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(*Particle-in-box-M4*)
(*Jared Frazier*)
(*Description:

Plot the probability density functions for the time-independent wave function
in one and two dimensions. Derive the expectation of position and momentum.
Determine the normalization constants.

*)
(*Due: 10-12-2020*)

Clear["Global`*"];

(*------------------------------*)
   (*1-1 => Plotting 1D PDFs*)
(*------------------------------*)

Print["-----------------------------------------------
------------------Question 1------------------
---------------------------------------------------"
]

(*P(x) = ψn(x) for n[1,3]*)
waveN1 := 2*(Sin[Pi*x])^2;
waveN2 := 2*(Sin[2*Pi*x])^2;
waveN3 := 2*(Sin[3*Pi*x])^2;

(*Plot these wave functions from a = 0, a = L where L = 1*)
Print["Probability Density Functions For |ψn(x)|^2 In 1D"]
Show[
    Plot[
        waveN1,
        {x, 0, 1},
        PlotLabel→"|ψn(x)|^2 for n = 1,2,3" ,
        AxesLabel→{"Length x", "|ψn(x)|^2"},
        PlotStyle→{Red, Dashed},
        Filling->Axis,
        PlotLegends→{"ψ1(x) = 2sin^2πx"}
    ],
    Plot[
        waveN2,
        {x, 0, 1},
        PlotStyle→{Green,Thick},
        Filling->Axis,
        PlotLegends→{"ψ2(x) = 2sin^22πx"}
    ],
    Plot[
        waveN3,
        {x,0,1},
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        PlotRange→Full,
        Filling→Axis,
        PlotLegends→{"ψ3(x) = 2sin²3πx"}
    ]
]

(*------------------------------*)
   (*1-2 => Plotting 2D PDFs*)
(*------------------------------*)
Print["Density Functions for ψn(x)ψn(y)"]
(*2D wave functions for n=1,2,3,*)
waveN1X := Sqrt[2]*Sin[Pi*x];
waveN2X := Sqrt[2]*Sin[2*Pi*x];
waveN3X := Sqrt[2]*Sin[3*Pi*x];
waveN1Y := Sqrt[2]*Sin[Pi*y];
waveN2Y := Sqrt[2]*Sin[2*Pi*y];
waveN3Y := Sqrt[2]*Sin[2*Pi*y];
(*2D system*)
DensityPlot[
    waveN1X*waveN1Y,
    {x,0,1},
    {y,0,1},
    PlotLabel→"ψ1(x)ψ1(y) Density Plot"
]
DensityPlot[
    waveN2X*waveN2Y,
    {x,0,1},
    {y,0,1},
    PlotLabel→"ψ2(x)ψ2(y) Density Plot"
]
DensityPlot[
    waveN3X*waveN3Y,
    {x,0,1},
    {y,0,1},
    PlotLabel→"ψ3(x)ψ3(y)Density Plot"
]
(*------------------------------*)
  (*2 => Expectation Derivation*)
(*------------------------------*)
Print["---------------------------------------------
------------------Question 2------------------
---------------------------------------------"
]
(*Derive <x>*)
Print["Derive <x>"]
Print["(1) Steps 2-3 are the human intuition steps needed before Mathematica:"]
Print["(2) sin²(nπx/L) = (1 - cos(nπx/L))/2 in the integrand of <x> = 2/L∫xsin²(nπx/L)dx
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from the double angle identity"]
Print["(3) Then the sum of two integrals can be used to solve for <x>
such that <x> = 1/L [∫xdx + ∫cos(nπx/L) dx]"]
Print["(4) Given steps 2-3, I will use Mathematica to evaluate the integrals
∫xdx and ∫cos(nπx/L) dx] separately if 'n' is any positive integer on the interval
x = 0 to x = L"]
firstIntegral = Integrate[x, {x,0,L}]; (*Compute both integrals from 0 to L*)
secondIntegral = Assuming[
                    Element[n, PositiveIntegers],
                    Integrate[Cos[n*Pi*x/L], {x, 0, L}]
                  ];
Print["(5) From mathematica, '1/L * ", firstIntegral, " + ", secondIntegral,
"' is <x>."]
Print["(6) <x> = L/2"]
Print[]

(*Derive <px>*)
Print["Derive <p_x>"]
Print["(1) Since p̂_x = -iħ d/dx, then <p_x> = -iħ∫√(2/L) sin(nπx/L) d/dx √(2/L) sin(nπx/L) dx
simplifies to <p_x> = -iħ 2nπ/L^2 ∫sin(nπx/L) cos(nπx/L) dx"]
expectationOfMomentum = Assuming [ (*Compute expectation of momentum*)
                          Element[n, PositiveIntegers],
                          Integrate[Sin[n*Pi*x/L]*Cos[n*Pi*x/L], {x, 0, L}]
                        ];
Print["(2) Using mathematica to evaluate the second integral from
step 1 on
x = 0 to x = L where n is an element of the set of positive integers, then
<p_x> = -iħ 2nπ/L^2 ∫sin(nπx/L) cos(nπx/L) = -iħ 2nπ/L^2 *", expectationOfMomentum,
"\n(3) Therefore, <p_x> = 0"]
Print[]

(*Derive <x^2> for σ^2_x*)
Print["Derive <x^2> For σ^2_x "]
Print["(1) σ_x = √(σ^2_x) = √(<x^2> - <x>^2) . Therefore, I must derive <x^2> first
before calculating σ_x."]
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Print["(2) <x^2> = (2/L)∫x^2 sin^2(nπx/L)dx, just like with <x> except now x^2
is in the integrand."]
Print["(3) sin^2(nπx/L) = (1 - cos(nπx/L))/2 so the integral in step 2 expands
to (1/L)[∫x^2 dx + ∫cos(nπx/L)dx]"]
Print["(4) From step 5 of the derivation of <x>, ∫cos(nπx/L)dx is zero
if n is an element of the set of positive integers."]
Print["(5) ∫x^2 dx = ", Integrate[x^2, {x,0,L}], " so 1/L * ", Integrate[x^2, {x,0,L}]]
Print["(6) <x^2> = L^2/3"]
Print["(7) σx = Sqrt[σx^2] = Sqrt[<x^2> - <x>^2] = ", Sqrt[L^2/3 - L^2/4]] (*σx*)

(*Derive <px^2> for σ^2px*)
Print[]
Print["Derive <px^2> For σ^2px"]
Print["(1) σpx = Sqrt[σpx^2] = Sqrt[<px^2> - <px>^2] and some human intuition is required
to set-up the proper integral, as in previous steps."]
Print["(2) This is the general expression
for  <px^2> = ∫Sqrt[2/L] sin(nπx/L)(-iħ d/dx(-iħ d/dx Sqrt[2/L] sin(nπx/L)))dx."]
Print["(3) Several constants in the expression can be pulled
out of the integrand: (2i^2ħ^2/L)∫sin(nπx/L) d^2/dx^2 sin(nπx/L)dx"]
Print["(4) I will evaluate d^2/dx^2 sin(nπx/L) in the integrand using Mathematica: ",
Assuming[Element[n, PositiveIntegers], D[Sin[(n*Pi*x)/L] ,{x, 2}]]]
Print["(5) Then step 3 simplifies to -(2i^2ħ^2n^2π^2/L^3)∫sin(nπx/L)sin(nπx/L)dx, the
integrand of which was already computed in step 5 of 'Derive <x>'
by using the double angle identity"]
Print["(6) Step 5, therefore, simplifies to -(2i^2ħ^2n^2π^2/L^3)[∫xdx - ∫cos(nπx/L)], so
evaluating the second integral from x=0 to x=L using Mathematica,
∫cos(nπx/L) = ", Assuming[Element[n, PositiveIntegers],
Integrate[Cos[(n*Pi*x)/L], {x, 0, L}]]]
Print["(7)Then all that's left is -(2i^2ħ^2n^2π^2/L^3)∫xdx for x=0 to x=L,
and ∫xdx is simply ", Integrate[x, {x,0,L}]]
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Print["(8) <px^2> = ", (2ℏ^2 n^2 π^2)/L^3 * Integrate[x, {x,0,L}]]
Print["(9) Then σ_px = Sqrt[σ_px^2] = Sqrt[<px^2> - <px>^2] = ", Sqrt[(2ℏ^2 n^2 Pi^2)/L^3 * Integrate[x, {x,0,L}]]]

(*------------------------------*)
(*3 => Acceptable wave function*)
(*------------------------------*)
Print["---------------------------------------------
-----------------Question 3-----------------
---------------------------------------------"
]
(*Find normalization constant*)
Print["Find Normalization Constant 'A'"]
Print["(1) f(x) is normal if ∫f(x)f(x)dx = 1. Therefore,
I can solve for A from ∫A^2[x(x-L)(x-L)]dx = 1 since 'A' is a constant."]
Print["(2) A^2" , Integrate[(x*(x-L))^2, {x, 0, L}], " = 1"]
Print["(3) f(x) is normalized if A = ", Sqrt[1/(Integrate[(x*(x-L))^2, {x, 0, L}])]]
Print["(4) A = Sqrt[30/L^5] "]


Print[]
(*Plot f(x) with exact ground state wave function assuming L = 1*)
Print["Plot the PDFs assuming L = 1"]
L = 1;
groundStateWaveFunc = Sqrt[2/L]*Sin[(Pi*x)/L];
fx = Sqrt[30/L^5]*x*(L-x);
Show[
    Plot[ (*Plot fx squared*)
        (fx)^2,
        {x, 0, L},
        PlotRange→All,
        PlotLabel→"PDFs of |f(x)|^2, |ψ1(x)|^2, and f(x)ψ1(x)",
        AxesLabel→{"Length x","|ϕ(x)|^2"},
        PlotLegends→{"(f(x))^2 = (Sqrt[30/L^5] x(L-x))^2"},
        PlotStyle→{Red, Dashed},
        ImageSize→Large
    ],
    Plot[ (*Plot the ground state wave function squared*)
        (groundStateWaveFunc)^2,
        {x, 0, L},
        PlotLegends→{"(ψ1(x))^2 = (Sqrt[2/L] sin(πx/L))^2"},
        PlotStyle→{Orange, Bold}
```

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    ],
    Plot[ (*Plot difference between fx and ground state then square it*)
        (groundStateWaveFunc-fx)^2,
        {x, 0, L},
        PlotLegends→{"ψ1(x)-f(x))^2 = (Sqrt[2/L] sin(πx/L)-(Sqrt[30/L^5] x(L-x))^2"},
        PlotStyle→{Green, Thick}
    ]
]

(*Probability calculations for each PDF*)
Print["Calculate Probability Of x = 0 To x = L/3 For Each PDF |ϕ(x)|^2"]
probGroundState = Integrate[groundStateWaveFunc^2, {x, 0, L/3}];
probFx = Integrate[fx^2, {x, 0, L/3}];
probProduct = Integrate[(groundStateWaveFunc-fx)^2, {x, 0, L/3}];
Print["(i) ∫_0^(L/3)",groundStateWaveFunc^2, " = ", probGroundState]
Print["(ii) ∫_0^(L/3)",fx^2, " = ", probFx]
Print["(iii) ∫_0^(L/3)", (groundStateWaveFunc-fx)^2, " = ", probProduct]
Print[]
(*------------------------------*)
 (*4 => Superposition*)
(*------------------------------*)
Print["----------------------------------------------
------------------Question 4------------------
-------------------------------------------------"
]
Print["Solve for normalization constant A of initial PDF"]
Print["(1)  ∫_0^L ψψ* = 1, then A^2 ∫_0^L (c1ψ1+c2ψ2)(c1ψ*1+(c2ψ*2)dx = 1."]
Print["(2) Expanding the integral in step 2, and using the fact that the
dot product of two orthonormal eigenstates is 0,
A^2[(1/4)^2 ∫_0^L ψ1ψ*1dx + 0 + 0 + (3/4)^2 ∫_0^L ψ2ψ*2dx] = 1"]
Print["(3) Since ∫_0^L ψxψ*xdx = 1, then A^2(1/16 + 9/16) = 1.
Therefore, A = Sqrt[16/10] = 4/Sqrt[10]"]
Print[]
(*Plot Initial PDFs*)
normConstA = 4/Sqrt[10];
Print["Plot initial PDF Of |ψ|^2 Where n=1, m=2, c1=0.25, c2=0.75, and A = 4/Sqrt[10]"]
```

```
Plot[
    (normConstA*(0.25*waveN1X+0.75*waveN2X))^2,
    {x, 0, L},
    PlotRange→All,
    PlotLabel→"|ψ(x,t=0)|²= (A(0.25√(2/L) sin(πx)+0.75√(2/L) sin(2πx))² vs Length x",
    AxesLabel→{"Length x","|ψ(x,t=0)|²"},
    ImageSize→Large
]
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---------------------------------------------
-----------------Question 1-----------------
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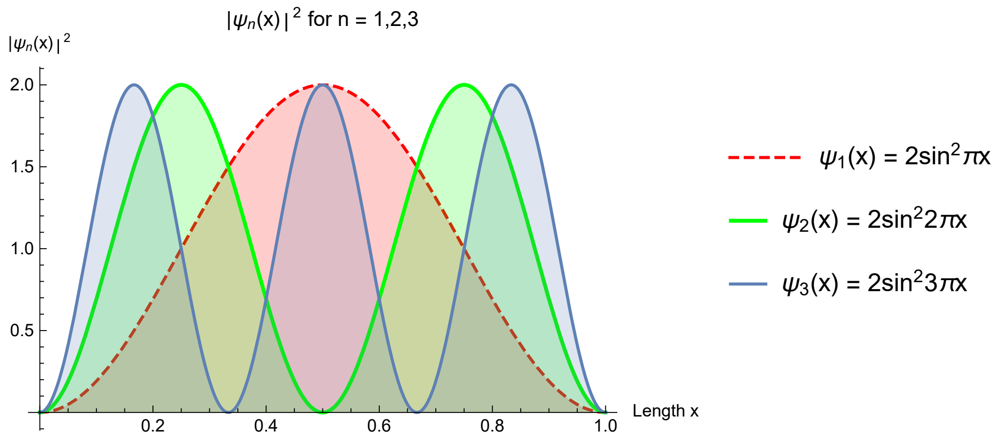
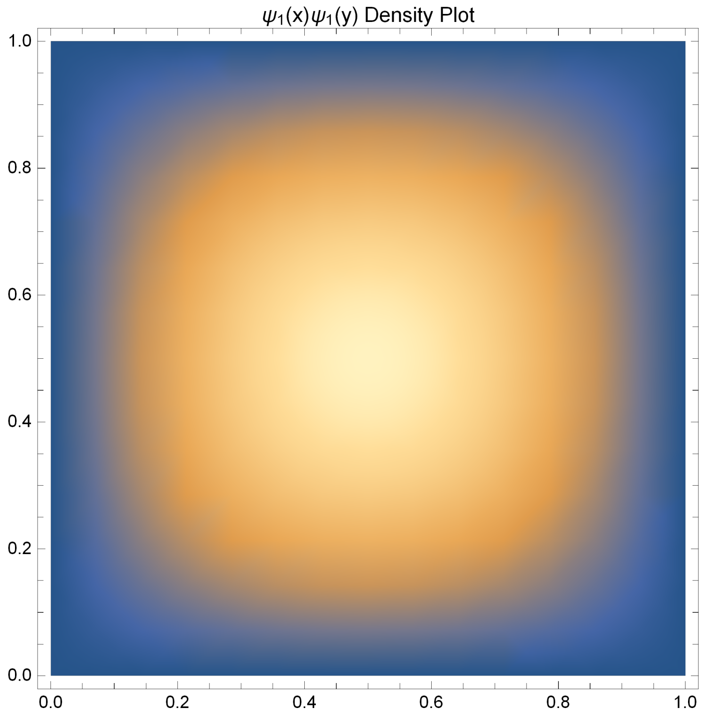
Probability Density Functions For $|\psi_n(x)|^2$ In 1D

Out[405]=

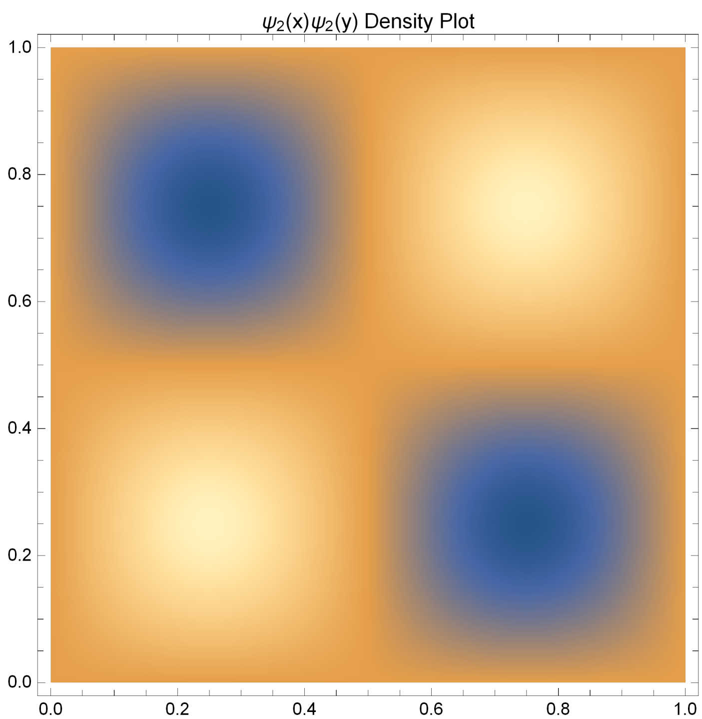


Density Functions for $\psi_n(x)\psi_n(y)$

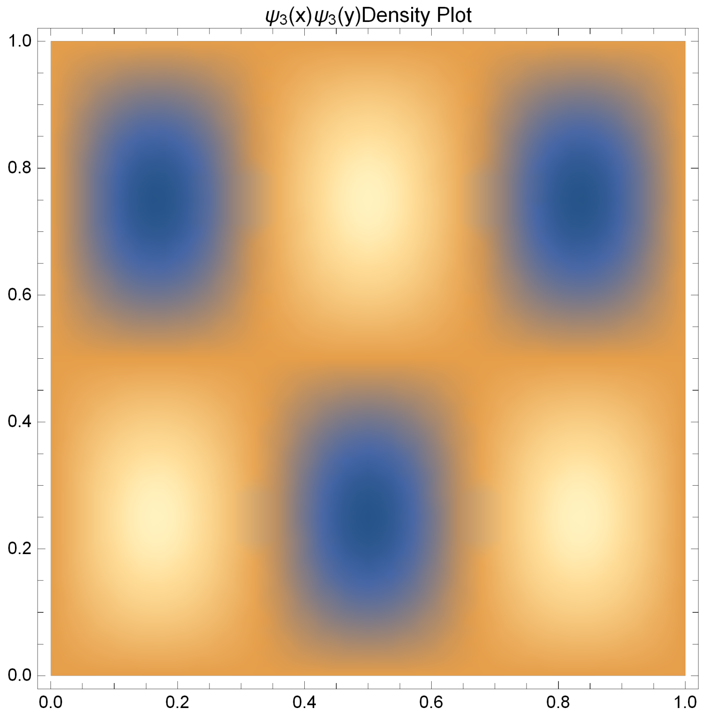
Out[413]=



Out[414]=



Out[415]=



-----------------Question 2-----------------

Derive <x>

(1) Steps 2-3 are the human intuition steps needed before Mathematica:

(2) $\sin^2\left(\frac{n\pi x}{L}\right) = \frac{1 - \cos\left(\frac{n\pi x}{L}\right)}{2}$ in the integrand of $\langle x\rangle = \frac{2}{L}\int x\sin^2\left(\frac{n\pi x}{L}\right)dx$

from the double angle identity

(3) Then the sum of two integrals can be used to solve for <x>

such that $\langle x\rangle = \frac{1}{L}\left[\int x dx + \int\cos\left(\frac{n\pi x}{L}\right)dx\right]$

(4) Given steps 2-3, I will use Mathematica to evaluate the integrals

$\int x dx$ and $\int\cos\left(\frac{n\pi x}{L}\right)dx]$ separately if 'n' is any positive integer on the interval

x = 0 to x = L

(5) From mathematica, '$\frac{1}{L} * \frac{L^2}{2} + \frac{L\,\mathrm{Sin}[n\,\pi]}{n\,\pi}$' is <x>.

(6) $\langle x\rangle = \frac{L}{2}$

Derive $\langle p_x\rangle$

(1) Since $\hat{p}_x = -i\hbar\frac{d}{dx}$, then $\langle p_x\rangle = -i\hbar\int\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\frac{d}{dx}\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)dx$

simplifies to $\langle p_x\rangle = -i\hbar\frac{2\,n\pi}{L^2}\int\sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right)dx$

(2) Using mathematica to evaluate the second integral from
step 1 on
x = 0 to x = L where n is an element of the set of positive integers, then
$<p_x> = -i\hbar \frac{2 n\pi}{L^2} \int \sin(\frac{n\pi x}{L}) \cos(\frac{n\pi x}{L}) = -i\hbar \frac{2 n\pi}{L^2} * \frac{L \, \text{Sin}[n \pi]^2}{2 n \pi}$
(3) Therefore, $<p_x> = 0$

Derive $<x^2>$ For $\sigma^2{}_x$

(1) $\sigma_x = \sqrt{\sigma^2{}_x} = \sqrt{<x^2> - <x>^2}$. Therefore, I must derive $<x^2>$ first
before calculating σ_x.

(2) $<x^2> = \frac{2}{L} \int x^2 \sin^2(\frac{n\pi x}{L}) dx$, just like with $<x>$ except now x^2
is in the integrand.

(3) $\sin^2(\frac{n\pi x}{L}) = \frac{1 - \cos\left(\frac{n\pi x}{L}\right)}{2}$ so the integral in step 2 expands
to $\frac{1}{L} [\int x^2 dx + \int \cos(\frac{n\pi x}{L}) dx]$

(4) From step 5 of the derivation of $<x>$, $\int \cos(\frac{n\pi x}{L}) dx$ is zero
if n is an element of the set of positive integers.

(5) $\int x^2 dx = \frac{L^3}{3}$ so $\frac{1}{L} * \frac{L^3}{3}$

(6) $<x^2> = \frac{L^2}{3}$

(7) $\sigma_x = \sqrt{\sigma_x{}^2} = \sqrt{<x^2> - <x>^2} = \frac{\sqrt{L^2}}{2\sqrt{3}}$

Derive $<p_x{}^2>$ For $\sigma^2{}_{p_x}$

(1) $\sigma_{p_x} = \sqrt{\sigma_{p_x}{}^2} = \sqrt{<p_x{}^2> - <p_x>^2}$ and some human intuition is required
to set-up the proper integral, as in previous steps.

(2) This is the general expression
for $<p_x{}^2> = \int \sqrt{\frac{2}{L}} \sin(\frac{n\pi x}{L}) (-i\hbar \frac{d}{dx} (-i\hbar \frac{d}{dx} \sqrt{\frac{2}{L}} \sin(\frac{n\pi x}{L}))) dx$.

(3) Several constants in the expression can be pulled
out of the integrand: $\frac{2 i^2 \hbar^2}{L} \int \sin(\frac{n\pi x}{L}) \frac{d^2}{dx^2} \sin(\frac{n\pi x}{L}) dx$

(4) I will evaluate $\frac{d^2}{dx^2} \sin(\frac{n\pi x}{L})$ in the integrand using Mathematica: $-\frac{n^2 \pi^2 \, \text{Sin}\left[\frac{n \pi x}{L}\right]}{L^2}$

(5) Then step 3 simplifies to $-\frac{2 i^2 \hbar^2 n^2 \pi^2}{L^3} \int \sin(\frac{n\pi x}{L}) \sin(\frac{n\pi x}{L}) dx$, the
integrand of which was already computed in step 5 of 'Derive $<x>$'
by using the double angle identity

(6) Step 5, therefore, simplifies to $-\frac{2\, i^2\, \hbar^2\, n^2\, \pi^2}{L^3} \left[\int x dx - \int \cos\left(\frac{n\pi x}{L}\right)\right]$, so evaluating the second integral from x=0 to x=L using Mathematica,

$\int \cos\left(\frac{n\pi x}{L}\right) = \frac{L\, \mathrm{Sin}[n\,\pi]}{n\,\pi}$

(7) Then all that's left is $-\frac{2\, i^2\, \hbar^2\, n^2\, \pi^2}{L^3} \int x dx$ for x=0 to x=L,

and $\int x dx$ is simply $\frac{L^2}{2}$

(8) $\langle p_x{}^2 \rangle = \frac{n^2\, \pi^2\, \hbar^2}{L}$

(9) Then $\sigma_{p_x} = \sqrt{\sigma_{p_x}{}^2} = \sqrt{\langle p_x{}^2 \rangle - \langle p_x \rangle^2} = \pi \sqrt{\frac{n^2\, \hbar^2}{L}}$

-----------------Question 3-----------------

Find Normalization Constant 'A'

(1) f(x) is normal if $\int f(x) f(x) dx = 1$. Therefore,
I can solve for A from $\int A^2 [x(x-L)(x-L)] dx = 1$ since 'A' is a constant.

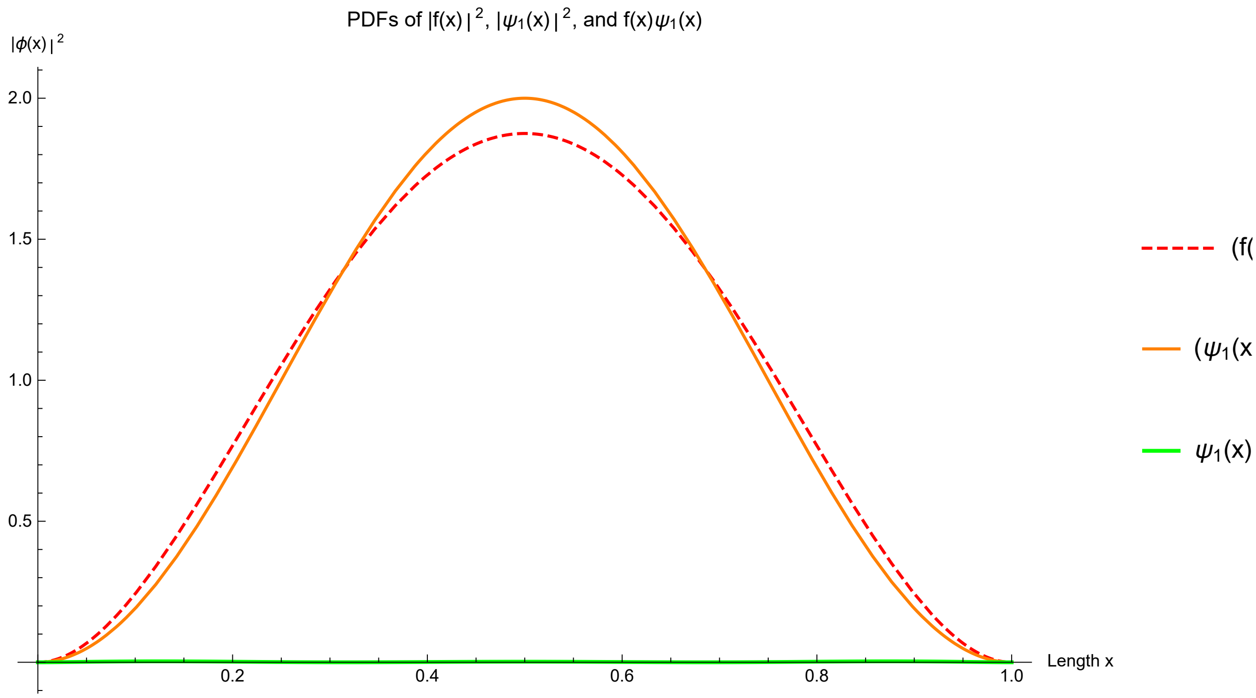
(2) $A^2 \frac{L^5}{30} = 1$

(3) f(x) is normalized if $A = \sqrt{30} \sqrt{\frac{1}{L^5}}$

(4) $A = \sqrt{\frac{30}{L^5}}$

Plot the PDFs assuming L = 1

Out[461]=


PDFs of |f(x)|², |ψ₁(x)|², and f(x)ψ₁(x)
|ϕ(x)|²
2.0
1.5
1.0
0.5
0.2
0.4
0.6
0.8
1.0
Length x
(f(
(ψ1(x
ψ1(x)

Calculate Probability Of $x = 0$ To $x = \frac{L}{3}$ For Each PDF $|\phi(x)|^2$

(i) $\int_0^{\frac{L}{3}} 2\,\mathrm{Sin}[\pi x]^2 = \frac{1}{3} - \frac{\sqrt{3}}{4\pi}$

(ii) $\int_0^{\frac{L}{3}} 30\,(1-x)^2 x^2 = \frac{17}{81}$

(iii) $\int_0^{\frac{L}{3}} \left(-\sqrt{30}\,(1-x)\,x + \sqrt{2}\,\mathrm{Sin}[\pi x]\right)^2 = \frac{44}{81} - \frac{4\sqrt{15}}{\pi^3} - \frac{2\sqrt{5}}{\pi^2} + \frac{-9+16\sqrt{5}}{12\sqrt{3}\,\pi}$

------------------Question 4------------------

Solve for normalization constant A of initial PDF

(1) $\int_0^L \psi\psi^* = 1$, then $A^2\int_0^L (c_1\psi_1+c_2\psi_2)\,(c_1\psi^*{}_1+(c_2\psi^*{}_2)\,dx = 1$.

(2) Expanding the integral in step 2, and using the fact that the dot product of two orthonormal eigenstates is 0,

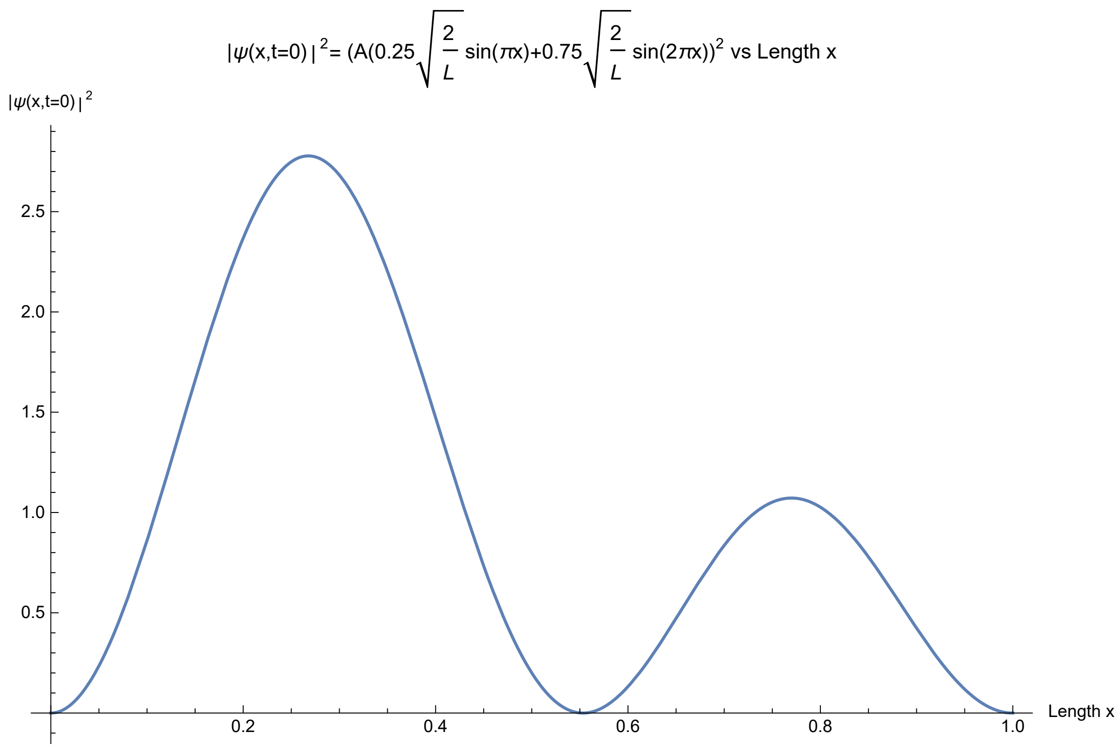
$A^2\left[\left(\frac{1}{4}\right)^2\int_0^L \psi_1\psi^*{}_1 dx + 0 + 0 + \left(\frac{3}{4}\right)^2\int_0^L \psi_2\psi^*{}_2 dx\right] = 1$

(3) Since $\int_0^L \psi_x\psi^*{}_x dx = 1$, then $A^2\left(\frac{1}{16} + \frac{9}{16}\right) = 1$.

Therefore, $A = \sqrt{\frac{16}{10}} = \frac{4}{\sqrt{10}}$

Plot initial PDF Of $|\psi|^2$ Where $n=1$, $m=2$, $c_1=0.25$, $c_2=0.75$, and $A = \frac{4}{\sqrt{10}}$

Out[478]=


$|\psi(x,t=0)|^2 = (A(0.25\sqrt{\frac{2}{L}}\sin(\pi x)+0.75\sqrt{\frac{2}{L}}\sin(2\pi x))^2$ vs Length x
$|\psi(x,t=0)|^2$
2.5
2.0
1.5
1.0
0.5
0.2
0.4
0.6
0.8
1.0
Length x