Solution to Problem Set 5
Physics 480 / Fall 1999
Prof. Klaus Schulten / Prepared by Pinaki Sengupta & Ioan Kosztin

Problem 1: Energies of the Bound States of the Morse Potential in the Semiclassical Approximation

The Bohr–Sommerfeld quantization condition can be expressed as follows

$$\int_{y_\ell(E)}^{y_r(E)} dy \sqrt{\frac{2m}{\hbar^2}\left[E \,-\, D(e^{-2ay} \,-\, 2\,e^{-ay})\right]} \;=\; \pi\,(n \,+\, \frac{1}{2}) \tag{1}$$

where $y_\ell(E)$ and $y_r(E)$ are the left and right classical turning points, respectively. The latter are determined trough the roots of

$$E \,-\, D(e^{-2ay} \,-\, 2\,e^{-ay}) \;=\; 0 \tag{2}$$

where $E \,<\, 0$ and

$$y_\ell(E) \;<\; y_r(E)\;. \tag{3}$$

In order to determine the integral in (1) we simplify by transforming to dimensionless variables $y' \,=\, a\,y$

$$\int_{ay_\ell(E)}^{ay_r(E)} dy \sqrt{\epsilon \,-\, e^{-2ay} \,+\, 2\,e^{-ay}} \;=\; \pi\,(n \,+\, \frac{1}{2})\sqrt{\frac{\hbar^2 a^2}{2mD}} \tag{4}$$

$$\epsilon \;=\; \frac{E}{D}\;. \tag{5}$$

Let us define the new variable $x \,=\, e^{-y}$. It holds then $dy \,=\, -dx/x$ and the Bohr–Sommerfeld condition reads

$$\int_{x_r(E)}^{x_\ell(E)} \frac{dx}{x}\sqrt{\epsilon \,-\, x^2 \,+\, 2\,x} \;=\; \pi\,(n \,+\, \frac{1}{2})\sqrt{\frac{\hbar^2 a^2}{2mD}}\;. \tag{6}$$

The left and right turning points correspond to $x_\ell(\epsilon)$ and $x_r(\epsilon)$, respectively, and are defined through

$$x_\ell(\epsilon) \;=\; \exp\left[\,-\,y_\ell(E)\right]\;, \quad x_r(\epsilon) \;=\; \exp\left[\,-\,y_r(E)\right]\;. \tag{7}$$

Note that the following property holds

$$x_\ell(\epsilon) \; > \; x_r(\epsilon) \tag{8}$$

which is consistent with (3). According to (2) holds

$$\epsilon \; - \; x_{\ell,r}^2 \; + \; 2\, x_{\ell,r} \; = \; 0 \, . \tag{9}$$

The two solutions of this equation are

$$x_\ell(\epsilon) \; = \; 1 \; + \; \sqrt{\epsilon \; + \; 1} \, , \quad x_\ell(\epsilon) \; = \; 1 \; - \; \sqrt{\epsilon \; + \; 1} \tag{10}$$

From this one can derive the following properties

$$\frac{1 \; - \; x_\ell}{\sqrt{\epsilon + 1}} \; = \; -1 \, , \quad \frac{1 \; - \; x_r}{\sqrt{\epsilon + 1}} \; = \; 1 \tag{11}$$

as well as

$$\frac{x_\ell \; + \; \epsilon}{x_\ell \, \sqrt{\epsilon + 1}} \; = \; 1 \, , \quad \frac{x_r \; + \; \epsilon}{x_r \, \sqrt{\epsilon + 1}} \; = \; -1 \, . \tag{12}$$

The integral in (6) can be evaluated analytically. Consulting an integral table one obtains (note $\epsilon < 0$ and $1 + \epsilon > 0$, see previous problem)

$$\begin{aligned} \int \frac{dx}{x} \sqrt{\epsilon \; - \; x^2 \; + \; 2x} \; = \; & \sqrt{\epsilon \; - \; x^2 \; + \; 2x} \; - \; \sqrt{-\epsilon} \arcsin\left(\frac{\epsilon + x}{x \sqrt{\epsilon + 1}} \right) \\ & + \quad \arcsin\left(\frac{1 - x}{\sqrt{\epsilon + 1}} \right) \, . \end{aligned} \tag{13}$$

Noting properties (9, 11, 12) one can state (6) immediately in the form

$$\left(\sqrt{-\epsilon} \; + \; 1 \right) \pi \; = \; \pi \left(n \; + \; \frac{1}{2} \right) \sqrt{\frac{\hbar^2 a^2}{2mD}} \, . \tag{14}$$

This can be expressed using (5)

$$E \; = \; -D \left(1 \; - \; \sqrt{\frac{\hbar^2 a^2}{2mD}} \, (n + \frac{1}{2}) \right)^2 \tag{15}$$

which is indeed identical to the exact solution. An upper limit for n follows from the derivation.

Problem 2: Electron at Surface of a Semiconductor

(a) We can see that the classical turning points for the electron with energy E_n will be at $x = 0$ and $x = E_n/e\mathcal{E}$. Using these in the Born-Sommerfeld condition, we get

$$S(E_n) \; = \; 2\int_0^{E_n/e\mathcal{E}} dx\sqrt{\frac{2m}{\hbar^2}\left(E_n - e\mathcal{E}x\right)} \; = \; \left(n+\frac{1}{2}\right)2\pi \; . \tag{16}$$

Making the substitutions

$$y \; = \; \frac{2m}{\hbar^2}\left(E_n - e\mathcal{E}x\right), \; dy \; = \; -\frac{2me\mathcal{E}}{\hbar^2}dx, \tag{17}$$

we get

$$\begin{aligned} S(E_n) \; &= \; 2\frac{\hbar^2}{2me\mathcal{E}}\int_0^{\frac{2mE_n}{\hbar^2}} dy\sqrt{y} \\ &= \; \frac{2\hbar^2}{3me\mathcal{E}}\left(\frac{2mE_n}{\hbar^2}\right)^{\frac{3}{2}} \\ &= \; \frac{2}{3}\frac{\left(2mE_n\right)^{\frac{3}{2}}}{me\mathcal{E}\hbar} \; = \; \left(n+\frac{1}{2}\right)2\pi \end{aligned} \tag{18}$$

which, when solved for E_n, gives the semiclassical energy levels

$$E_n^{(semi)} \; = \; \frac{\hbar^2}{2m}\left[\frac{3\pi me\mathcal{E}}{\hbar^2}\left(n+\frac{1}{2}\right)\right]^{\frac{2}{3}}, n \; = \; 0, 1, 2, \ldots \tag{19}$$

(b) The Schrödinger equation for this problem is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_E}{dx^2} + e\mathcal{E}x\phi_E \; = \; E\,\phi_E \; . \tag{20}$$

For $x < 0$,

$$\phi_E(x) \; = \; 0 \; . \tag{21}$$

For $x \geq 0$, employing new variable

$$\xi \; = \; \left(\frac{2me\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}\left(x - \frac{E}{e\mathcal{E}}\right) \; , \tag{22}$$

we obtain

$$\frac{d^2}{dx^2} \;=\; \left(\frac{2me\mathcal{E}}{\hbar^2}\right)^{\frac{2}{3}} \frac{d^2}{d\xi^2} \;, \tag{23}$$

so that (20) can be written as

$$-\frac{d^2\phi_E(\xi)}{d\xi^2} + \xi\phi_E(\xi) \;=\; 0 \;. \tag{24}$$

The solution of the differential equation, which is finite everywhere, is the so-called *Airy function*

$$Ai(\xi) \;=\; \frac{1}{\sqrt{\pi}} \int_0^\infty du \cos\left(\frac{1}{3}u^3 + u\xi\right) . \tag{25}$$

Thus, for $x > 0$, we have

$$\phi_E(x) \;=\; const \times Ai\left[\left(\frac{2me\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}} \left(x - \frac{E}{e\mathcal{E}}\right)\right] . \tag{26}$$

And, at the boundary $x = 0$, we have

$$\phi_E(0) \;=\; 0 \;. \tag{27}$$

(c) From (26) and (27), we have

$$Ai\left[-\left(\frac{2m}{e^2\mathcal{E}^2\,\hbar^2}\right)^{\frac{1}{3}} E\right] \;=\; 0 \;. \tag{28}$$

If x_n is n-th zero of the *Airy function* $Ai(-x)$, $n = 0, 1, 2, ...$, the n-th exact quantum mechanical eigen energy is

$$E_n^{(qm)} \;=\; \left(\frac{e^2\mathcal{E}^2\,\hbar^2}{2m}\right) x_n \tag{29}$$

One can see the Airy function $Ai\,(-x)$ in Fig 1. First, we estimate 10 zeros for Ai[-x] by reading from the plot

$$x \;=\; \{2.2,\, 4.0,\, 5.8,\, 7.0,\, 8.0,\, 9.1,\, 10.0,\, 11.0,\, 12.0,\, 13.0\} \;. \tag{30}$$

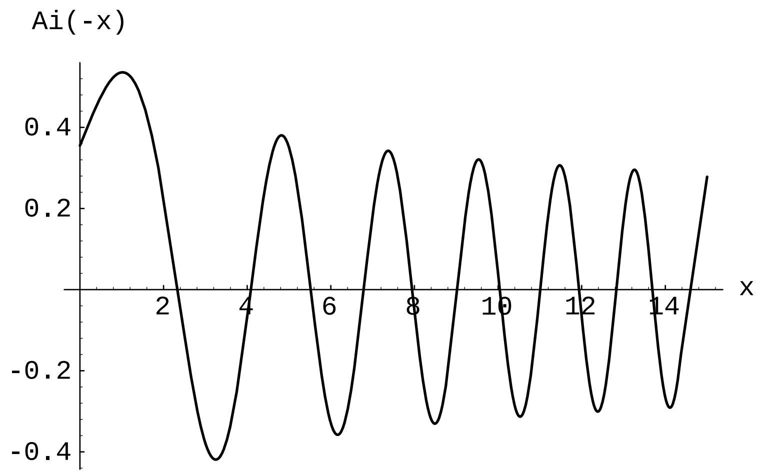

Figure 1: *Airy function* $Ai\,(-x)$.

Now we use the `Mathematica` built-in function `FindRoot` to evaluate the exact solution for the zeros of the *Airy function* near the estimated points in (30). It gives the following result

$$\begin{aligned} x \;&=\; \{2.33811,\, 4.08795,\, 5.52056,\, 6.78671,\, 7.94413, \\ &\qquad 9.02265,\, 10.0402,\, 11.0085,\, 11.936,\, 12.8288\}\;. \end{aligned} \tag{31}$$

The exact eigen energies $E_n^{(qm)}$ can be calculated from (29), and can be compared with the semiclassical result in (19). Evaluate the percentage error by

$$error\,[n] \;=\; \frac{E_n^{(qm)} \;-\; E_n^{(semi)}}{E_n^{(qm)}}\;. \tag{32}$$

Then one can get the percentage error of semiclassical energy levels as a function of quantum number n, which is shown in Fig. 2. From the figure, it is shown that the larger the quantum number is, the better the semi-classical approximation can be.

(d) The wave function $\phi_{E_n}(x)$ can be written as

$$\phi_{E_n}(x) \;=\; C_n\,Ai\left[\left(\frac{2me\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}\left(x - \frac{E_n}{e\mathcal{E}}\right)\right] \tag{33}$$

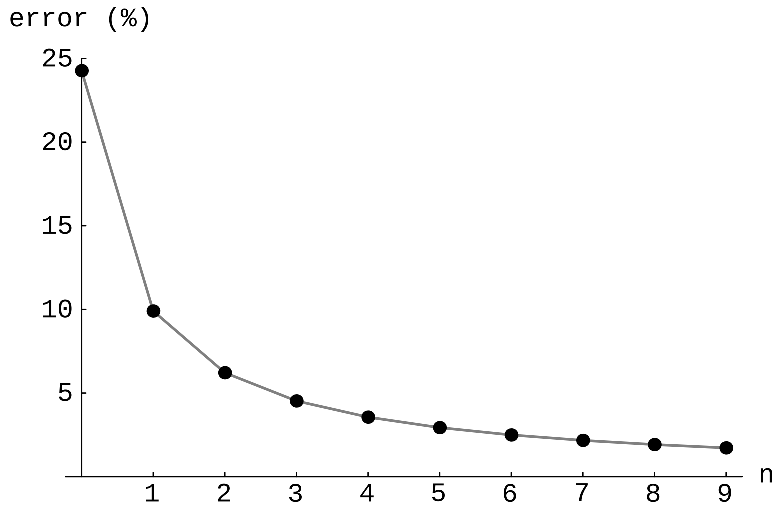

Figure 2: percentage error of semiclassical energy levels as a function of quantum number n.

where C_n is

$$C_n = \left\{ \int_0^\infty \mathrm{d}x \, Ai^2 \left[\left(\frac{2me\mathcal{E}}{\hbar^2} \right)^{\frac{1}{3}} \left(x - \frac{E_n}{e\mathcal{E}} \right) \right] \right\}^{-\frac{1}{2}} . \tag{34}$$

Hence, we can use (34) and (33) to plot the wave function for $n = 0, 2, 4, 6, 8$, by using both the semiclassical energies obtained in **(a)** and the exact energies obtained in **(c)**. The wave functions are shown in Fig. 3.

Fig. 3 clearly demonstrates for the exact solution that the wave functions have the characteristics we require: they are zero at the origin, and decay to zero once they are past the potential boundary. Also, the n-th wave has n inflection points, as we expect. For the semiclassical plot, the wave functions are not quite vanishing at the origin due to the error of semiclassical eigen energies.

(e) The classical turning points x' for the electron is

$$x' = \frac{E_n}{e\mathcal{E}} . \tag{35}$$

The probabilities for the electron to penetrate into the classically forbid-

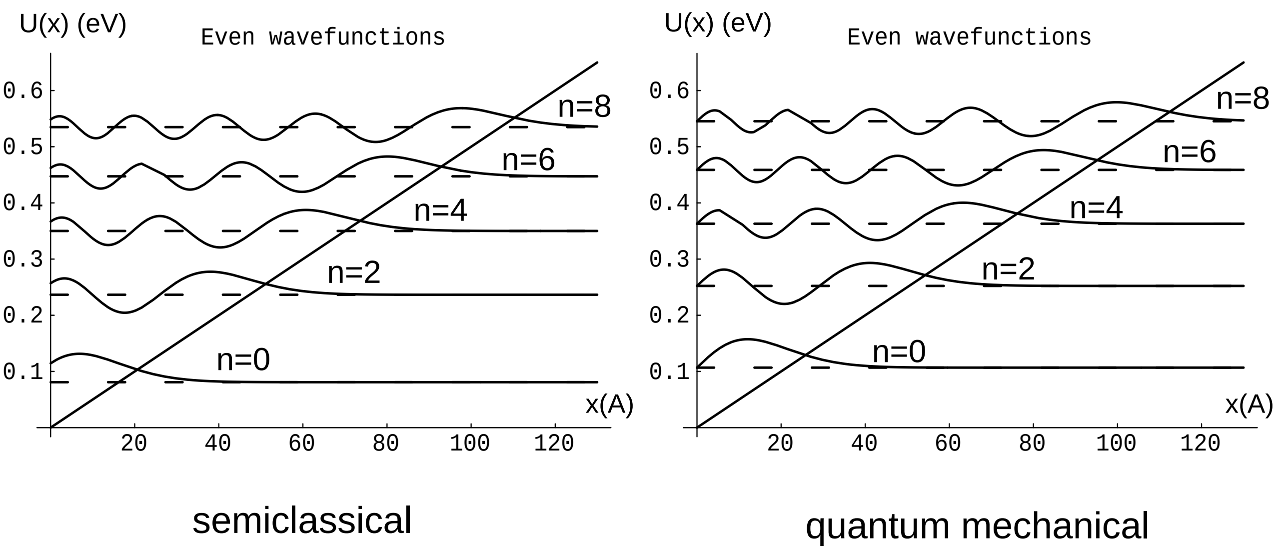

Figure 3: Plot of the even-n wave functions along with the potential well. The energy of each wave function will be indicated by a dashed line. Note that the scale of the wave function here is rescaled. All the wave functions have been multiplied by a factor of 0.2 simply to fit the potential plot.

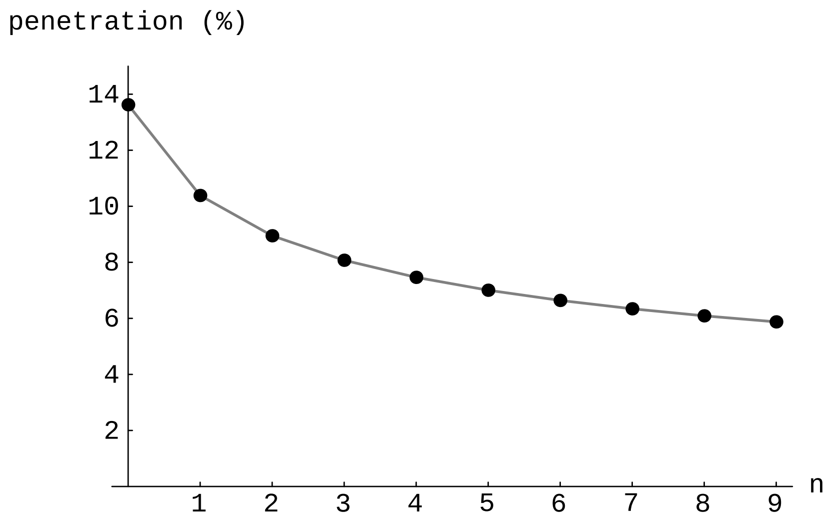

Figure 4: The probabilities for the electron to penetrate into the classically forbidden region as a function of quantum number n

.

den region is

$$P_n \;=\; C_n^2 \int_{x_n'}^{\infty} \mathrm{d}x\, Ai^2\left[\left(\frac{2me\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}\left(x-\frac{E_n}{e\mathcal{E}}\right)\right] \tag{36}$$

which is shown in the Fig. 4. One can see that the larger the quantum numbers are, the less the electron can penetrate into the classical forbidden region.

The mean values of x is

$$\bar{x}_n \;=\; C_n^2 \int_{0}^{\infty} \mathrm{d}x\, x\, Ai^2\left[\left(\frac{2me\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}\left(x-\frac{E_n}{e\mathcal{E}}\right)\right] \tag{37}$$

which is shown in the Fig. 5.

1 Mathematica notebook

(c)

Input the following parameters in units (eV, Angstrom, second):

(1) e – charge of electron (electron unit);

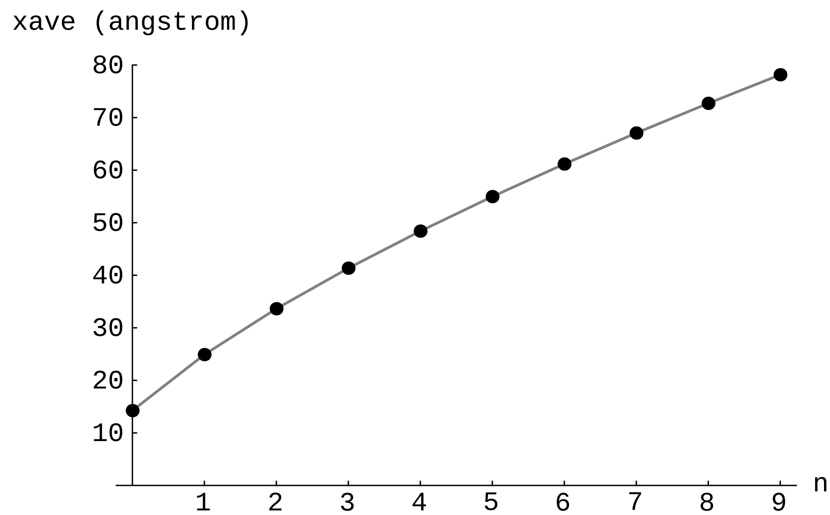

Figure 5: The mean values of x as a function of quantum number n

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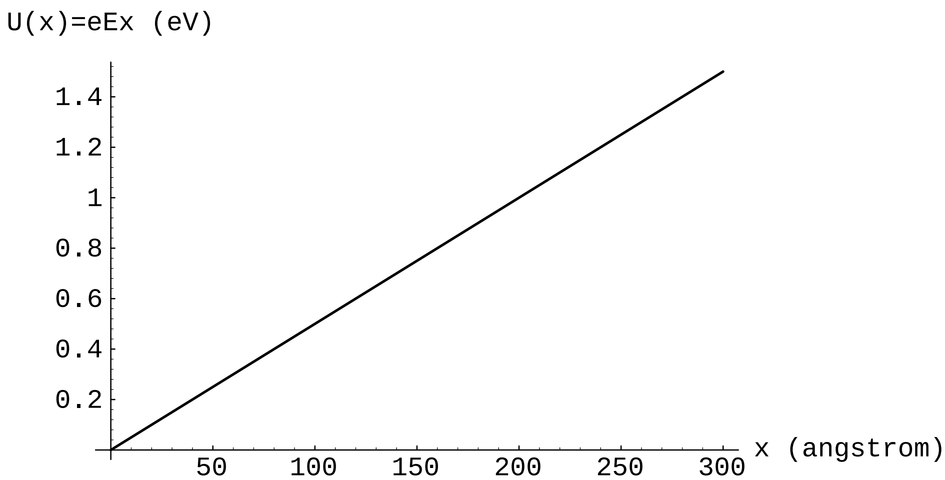
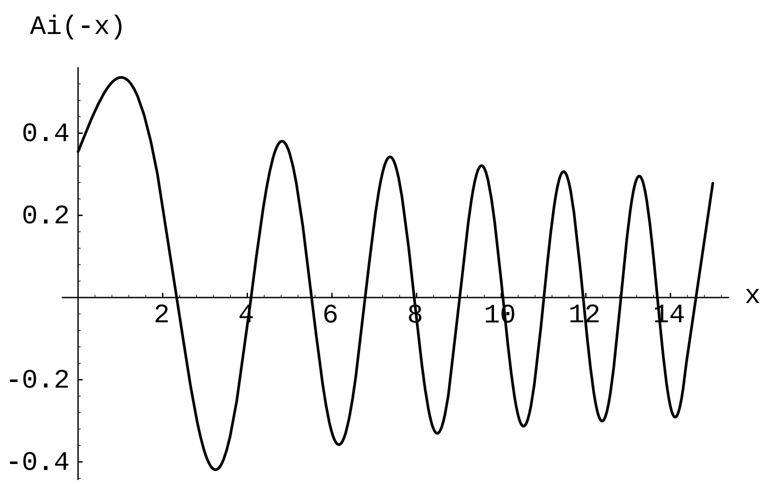
(2) Ef – electric field (eV/Angstrom);
(3) m – mass (eV secˆ2 / Angstromˆ2);
(4) hbar– Planck constant (eV sec).

```
In[1]:=    e=1;
           Ef=500 1000/10^8;
           m= 5.11 10^5 / (3 10^8 10^10)^2;
           hbar=6.5822 10^(-16);

In[2]:=    f=e Ef
Out[2]=     1
           ---
           200

In[3]:=
           Plot[f x,{x,0,300},AxesLabel->{"x (angstrom)","U(x)=eEx
(eV)"},
              PlotRange -> All]
```



Out[3]= -Graphics-

In[4]:=
```
Plot[AiryAi[-e],{e,0,15},
   AxesLabel->{"x","Ai(-x)"},
   PlotRange->All]
```



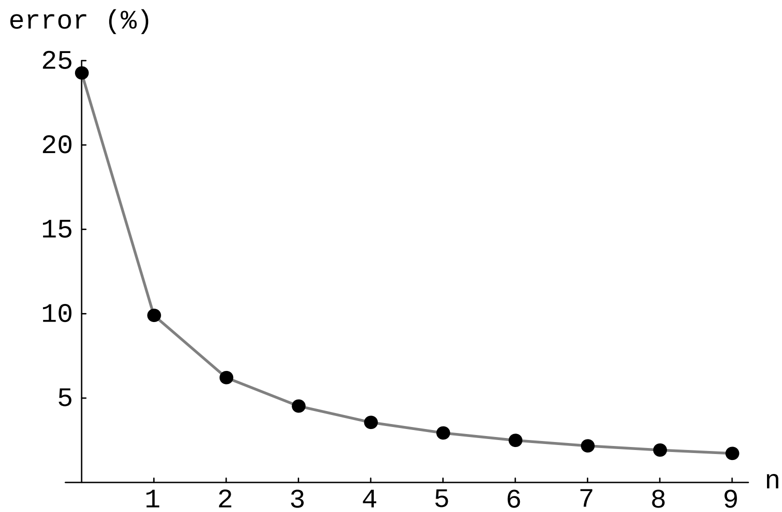
Out[4]= -Graphics-

From the solution for part (b) of this problem, we can use the equations (b-11) and (b-12), which leads to solve the zeroes of the Airy function.

In the following, we read 10 zeroes for Ai[-e] from the plot:

```
In[5]:=    guesses = {2.2,4.0,5.8,7.0,8.0,9.1,10.0,11.0,12.0,13.0};

In[6]:=    epsilon = Table[0.0,{n,1,Length[guesses]}];

In[7]:=    Clear[j];
           For[j = 1, j <= Length[guesses], j++,
              epsilon[[j]]=e /. FindRoot[AiryAi[-e]==0,
                                   {e,guesses[[j]]}];
              Print["epsilon",j-1," = ",epsilon[[j]]]
           ]

epsilon0 = 2.33811
epsilon1 = 4.08795
epsilon2 = 5.52056
epsilon3 = 6.78671
epsilon4 = 7.94413
epsilon5 = 9.02265
epsilon6 = 10.0402
epsilon7 = 11.0085
epsilon8 = 11.936
epsilon9 = 12.8288

In[8]:=    ff = N[ (2 m f / hbar^2)^(1/3)]

Out[8]=    0.109432

In[9]:=    epsilon1= f epsilon / ff
Out[9]=    {0.106829, 0.18678, 0.252236, 0.310087, 0.36297, 0.412248,
             0.458739, 0.502983, 0.545361, 0.586151}

In[10]:=   epsilon2 = Table[N[(hbar^2 /2/m) ((3 Pi m f/hbar^2)
           (n+.5))^(2/3)],
           {n,0,9}]
Out[10]=   {0.0809031, 0.168285, 0.236562, 0.296049, 0.350048,
             0.400154, 0.447295, 0.492069, 0.53489, 0.57606}

In[11]:=   error= (epsilon1 -epsilon2)/epsilon1
Out[11]=   {0.242685, 0.0990181, 0.0621408, 0.0452706, 0.0356029,
             0.0293372, 0.0249466, 0.021699, 0.0191995, 0.0172164}
```

```
In[12]:=  p=Table[{n-1, 100 error[[n]]},{n,10}];
          perr=ListPlot[p,
          AxesLabel->{"n","error (%)"},
          PlotRange->{0,25}, Prolog->{{GrayLevel[.5],
          Line[p]},AbsolutePointSize[5]},
          Ticks->{{1,2,3,4,5,6,7,8,9}, {0,5,10,15,20,25}}]
```




```
Out[12]=  -Graphics-
```

(d)
Plot the potential well for comparison

```
In[13]:=  Pplot=Plot[f x, {x,0,130},
            DisplayFunction->Identity];
```

For semiclassical solution:
Define the constant epsilon3 as

```
In[14]:=  epsilon3 = epsilon2 ff/f
Out[14]=  {1.77068, 3.68317, 5.17751, 6.47947, 7.6613, 8.75795,
            9.78971, 10.7697, 11.7068, 12.6079}
```

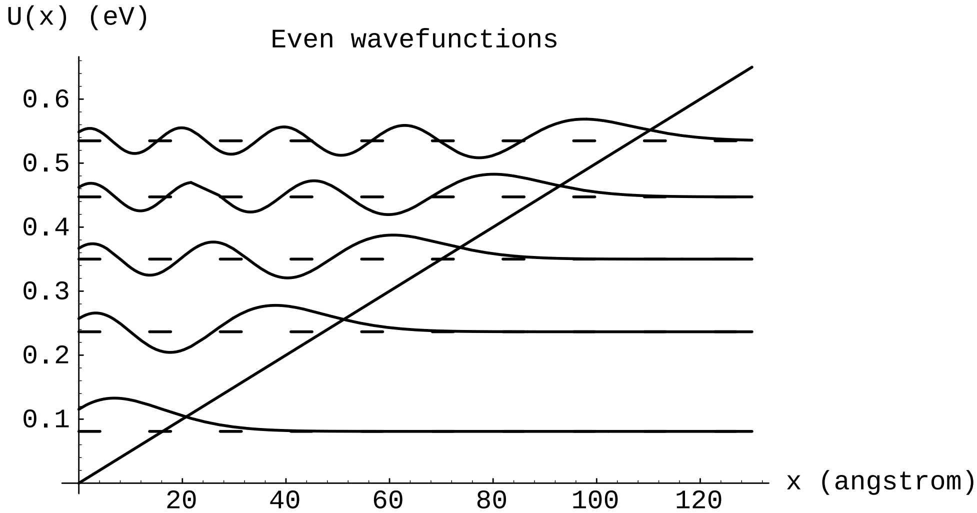
Find out the normalized factor by evaluating

```
In[15]:=  norm = Table[NIntegrate[AiryAi[ff x-epsilon3[[n]]]^2,
          {x,0, Infinity}], {n,1,10}]
Out[15]=  {4.25429, 5.7794, 6.75948, 7.51678, 8.14637, 8.69137,
            9.17551, 9.61335, 10.0146, 10.386}
```

```
In[16]:=  WFF1=Plot[epsilon2[[1]]+
                .2 AiryAi[ff x-epsilon3[[1]]]/Sqrt[norm[[1]]],
            {x,0,130}, DisplayFunction->Identity];
          WFF3=Plot[epsilon2[[3]]+
                .2 AiryAi[ff x-epsilon3[[3]]]/Sqrt[norm[[3]]],
            {x,0,130}, DisplayFunction->Identity];
          WFF5=Plot[epsilon2[[5]]+
                .2 AiryAi[ff x-epsilon3[[5]]]/Sqrt[norm[[5]]],
            {x,0,130}, DisplayFunction->Identity];
          WFF7=Plot[epsilon2[[7]]+
                .2 AiryAi[ff x-epsilon3[[7]]]/Sqrt[norm[[7]]],
            {x,0,130}, DisplayFunction->Identity];
          WFF9=Plot[epsilon2[[9]]+
                .2 AiryAi[ff x-epsilon3[[9]]]/Sqrt[norm[[9]]],
            {x,0,130}, DisplayFunction->Identity];
```

The following commands will create a plot of the even-n wavefunctions within the potential well. The energy of each wavefunction will be indicated by a dashed line. Note that the scale of the wavefunction here is rescaled - since we are plotting the wavefunction on the same scale as the potential. All wavefunctions have been multiplied by a factor of 0.2 simply to fit into the potential plot.

```
In[17]:=  Show[WFF1,WFF3,WFF5,WFF7,WFF9,Pplot,
               Graphics[{Dashing[{0.03,0.07}],
                Line[{{0,epsilon2[[1]]},{130,epsilon2[[1]]}}]}],
               Graphics[{Dashing[{0.03,0.07}],
                Line[{{0,epsilon2[[3]]},{130,epsilon2[[3]]}}]}],
               Graphics[{Dashing[{0.03,0.07}],
                Line[{{0,epsilon2[[5]]},{130,epsilon2[[5]]}}]}],
               Graphics[{Dashing[{0.03,0.07}],
                Line[{{0,epsilon2[[7]]},{130,epsilon2[[7]]}}]}],
               Graphics[{Dashing[{0.03,0.07}],
                Line[{{0,epsilon2[[9]]},{130,epsilon2[[9]]}}]}],
               DisplayFunction->$DisplayFunction,
               AxesLabel->{"x (angstrom)","U(x) (eV)"},
               PlotRange->All,
               PlotLabel->"Even wavefunctions"]
```



Out[17]= -Graphics-

For exact solution:
Find out the normalized factor by evaluating

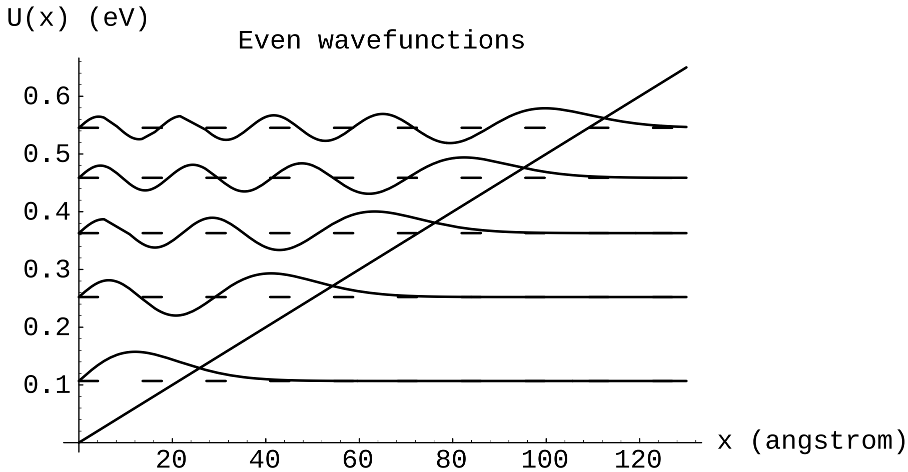
In[18]:=
```
norm1 = Table[NIntegrate[AiryAi[ff x-epsilon[[n]]]^2,
{x,0, Infinity}], {n,1,10}]
```

Out[18]= {4.49316, 5.89395, 6.84056, 7.58139, 8.20092, 8.73904, 9.21812, 9.65206, 10.0502, 10.4191}

Generating the exact energy level and its wavefunction
(multiply by 0.2 to fit the scale)

In[19]:=
```
WF1=Plot[epsilon1[[1]]+
.2 AiryAi[ff x-epsilon[[1]]]/Sqrt[norm1[[1]]],
   {x,0,130}, DisplayFunction->Identity];
WF3=Plot[epsilon1[[3]]+
.2 AiryAi[ff x-epsilon[[3]]]/Sqrt[norm1[[3]]],
   {x,0,130}, DisplayFunction->Identity];
WF5=Plot[epsilon1[[5]]+
.2 AiryAi[ff x-epsilon[[5]]]/Sqrt[norm1[[5]]],
   {x,0,130}, DisplayFunction->Identity];
WF7=Plot[epsilon1[[7]]+
.2 AiryAi[ff x-epsilon[[7]]]/Sqrt[norm1[[7]]],
   {x,0,130}, DisplayFunction->Identity];
WF9=Plot[epsilon1[[9]]+
.2 AiryAi[ff x-epsilon[[9]]]/Sqrt[norm1[[9]]],
   {x,0,130}, DisplayFunction->Identity];
```

In[20]:=
```
Show[WF1,WF3,WF5,WF7,WF9,Pplot,
     Graphics[{Dashing[{0.03,0.07}],
      Line[{{0,epsilon1[[1]]},{130,epsilon1[[1]]}}]}],
     Graphics[{Dashing[{0.03,0.07}],
      Line[{{0,epsilon1[[3]]},{130,epsilon1[[3]]}}]}],
     Graphics[{Dashing[{0.03,0.07}],
      Line[{{0,epsilon1[[5]]},{130,epsilon1[[5]]}}]}],
     Graphics[{Dashing[{0.03,0.07}],
      Line[{{0,epsilon1[[7]]},{130,epsilon1[[7]]}}]}],
     Graphics[{Dashing[{0.03,0.07}],
      Line[{{0,epsilon1[[9]]},{130,epsilon1[[9]]}}]}],
     DisplayFunction->$DisplayFunction,
     AxesLabel->{"x (angstrom)","U(x) (eV)"},
     PlotRange->All,
     PlotLabel->"Even wavefunctions"]
```



Out[20]= -Graphics-

(e)
the classical turning points for the electron

In[21]:=
```
cross=epsilon1/f
```

Out[21]= {21.3658, 37.356, 50.4473, 62.0174, 72.5941, 82.4496, 91.7478, 100.597, 109.072, 117.23}

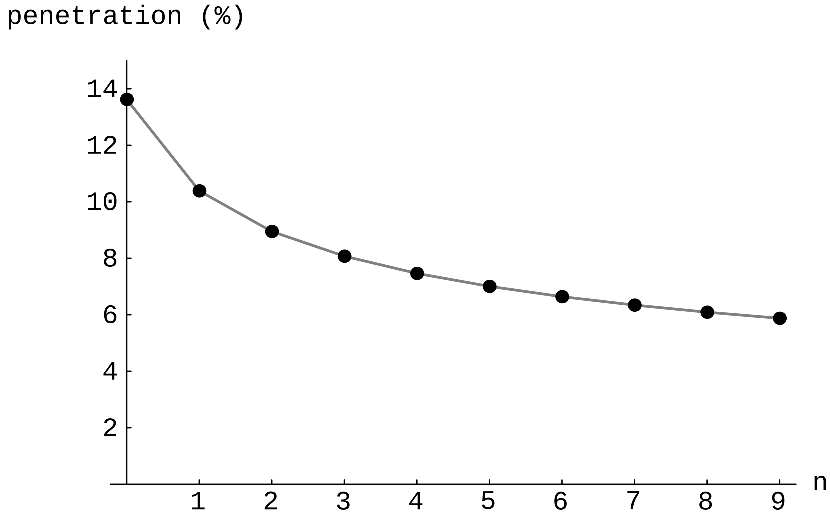
The probabilities for the electron to penetrate into the classically forbidden region

In[22]:=
```
penetr = Table[NIntegrate[AiryAi[ff x-epsilon[[n]]]^2
/norm1[[n]],{x,cross[[n]], Infinity}], {n,1,10}]
```

Out[22]= {0.136237, 0.103859, 0.0894863, 0.080742, 0.0746424,
0.0700462, 0.0664058, 0.0634203, 0.060908, 0.0587515}

which can be shown

```
In[23]:=  p1=Table[{n-1, 100 penetr[[n]]},{n,10}];
ppen=ListPlot[p1,
AxesLabel->{"n", "penetration (%)"},
PlotRange->{0,15},
Prolog->{{GrayLevel[.5],
Line[p1]},AbsolutePointSize[5]},
Ticks->{{1,2,3,4,5,6,7,8,9}, {0,2,4,6,8,10,12,14}}]
```



Out[23]= -Graphics-

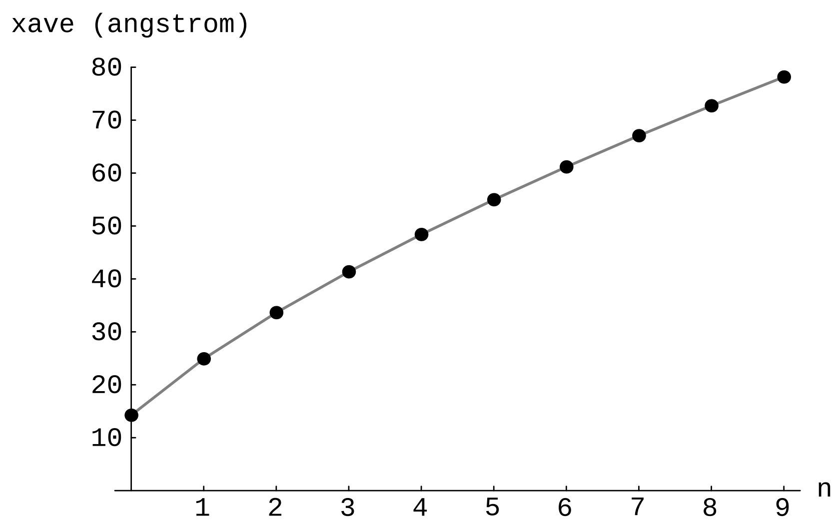
the mean values of x

```
In[24]:=  xave = Table[NIntegrate[x AiryAi[ff x-epsilon[[n]]]^2
/norm1[[n]],{x,0, Infinity}], {n,1,10}]
```

Out[24]= {14.2439, 24.904, 33.6315, 41.345, 48.396, 54.9664,
61.1652,
67.0645, 72.7148, 78.1535}

which is shown in the following figure

```
In[25]:=  p2=Table[{n-1,  xave[[n]]},{n,10}];
ListPlot[p2,
AxesLabel->{"n", "xave (angstrom)"},
PlotRange->{0,80},
Prolog->{{GrayLevel[.5],
Line[p2]},AbsolutePointSize[5]},
Ticks->{{1,2,3,4,5,6,7,8,9},
{0,10,20,30,40,50,60,70,80}}]
```



Out[25]= -Graphics-

Problem 3: Semiclassical Tunneling

(a) Using the formula

$$\mathbf{j} \; = \; \frac{i\hbar}{2m} \left[\psi(x)\nabla\psi^*(x) - \psi^*(x)\nabla\psi(x) \right] \tag{38}$$

for the current and the explicit form of $\psi(x)$ in the region I

$$\psi_I(x) \; = \; \frac{d}{\sqrt{k(x)}} \exp(i \int_x^a k(x^{'})dx^{'}) + \frac{d^*}{\sqrt{k(x)}} \exp(-i \int_x^a k(x^{'})dx^{'}) \tag{39}$$

one obtains $j_x = 0$, which means that the incident and reflected currents have equal values and opposite directions.

(b) We assumed that the wave function in region I is of the type

$$\psi_I(x) \; = \; \frac{c}{\sqrt{k(x)}} \sin\left(\int_x^a k(x')dx' + \gamma \right) \tag{40}$$

where c and γ are some constants and $k(x) = \sqrt{2m(E - U(x))/\hbar^2}$. A particle in the classically forbidden region II will have a wave function of the type

$$\psi_{II}^{gen}(x) \;=\; \frac{c_1}{\sqrt{|k(x)|}}\exp\left(\int_a^x |k(x')|dx'\right)+\frac{c_2}{\sqrt{|k(x)|}}\exp\left(-\int_a^x |k(x')|dx'\right). \tag{41}$$

Since we assumed that the probability for tunneling is very small we put $c_1 = 0$, otherwise the wave function will be exponentially large for points far from $x = a$ and a smoothly continued wave function in region III will not be small.

$$\psi_{II}(x) \;=\; \frac{c_2}{\sqrt{|k(x)|}}\exp\left(-\int_a^x |k(x')|dx'\right). \tag{42}$$

So we have now to find equations which relate c, γ and c_2. For this purpose we will approximate $U(x)$ near $x = a$ as

$$U(x) \approx U_a(x) \;=\; E + F_a(x-a),\; F_a > 0 \tag{43}$$

and solve *exactly* the corresponding Schrödinger equation:

$$\frac{d^2\psi_{I,II}(x)}{dx^2} - \frac{2m}{\hbar^2}\,F_a(x-a)\,\psi_{I,II}(x) \;=\; 0. \tag{44}$$

Introducing a new dimensionless variable z

$$z \;=\; \left(\frac{2mF_a}{\hbar^2}\right)^{(1/3)}(x-a) \tag{45}$$

we rewrite (44) as

$$\frac{d^2\psi_{I,II}(z)}{dz^2} - z\psi_{I,II}(z) \;=\; 0. \tag{46}$$

The combination

$$\lambda \;=\; \left(\frac{2mF_a}{\hbar^2}\right)^{(1/3)} \tag{47}$$

has dimension one over length and its reciprocal value plays a role of a characteristic length in this problem.

Equation (46) has generally two types of solutions called regular and irregular Airy functions. We consider here only the regular Airy function Ai (z) because the irregular Airy function Bi (z) diverges as $z \to \infty$. Ai (z) is usually written in the form

$$\mathrm{Ai}(z) \;=\; \frac{1}{\pi}\int_0^\infty \cos\,(\,\frac{u^3}{3} + uz\,)\,du. \tag{48}$$

The solution of (44) is given by

$$\psi_{I,II}(x) \;=\; \text{Const Ai}\,[\,\lambda\,(x-a)\,]\,. \tag{49}$$

We assume that (43) holds in a sufficiently broad interval $x \in [a-\epsilon, a+\epsilon]$ such that

$$\lambda\,\epsilon \;\gg\; 1. \tag{50}$$

We require (50) because the argument in (49) is essentially $\lambda\epsilon$ at the end points of the interval and we want to use the asymptotic forms of Ai (z) for $z \to \infty$

$$\mathrm{Ai}(z) \;\approx\; \frac{1}{2}\pi^{-1/2}z^{-1/4}e^{-\frac{2}{3}(z)^{3/2}} \tag{51}$$

and for $z \to -\infty$

$$\mathrm{Ai}(z) \;\approx\; \pi^{-1/2}(-z)^{-1/4}\sin(\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}) \tag{52}$$

We give here for later reference the asymptotic forms of $\mathrm{Bi}(z)$ for $z \to \infty$

$$\mathrm{Bi}(z) \;\approx\; \pi^{-1/2}z^{-1/4}e^{\frac{2}{3}(z)^{3/2}} \tag{53}$$

and for $z \to -\infty$

$$\mathrm{Bi}(z) \;\approx\; \pi^{-1/2}(-z)^{-1/4}\cos(\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}) \tag{54}$$

For the semiclassical approximate wave functions (40) and (42) one obtains in the framework of (43)

$$k(x) \;\approx\; \sqrt{\frac{2m}{\hbar^2}(\,E - E - F_a(x-a)\,)} \;=\; \sqrt{-\lambda^3\,(x-a)}. \tag{55}$$

One now uses (55) to take the definite integrals in (40) and (42) and obtain correspondingly

$$\psi_I(x) \;=\; c\,\lambda^{-1/2}\,[\,\lambda\,(a-x)\,]^{-1/4}\sin\left(\frac{2}{3}\;[\,\lambda\,(a-x)\,]^{3/2} + \gamma\right) \tag{56}$$

and

$$\psi_{II}(x) \;=\; c_2\,\lambda^{-1/2}\,[\,\lambda\,(a-x)\,]^{-1/4}\,\exp\left(-\frac{2}{3}\,[\,\lambda\,(x-a)\,]^{3/2}\right). \qquad (57)$$

At this point we have obtained the exact solution of (44) in some interval around $x=a$ and want to connect it with the semiclassical wave functions in the corresponding extended regions. So we consider the asymptotic behavior of the exact solution and impose the necessary conditions so that the continuation is smooth.

Equations (45), (49), (51) and (57) are consistent if

$$\frac{1}{2}\pi^{-1/2}\ \mathrm{Const} \;=\; c_2\,\lambda^{-1/2}. \qquad (58)$$

Similarly, equations (45), (49), (52) and (56) lead to

$$\pi^{-1/2}\ \mathrm{Const} \;=\; c\,\lambda^{-1/2} \qquad (59)$$

and

$$\gamma \;=\; \frac{\pi}{4}. \qquad (60)$$

From equations (58) and (59) one finally finds the relation between the normalization constants of the wave functions in the regions I and II.

$$c_2 \;=\; c/2 \qquad (61)$$

(c) The general semiclassical wave function of a particle of mass m and energy E moving in the classically allowed region III is given by

$$\psi_I(x) \;=\; \frac{d'}{\sqrt{k(x)}}\exp\left(i\int_x^a k(x^{'})\,dx^{'}\right)+\frac{f'}{\sqrt{k(x)}}\exp\left(-i\int_x^a k(x^{'})\,dx^{'}\right) \qquad (62)$$

where the first term corresponds to a particle moving in the positive direction and the second term — to a particle moving in the negative direction, $k(x)$ was defined earlier. Since we consider particles (incident and reflected) moving in the region I we have to assume that in the region III there are no particles moving in the negative direction, some particles could be moving in the positive direction due to tunneling from region I. Hence the normalization coefficient f' must be zero.

(d) The plots of Ai(z) and Bi(z) produced by `Mathematica` are given in Fig. 1 and Fig. 1 . We used the built-in functions `AiryAi[z]` and `AiryBi[z]`. Note the asymptotic behavior of these functions.

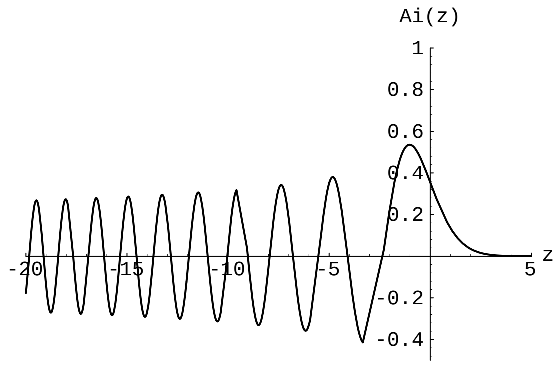


Figure 6: The regular Airy function Ai(z)

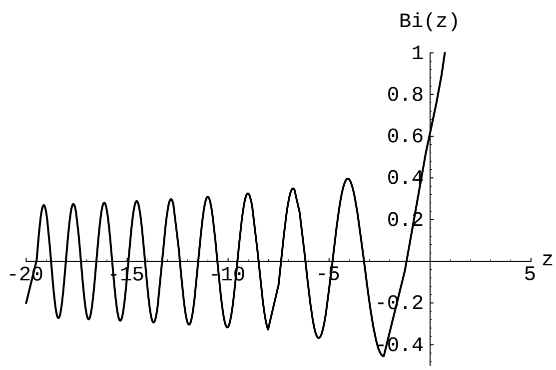


Figure 7: The irregular Airy function Bi(z)

(e) We approximate $U(x)$ near $x = b$ as

$$U(x) \approx U_b(x) = E + F_b(b - x), F_b > 0 \tag{63}$$

and write the corresponding Schrödinger equation for $U(x) = U_b(x)$

$$\frac{d^2\psi_{II,III}(x)}{dx^2} - \frac{2m}{\hbar^2}\, F_b(b - x)\, \psi_{I,II}(x) \;=\; 0. \tag{64}$$

A substitution similar to the one made before

$$z = \left(\frac{2mF_b}{\hbar^2}\right)^{(1/3)} (b - x) \tag{65}$$

allows us to rewrite (64) as

$$\frac{d^2\psi_{II,III}(z)}{dz^2} - z\psi_{II,III}(z) = 0. \tag{66}$$

We define as before the parameter

$$\lambda = \left(\frac{2mF_b}{\hbar^2}\right)^{(1/3)} \tag{67}$$

The regular and the irregular Airy functions — Ai(z) and Bi(z) are linearly independent and the general solution of (66) is a linear combination of these two functions. Thus, the general solution of (64) is

$$\psi_{II,III}(x) = c^{''}\mathrm{Ai}[\,\lambda\,(b - x)\,] + c^{'''}\mathrm{Bi}[\,\lambda\,(b - x)\,] \tag{68}$$

It is important to emphasize once again that this solution is valid for points close to $x = b$, where the approximation (63) is valid. We want to connect (68) to the function

$$\psi_{III}(x) = \frac{g}{\sqrt{k(x)}} \exp(i\int_b^x k(x')dx' + i\frac{\pi}{4}) \tag{69}$$

which is valid in region III. Following the procedure from part **(b)** we assume that (63) is valid in a sufficiently broad interval $x \in [b-\epsilon, b+\epsilon]$ such that

$$\lambda\,\epsilon \gg 1. \tag{70}$$

Using (55) and the Euler formula $e^{i\phi} = \cos(\phi) + i\sin(\phi)$ we rewrite (69)

$$\psi_{III}(x) = \frac{g\left[\cos\left(\frac{2}{3}\,[\,\lambda\,(x-b)\,]^{3/2} + \frac{\pi}{4}\right) + i\sin\left(\frac{2}{3}\,[\,\lambda\,(x-b)\,]^{3/2} + \frac{\pi}{4}\right)\right]}{\lambda^{1/2}\,[\,\lambda\,(x-b)\,]^{1/4}}. \tag{71}$$

A comparison between this equation and the asymptotic forms of Ai(z) and Bi(z) for $z \to -\infty$ confirms that (68) has, indeed, the form

$$\psi_{II,III}(x) \;=\; g\,\{\,\mathrm{Bi}\,[\,\lambda\,(b-x)\,] + i\,\mathrm{Ai}\,[\,\lambda\,(b-x)\,]\,\} \tag{72}$$

(f) Both terms in (72) have exponential behavior for x far enough from $x = b$, as $x \to a$. The first one is growing and second one is decaying. The rates of change are related to the parameter λ, which as we assumed above is large. So in region II we will neglect the exponentially small second term in (72)

$$\psi_{II,III}(x) \;=\; g\,\mathrm{Bi}\,[\,\lambda\,(b-x)\,],\ \text{in region } II, \tag{73}$$

The equation (73) is smoothly connected to a general solution for the wave function in region II

$$\psi_{II}(x) \;=\; \frac{g}{\sqrt{|k(x)|}}\exp\left(\int_x^b |k(x')|dx'\right). \tag{74}$$

It is now easy to verify that in order that equations (42) and (74) be consistent everywhere in the region II the following relation should hold

$$c_2\exp\left(-\int_a^x |k(x')|dx'\right) \;=\; g\exp\left(\int_x^b |k(x')|dx'\right),\ x \in [a,b]. \tag{75}$$

Taking into account (61) one finds from (75) the necessary condition

$$g \;=\; \frac{c}{2}\exp\left(-\int_a^b |k(x)|\,dx\right). \tag{76}$$

(g) In order to calculate the current of the incident particles at $x \to -\infty$ we use that $U(x \to \pm\infty) = 0$ and write (39) as

$$\psi_I(x \to -\infty) \;=\; \frac{c}{2i\sqrt{2mE/\hbar^2}}\left[\exp\left(i\int_x^a k(x^{'})dx^{'}\right) - \exp\left(-i\int_x^a k(x^{'})dx^{'}\right)\right] \tag{77}$$

The first term in this expression corresponds to incoming particles. We apply (38) to obtain

$$j_i(x \to -\infty) \;=\; \frac{|c|^2\hbar^2}{8}\sqrt{2mE} \tag{78}$$

Similarly from (69) and (38) one obtains

$$j_t(x \to +\infty) \;=\; \frac{|g|^2\hbar^2}{8}\sqrt{2mE}. \tag{79}$$

One uses the definition of the transition coefficient $T = j_t/j_i$ and (76) to obtain

$$T \;=\; \exp(-2\int_a^b |k(x)|dx). \tag{80}$$

(h) We consider now a potential

$$U(x) \quad = \quad \begin{cases} 0, & \text{for } x < -a \\ U_0 - \alpha x^2, & \text{for } -a < x < a, a = \sqrt{U_0/\alpha} \\ 0, & \text{for } a < x \end{cases} \tag{81}$$

and want to calculate the transition coefficient for particles om mass m and energy E, scattered by such a potential. We find first the turning points for which $U(x) = E$, $x = \pm x_0(E); x_0(E) = \sqrt{(U_0 - E)/\alpha}$. We then have to calculate the integral

$$I(E) \;=\; \frac{1}{\hbar}\int_{-x_0}^{x_0} \sqrt{2m(E - U_0 + \alpha x^2)}\,dx. \tag{82}$$

Substituting $z = \sqrt{\alpha/(U_0 - E)}\,x$ one brings $I(E)$ to the form

$$I(E) \;=\; \sqrt{\frac{2m(U_0 - E)^2}{\alpha\hbar^2}}\int_{-1}^{1}\sqrt{1 - z^2)}\,dz. \tag{83}$$

Using that $\alpha = 2m{U_0}^2/\hbar^2$ one finds $I(E) = (1 - E/U_0)\pi/2$. Thus the sought transition coefficient is

$$T(E) \;=\; \exp\left[-\pi\left(1 - \frac{E}{U_0}\right)\right]. \tag{84}$$

A plot of this function is given in Fig. 1.

It should be pointed out that (84) is valid for values of the energy E for which $\left|\frac{dU(x)}{dx}\right|$ at $x = \pm x_0(E)$ is sufficiently large. This condition can be traced back to equations (50) and (70) where we needed λ be sufficiently large. Hence, for energies close to the pick of the potential (81) the formula (84) is not valid. Indeed, an exact calculation shows that $T(E)$ exhibits oscillatory behavior for E close to U_{max}.

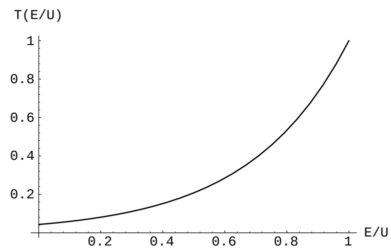
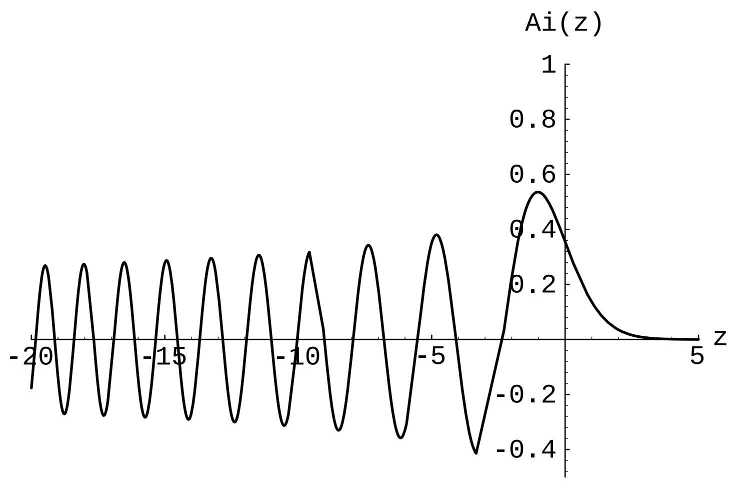


Figure 8: The transition coefficient for the potential as a function of E/U_0. Semi-classical approximation.

2 `Mathematica` notebook

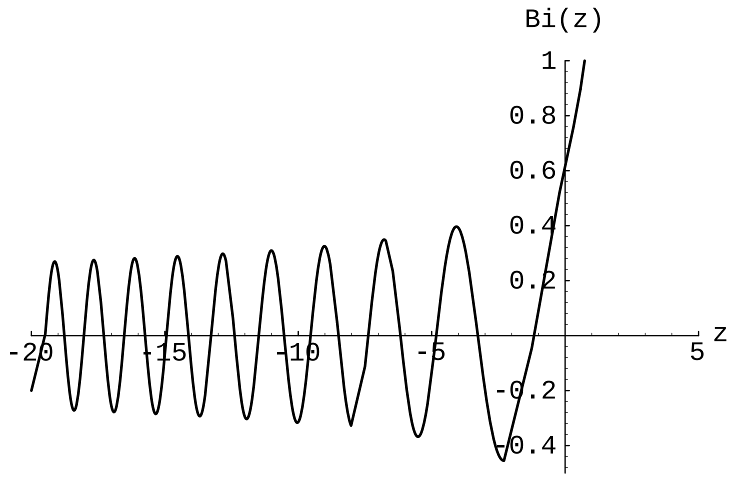
(i) Regular Airy Function:
With this command we plot the regular Airy function A[z].

```
In[26]:=   Plot[ AiryAi[x],{x,-20,5}, AxesLabel->{"z", "Ai(z)"},
           PlotRange->{ {-20,5},{-.5,1} }];
```



(ii) Irregular Airy Function:
Here we plot the irregular Airy function B[z]

```
In[27]:=   Plot[ AiryBi[x],{x,-20,5}, AxesLabel->{"z", "Bi(z)"},
           PlotRange->{ {-20,5},{-.5,1} }];
```



(iii) The Transition Coefficient :

A plot of the analytically calculated transition coefficient. T[E/U].

```
In[28]:=   U=1;
           Plot[ Exp [ -Pi ( 1 - E / U ) ], {E, 0, 1},
           AxesLabel->{"E/U", "T(E/U)"}];
```