates as the wavevector k is continuously increased. Enter the command if you like, but please remove the movie after watching it since it uses a lot of space.

In[24]:= `Table[EigenPlot[k,2,1,10,-15,10],{k,0.05,3,0.05}]`

If we want to study a different Barrel Geometry, we again have to invoke BarrelSetup first:

In[25]:= `BarrelSetup[2.5,0.5,10]`

In[26]:= `EigenPlot[3.5,2.5,0.5,10,-4.1,4]`