Physics 220
Homework #2
Spring 2017
Due Wednesday, 4/12/17

1. Griffith's 1.8
We start with by adding V_0 to the potential V to get $V+V_0$. The Schrödinger equation reads: $i\hbar\frac{d\Psi}{dt}=-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+V\Psi+V_0\Psi$. Let $\Psi(x,t)=\psi(x)P(t)=\psi P$ and inserting this into the SWE we get: $i\hbar\psi\frac{dP}{dt}=-\frac{\hbar^2 P}{2m}\frac{d^2\psi}{dx^2}+VP\psi+V_0P\psi$. Now divide by ψP and notice that both sides equal a constant. We call this constant the energy, E. Thus we have $i\hbar\frac{1}{P}\frac{dP}{dt}-V_0=-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2}+V=E$. From the left hand side we get,
$i\hbar\frac{1}{P}\frac{dP}{dt}-V_0=E\rightarrow\frac{dP}{P}=-i\left(\frac{E+V_0}{\hbar}\right)dt\rightarrow\ln P=-i\left(\frac{E+V_0}{\hbar}\right)t\rightarrow P(t)=e^{-i\left(\frac{E+V_0}{\hbar}\right)t}$.
The right hand side gives the solutions to the time independent Schrödinger wave equation. And we have that the wave function
$\Psi(x,t)=\psi(x)P(t)=\psi e^{-i\left(\frac{E+V_0}{\hbar}\right)t}=\left[\psi e^{-i\frac{E}{\hbar}t}\right]e^{-i\frac{V_0}{\hbar}t}$, which picks up a phase factor $e^{-i\frac{V_0}{\hbar}t}$.
Since this is in the time component, the expectation values are unaffected by the phase factor.

2. Griffith's 1.18
Quantum mechanics is important when the deBroglie wavelength of the particle λ is greater than the characteristic size of the system d. Thus $\lambda>d$, where $\lambda=\frac{h}{\sqrt{3mk_BT}}$. Or, $d<\lambda=\frac{h}{\sqrt{3mk_BT}}$. We can relate this to the temperature of the system, $d^2<\frac{h^2}{3mk_BT}\rightarrow T<\frac{h^2}{3mk_Bd^2}$. Thus when the temperature of the system is less than $\frac{h^2}{3mk_Bd^2}$, quantum mechanics is relevant.

   a. For electrons:
   $$T<\frac{h^2}{3mk_Bd^2}=\frac{\left(6.63\times10^{-34}\,Js\right)^2}{3\left(9.11\times10^{-31}\,kg\right)\times1.38\times10^{-23}\,\frac{J}{K}\times\left(0.3\times10^{-9}\,m\right)^2}=1.3\times10^5\,K$$
   and thus free electrons in a solid are always quantum mechanical.

b. For sodium nuclei:

$$T < \frac{h^2}{3m_{Na}k_B d^2} = \frac{\left(6.63\times10^{-34}\,Js\right)^2}{3\left(23\times1.67\times10^{-27}\,kg\right)\times1.38\times10^{-23}\,\tfrac{J}{K}\times\left(0.3\times10^{-9}\,m\right)^2} = 3.1K$$

and thus nuclei are most always not quantum mechanical.

c. For gasses we use the ideal gas law, where for one molecule ($N = 1$) we assume that the molecule takes up a volume of approximately d^3. Thus

$PV = Nk_BT \to P\left(d^3\right) = k_BT \to d = \left(\frac{k_BT}{P}\right)^{\frac{1}{3}}$ and

$T < \frac{h^2}{3m_{Na}k_Bd^2} = \frac{h^2}{3m_{Na}k_B}\left(\frac{P}{k_BT}\right)^{\frac{2}{3}} \to T^{\frac{5}{3}} < \frac{h^2}{3m_{Na}\left(k_B\right)^{\frac{5}{3}}}P^{\frac{2}{3}}$. Thus we have

$$T < \frac{1}{k_B}\left(\frac{h^2}{3m_{Na}}\right)^{\frac{3}{5}}P^{\frac{2}{5}}$$

For helium at atmospheric pressure:

$$T < \frac{1}{k_B}\left(\frac{h^2}{3m}\right)^{\frac{3}{5}}P^{\frac{2}{5}} = \left(\frac{1}{1.38\times10^{-23}\,\frac{J}{K}}\right)\left(\frac{\left(6.63\times10^{-34}\,Js\right)^2}{3\left(4\times1.67\times10^{-27}\,kg\right)}\right)^{\frac{3}{5}}\left(1.01\times10^5\,\tfrac{N}{m^2}\right)^{\frac{2}{5}} = 2.93K$$

and helium nuclei at atmospheric pressure is quantum mechanical.

d. For hydrogen in outer space:

$$T < \frac{h^2}{3m_{Na}k_Bd^2} = \frac{\left(6.63\times10^{-34}\,Js\right)^2}{3\left(1.67\times10^{-27}\,kg\right)\times1.38\times10^{-23}\,\tfrac{J}{K}\times\left(0.01m\right)^2} = 6.4\times10^{-14}\,K$$

and hydrogen in outer space is not quantum mechanical.

3. Griffith's 2.3

There are two ways to answer this problem.

Method I: The SWE reads: $\frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi$.

The two cases we have are:

Case 1:

$$E = 0 \to \frac{d^2\psi}{dx^2} = 0 \to \psi = A + Bx$$

$$BC's: \psi(0) = 0 = A + B(0) \to A = 0$$

$$\psi(a) = 0 = B(a) \to B = 0$$

$$\therefore \psi = 0$$

Case 2:

$$E<0 \rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = k^2\psi \rightarrow \psi = Ae^{kx} + Be^{-kx}$$

$$BC's: \psi(0) = 0 = A + B \rightarrow A = -B \rightarrow \psi = B\left(e^{kx} - e^{-kx}\right)$$

$$\psi(a) = 0 = B\left(e^{ka} - e^{-ka}\right) \rightarrow \begin{cases} B = 0 \\ e^{-ka} = e^{ka} \rightarrow 1 = e^{2ka} \rightarrow \ln(1) = 0 = 2ka \rightarrow k = 0 \end{cases}$$

$$\therefore \psi = 0$$

Method II: The lowest energy in the infinite square well is $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$. Why cannot the energy be zero or negative? For the case of $E = \frac{p^2}{2m} < 0$ implies that the momentum is imaginary and a measurement would not yield a real value. For the case of $E = 0$, the uncertainty principle, the uncertainty in the position of the particle is $\Delta x \sim a$ and therefore $\Delta x \Delta p \geq \frac{\hbar}{2} \rightarrow \Delta p \geq \frac{\hbar}{2a}$. But $E = 0$ if then $E = 0 = \frac{p^2}{2m} \rightarrow \Delta p = 0$, which violates the uncertainty principle.

4. Griffith's 2.9

First we normalize the wave function over the given region,

$P = 1 = \int_0^a A^2 x^2 (a-x)^2\, dx$. On Mathematica we have that $A = \sqrt{\frac{30}{a^5}}$. The Mathematica code for the problem is below. To determine the expectation value of the Hamiltonian, we perform

$$\langle H \rangle = \int_0^a \psi^* H \psi\, dx = \int_0^a \psi^* \left(-\tfrac{\hbar^2}{2m}\right)\tfrac{d^2\psi}{dx^2}\, dx = \int_0^a \left[Ax(a-x)\right]^* \left[-\tfrac{\hbar^2}{2m}\tfrac{d^2}{dx^2}\left(Ax(a-x)\right)\right] dx = \frac{5\hbar^2}{ma^2},$$

where the integral was done on Mathematica. See the code below.

```
(* Normlization of the wave fucntion given in example 2.3. *)

psi = A*x*(a - x)
Solve[Integrate[psi*psi, {x, 0, a}] == 1, A]

Out[1]= A (a - x) x

Out[2]= {{A -> -Sqrt[30]/a^(5/2)}, {A -> Sqrt[30]/a^(5/2)}}


(* Expectation value of the Hamiltonina operator.  *)

In[8]:= Clear[A, a, x, psi]
A := Sqrt[30 / a^5]
psi := A*x*(a - x)
Hpsi = (-hbar^2 / (2*m))*D[D[psi, x], x]
Integrate[psi*Hpsi, {x, 0, a}]

Out[11]= Sqrt[30] Sqrt[1/a^5] hbar^2 / m

Out[12]= 5 hbar^2 / (a^2 m)
```

5. Consider a particle bound in a 1D potential with wave function given by

$$\psi(x) = \begin{cases} Ae^{5ikx}\cos\left(\frac{3\pi}{a}x\right) & -\frac{a}{2} \le x \le \frac{a}{2} \\ 0 & |x| > \frac{a}{2} \end{cases}$$

a. What is the normalization constant A?
To normalize the wave function we compute

$$P = 1 = \int_{-a/2}^{a/2} \psi^*\psi\, dx = \int_{-a/2}^{a/2} \left[Ae^{-5ikx}\cos(\tfrac{3\pi}{a}x) \times Ae^{5ikx}\cos(\tfrac{3\pi}{a}x)\right]dx = \int_{-a/2}^{a/2} A^2\cos^2(\tfrac{3\pi}{a}x)dx$$

and we find that the normalization constant is $A = \sqrt{\frac{2}{a}}$. The normalization was done on Mathematica. The code follows.

b. What is the probability of finding the particle between $0 \le x \le \frac{a}{4}$?
From the normalized wavefunction we can calculate the probability and

$$P = 1 = \int_{-a/2}^{a/2} \psi^*\psi\, dx = \int_{-a/2}^{a/2} \left[\sqrt{\frac{2}{a}}e^{-5ikx}\cos(\tfrac{3\pi}{a}x) \times \sqrt{\frac{2}{a}}e^{5ikx}\cos(\tfrac{3\pi}{a}x)\right]dx = \frac{1}{4} - \frac{1}{6\pi} = 0.197$$

The integral was done on Mathematica and the code follows.

c. What are the expectation values of $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$, & $\langle p^2\rangle$?

$$\langle x\rangle = \int_{-a/2}^{a/2} \psi^* x\psi\, dx = \int_{-a/2}^{a/2}\left[\sqrt{\frac{2}{a}}e^{-5ikx}\cos(\tfrac{3\pi}{a}x)x\sqrt{\frac{2}{a}}e^{5ikx}\cos(\tfrac{3\pi}{a}x)\right]dx = 0$$

$$\langle x^2\rangle = \int_{-a/2}^{a/2} \psi^* x^2\psi\, dx = \int_{-a/2}^{a/2}\left[\sqrt{\frac{2}{a}}e^{-5ikx}\cos(\tfrac{3\pi}{a}x)x^2\sqrt{\frac{2}{a}}e^{5ikx}\cos(\tfrac{3\pi}{a}x)\right]dx = \left(\frac{3\pi^2-2}{36\pi^2}\right)a^2$$

$$\langle p\rangle = \int_{-a/2}^{a/2} \psi^*\left(-i\hbar\frac{d}{dx}\right)\psi\, dx = -i\hbar\int_{-a/2}^{a/2}\left[\sqrt{\frac{2}{a}}e^{-5ikx}\cos(\tfrac{3\pi}{a}x)\frac{d}{dx}\left(\sqrt{\frac{2}{a}}e^{5ikx}\cos(\tfrac{3\pi}{a}x)\right)\right]dx = 5\hbar k$$

$$\langle p^2\rangle = \int_{-a/2}^{a/2} \psi^*\left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right)\psi\, dx = -\hbar^2\int_{-a/2}^{a/2}\left[\sqrt{\frac{2}{a}}e^{-5ikx}\cos(\tfrac{3\pi}{a}x)\frac{d^2}{dx^2}\left(\sqrt{\frac{2}{a}}e^{5ikx}\cos(\tfrac{3\pi}{a}x)\right)\right]dx = \hbar^2k^2\left(\frac{9\pi^2}{k^2a^2}+25\right)$$

```
Clear[k, a, x, psi, A]

(*  Normalization:  To determine the normalization,
we integrate the square of the wave function over the given interval and set
 the result equal to one.  *)

Solve[Integrate[(A*Cos[3*Pi*x/a])^2, {x, -a/2, a/2}] == 1, A]
```

Out[16]= $\left\{\left\{A \to -\frac{\sqrt{2}}{\sqrt{a}}\right\}, \left\{A \to \frac{\sqrt{2}}{\sqrt{a}}\right\}\right\}$

In[51]:=

```
(* Using the normalizaiton constant,
we can calculate the probability of finding the particle in the given region.  *)

Clear[a, k, x, A, psi, psistar, xexp, xsquaredexp, pexp, psquaredexp]
A := Sqrt[2/a]
psi := A*Exp[5*I*k*x] Cos[3*Pi*x/a]
psistar := A*Exp[-5*I*k*x] Cos[3*Pi*x/a]
Integrate[psistar*psi, {x, 0, a/4}]
```

Out[55]= $\frac{1}{4} - \frac{1}{6\pi}$

In[56]:=

```
(*  Expectation values  *)

(* Expectation value of the position and position squared *)
xexp = Integrate[psistar*x*psi, {x, -a/2, a/2}]
xsquaredexp = Integrate[psistar*x^2*psi, {x, -a/2, a/2}]
```

Out[56]= 0

Out[57]= $\frac{a^2\left(-2+3\pi^2\right)}{36\pi^2}$

In[58]:=

```
(* Expectation value of the momentum and square of the momentum *)
pexp = -I*hbar*Integrate[psistar*D[psi, x], {x, -a/2, a/2}]
psquaredexp = -(hbar^2)*Integrate[psistar*D[D[psi, x], x], {x, -a/2, a/2}]
```

Out[58]= 5 hbar k

Out[59]= $-\text{hbar}^2\left(-25\,k^2 - \frac{9\pi^2}{a^2}\right)$

6. Determine the odd solutions to the finite square well. Determine the energy of the single bound state with $E < V_0$. Normalize your solutions in each region to determine the unknown coefficient A in each region. Plot your solution for $\psi_2(x)$.

   The mathematica code and plots are given in the attached file.

7. Determine the normalization coefficients for the second energy state of the even solutions to the finite square well. That is, renormalize the solutions and determine B in each region for E_3. Plot your solution for $\psi_3(x)$, along with the solutions for $\psi_2(x)$ from above and $\psi_1(x)$ from class.

   The mathematica code and plots are given in the attached file.

In[183]:=
```
(*  This Mathematica notebook is specifically for problem
 #6 on homework set #2. It can also be used for problem #7 on
 homework set #2 as well.  You'll have to modify it for use with
 problem #7 if you choose to use this notebook for that problem. *)

ClearAll["Global`*"]
```

In[184]:=
```
(* Problem #6  *)

(*  This section defines has you define your wavefunctions
 and then normalize them over all space.  You will need to
 use the solve command to determine an expression for A,
the normalization coefficient.  *)psistarpsiL := Integrate[
  (A * Sin[k * a / 2] * Exp[kprime * a / 2] * Exp[kprime * x]) ^2, {x, -Infinity, -a / 2}]
psistarpsiM := Integrate[(A * Sin[k * x]) ^2, {x, -a / 2, a / 2}]
psistarpsiR := Integrate[
  (-A * Sin[k * a / 2] * Exp[kprime * a / 2] * Exp[-kprime * x]) ^2, {x, a / 2, Infinity}]

psistarpsiL + psistarpsiM + psistarpsiR
```

Out[187]= $\text{ConditionalExpression}\left[\frac{A^2 \,\text{Sin}\left[\frac{a\,k}{2}\right]^2}{\text{kprime}} + \frac{1}{2} A^2 \left(a - \frac{\text{Sin}[a\,k]}{k}\right), \text{Re}[\text{kprime}] > 0\right]$

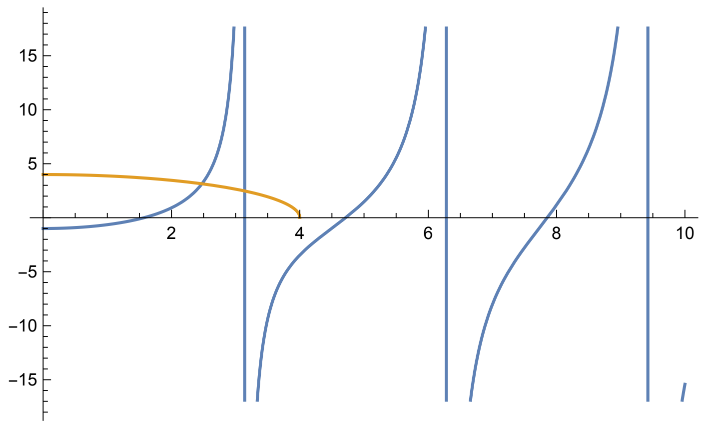
In[188]:= $\text{Solve}\left[\frac{A^2 \,\text{Sin}\left[\frac{a\,k}{2}\right]^2}{\text{kprime}} + \frac{1}{2} A^2 \left(a - \frac{\text{Sin}[a\,k]}{k}\right) == 1, A\right]$

Out[188]= $\left\{\left\{A \to -\left(\left(\sqrt{2}\right) \Big/ \left(\sqrt{\left(a + \frac{2\,\text{Sin}\left[\frac{a\,k}{2}\right]^2}{\text{kprime}} - \frac{\text{Sin}[a\,k]}{k}\right)}\right)\right)\right\},\right.$

$\left.\left\{A \to \left(\sqrt{2}\right) \Big/ \left(\sqrt{\left(a + \frac{2\,\text{Sin}\left[\frac{a\,k}{2}\right]^2}{\text{kprime}} - \frac{\text{Sin}[a\,k]}{k}\right)}\right)\right\}\right\}$

In[189]:=
```
(*  To determine the numerical solution to the odd
 bound state we make a plot and use the FindRoot command.   *)

Clear[a, r, x]
Plot[{-a * Cot[a], Sqrt[16 - a^2]}, {a, 0, 10}]
FindRoot[-a * Cot[a] == Sqrt[16 - a^2], {a, 2.5}]
```

Out[190]=



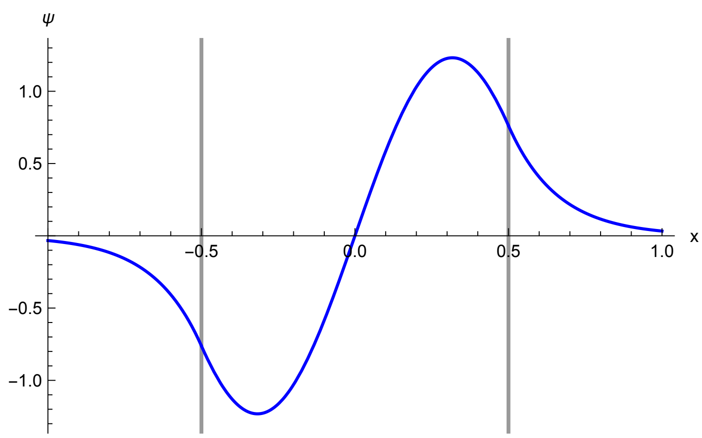
Out[191]= {a → 2.47458}

```
(*  Define and plot the Odd solutions for a finite well with r = 4.   *)

Clear[A, alpha, r, beta, well, psiLeftO1, psimiddleO1,
 psirightO1, plotleftO1, plotmiddleO1, plotrightO1]

(*  Define the normalization coefficient.  You need to enter your
 expression for the normalization coefficient and enter it below.   *)
A := Sqrt[2 / well] * ((Sin[alpha]^2 / beta) + 1 - (Sin[2 * alpha] / (2 * alpha)))^(-1 / 2)

(*  Define alpha, beta,
r and the width of the well.  Here the well has limits of -a/2 to a/2.

  Note: the colon after the name of the function tells Mathematica
    to evaluate the expression but do not display the result.  The
    normalization coefficient will be evaluated though. You need
    to determine alpha for the odd solution and enter it below *)


(* Now we use the value of a the calculation above and define it as alpha.*)
alpha := 2.4746
r := 4
beta := Sqrt[r^2 - alpha^2]
well := 1
A

(*  This defines the wavefunction in each of the three
 regions.  psileft is the wavefunctin to the left of the well,
psimiddle is the wavefunction in the well,
and psiright is the wavefunction to the right of the well.  You need
 to input your expressions for the wavefunctions in each region.*)

psileftO1 := -A * Exp[beta] * Sin[alpha] * Exp[2 * beta * x / well]
```

```
psimiddle01 := A * Sin[2 * alpha * x / well]
psiright01 := A * Exp[beta] * Sin[alpha] * Exp[-2 * beta * x / well]


(*  These set of commands defines the plot function for each of the three plots,
to the left of the well, in the well, and to the right of the well
 as well as the limits over which you want to plot each function.  *)

plotleft01 := Plot[psileft01, {x, -well, -well / 2}, PlotStyle → Blue]
plotmiddle01 := Plot[psimiddle01, {x, -well / 2, well / 2}, PlotStyle → Blue]
plotright01 := Plot[psiright01, {x, well / 2, well}, PlotStyle → Blue]


(*  The Show command lets you show each of the functions
 you want plotted on the same graph.  The plot range, automatic,
tells mathematica to use the plot ranges given in the definitions of the
  plots.  Gridlines denoting the well boundaries are shown at -a/2 and +a/2.  *)
Show[ plotleft01, plotmiddle01, plotright01, PlotRange → Automatic,
 GridLines → {{{-well / 2, {Black, Thick}}, {well / 2, {Black, Thick}}}, None},
 AxesLabel → {"x", "ψ"}]
```

Out[234]= 1.23176

Out[241]=



In[247]:=

```
(* Problem #7 *)

(*  This gives the normalization condition for the even
 solutions.  This is the same code that I used in class *)
Clear[B, k, a, r, alpha]
psistarpsiL := Integrate[
   (B * Cos[k * a / 2] * Exp[kprime * a / 2] * Exp[kprime * x]) ^2, {x, -Infinity, -a / 2}]
psistarpsiM := Integrate[(B * Cos[k * x]) ^2, {x, -a / 2, a / 2}]
psistarpsiR := Integrate[
   (B * Cos[k * a / 2] * Exp[kprime * a / 2] * Exp[-kprime * x]) ^2, {x, a / 2, Infinity}]

psistarpsiL + psistarpsiM + psistarpsiR
```

Out[251]= $\text{ConditionalExpression}\left[\frac{B^2 \text{Cos}\left[\frac{a k}{2}\right]^2}{\text{kprime}} + \frac{B^2 \left(a k + \text{Sin}[a k]\right)}{2 k}, \text{Re}[\text{kprime}] > 0\right]$

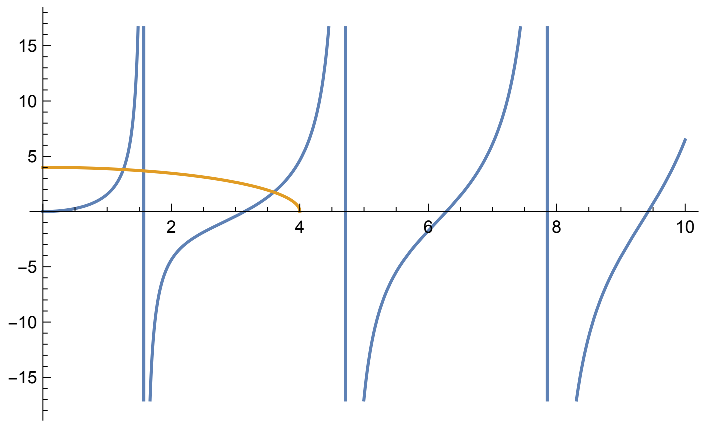
In[252]:= $\text{Solve}\left[\frac{B^2 \text{Cos}\left[\frac{a k}{2}\right]^2}{\text{kprime}} + \frac{B^2 \left(a k + \text{Sin}[a k]\right)}{2 k} == 1, B\right]$

Out[252]= $\left\{\left\{B \to -\left(\left(\sqrt{2}\right) \middle/ \left(\sqrt{\left(a + \frac{2 \text{Cos}\left[\frac{a k}{2}\right]^2}{\text{kprime}} + \frac{\text{Sin}[a k]}{k}\right)}\right)\right)\right\}, \left\{B \to \left(\sqrt{2}\right) \middle/ \left(\sqrt{\left(a + \frac{2 \text{Cos}\left[\frac{a k}{2}\right]^2}{\text{kprime}} + \frac{\text{Sin}[a k]}{k}\right)}\right)\right\}\right\}$

```
(* Now the second even soltution to the finite well.  *)
```

In[253]:=
```
(*  To determine the numerical solution to the second eveb
 bound state we make a plot and use the FindRoot command.   *)

Clear[a, r, x]
Plot[{a * Tan[a], Sqrt[16 - a^2]}, {a, 0, 10}]
FindRoot[a * Tan[a] == Sqrt[16 - a^2], {a, 3.6}]
```

Out[254]=



Out[255]= {a → 3.5953}

In[256]:=
```
(*  Define and plot the second even solution for a finite well with r = 4.  *)

Clear[B, alpha, r, beta, well, psileftE2, psimiddleE2,
 psirightE2, plotleftE2, plotmiddleE2, plotrightE2]

(*  Define the normalization coefficient that was calculated above  *)
B := Sqrt[2 / well] * ((Cos[alpha] ^ 2 / beta) + 1 - (Sin[2 * alpha] / (2 * alpha))) ^ (-1 / 2)

(*  Define alpha, beta,
r and the width of the well.  Here the well has limits of -a/2 to a/2. *)

(* Now we use the value of a the calculation above and define it as alpha.*)
alpha := 3.5953
r := 4
beta := Sqrt[r ^ 2 - alpha ^ 2]
well := 1
B

(*  This defines the wavefunction in each of the three
 regions.  psileft is the wavefunctin to the left of the well,
psimiddle is the wavefunction in the well,
and psiright is the wavefunction to the right of the well.  You need
 to input your expressions for the wavefunctions in each region.*)

psileftE2 := B * Exp[beta] * Cos[alpha] * Exp[2 * beta * x / well]
psimiddleE2 := B * Cos[2 * alpha * x / well]
psirightE2 := B * Exp[beta] * Cos[alpha] * Exp[- 2 * beta * x / well]


(*  These set of commands defines the plot function for each of the three plots,
to the left of the well, in the well, and to the right of the well
 as well as the limits over which you want to plot each function.  *)

plotleftE2 := Plot[psileftE2, {x, -well, -well / 2}, PlotStyle → Green]
plotmiddleE2 := Plot[psimiddleE2, {x, -well / 2, well / 2}, PlotStyle → Green]
plotrightE2 := Plot[psirightE2, {x, well / 2, well}, PlotStyle → Green]
```

Out[262]=
```
1.21661
```

In[272]:=
```
(*  The Show command lets you show each of the functions
 you want plotted on the same graph.  The plot range, automatic,
tells mathematica to use the plot ranges given in the definitions of the
  plots.  Gridlines denoting the well boundaries are shown at -a/2 and +a/2.  *)
Show[ plotleftO1, plotmiddleO1, plotrightO1, plotleftE2,
 plotmiddleE2, plotrightE2, PlotRange → All,
 GridLines → {{{-well / 2, {Black, Thick}}, {well / 2, {Black, Thick}}}, None},
 AxesLabel → {"x", "ψ"}]
```

Out[272]=