

## TZDII Examples 7.2 & 7.3

Consider a particle in the ground state ( $n = 1$ ) of a rigid box of length  $a$ .

- Find the probability density
- Where is the particle most likely to be found?
- What is the probability of finding the particle in the interval  $0.50a \leq x \leq 0.51a$ ?
- What is the probability of finding the particle in the interval  $0.75a \leq x \leq 0.76a$ ?
- What would be the average result if the position of a particle in the ground state were measured many times?

7.3: Repeat for a particle in the first excited state ( $n = 2$ ).

The wave function (7.60) for a particle in a box is

$$\text{In[ ]:= } \psi[x_] := \sqrt{\frac{2}{a}} \text{Sin}\left[\frac{n \pi x}{a}\right]$$

$\psi[x]$

$$\text{Out[ ]:= } \sqrt{2} \sqrt{\frac{1}{a}} \text{Sin}\left[\frac{n \pi x}{a}\right]$$

a) The probability density is found from  $|\psi(x)|^2$  where  $n = 1$  in the ground state  $n = 1$ . This gives

$\text{In[ ]:= } n = 1;$

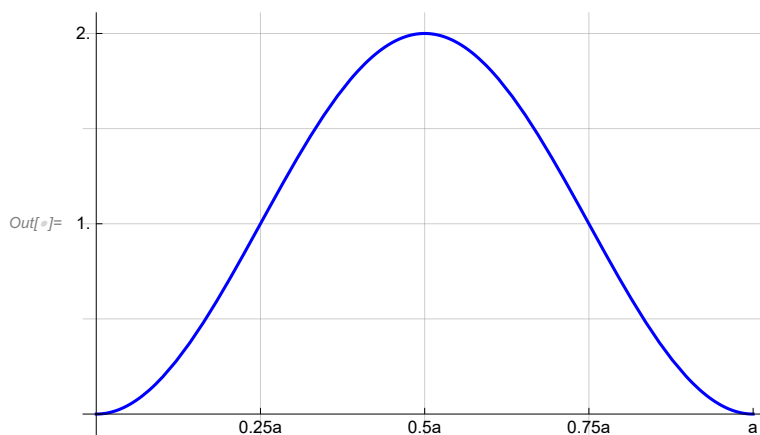
$\psi[x]^2$

$$\text{Out[ ]:= } \frac{2 \text{Sin}\left[\frac{\pi x}{a}\right]^2}{a}$$

b) The position where the particle is most likely to be found is the maximum of the probability function, which can be found from the plot. Define the constant as  $a = 1$  and plot  $|\psi(x)|^2$ .

$\text{In[ ]:= } a = 1;$

$\text{In[ ]:= } \text{Ppsisquard} = \text{Plot}[\psi[x]^2, \{x, 0, 1\}, \text{PlotStyle} \rightarrow \{\text{Blue}\},$   
 $\text{Ticks} \rightarrow \{\{0.25, "0.25a"\}, \{0.5, "0.5a"\}, \{0.75, "0.75a"\}, \{1.0, "a"\}\}, \{0, 1.0, 2.0\}\},$   
 $\text{GridLines} \rightarrow \{\{0.25, 0.5, 0.75\}, \{0.5, 1.0, 1.5, 2.0\}\}\}$



Thus the particle is most likely to be found at  $a/2$ .

c) The probability of finding the particle between  $x$  and  $x_1$  and  $x_2$  is the area under the curve between  $x_1$  and  $x_2$ . For  $x$  between  $0.5a$  and  $0.51a$ , this is

```
In[ ]:= ProbpositionMiddle = N[Integrate[psi[x]^2, {x, 0.5, 0.51}]]
```

```
Out[ ]:= 0.0199934
```

Which is approximately 2%. Compare to the approximate probability of  $|\psi(x)|^2 dx$  between  $0.5a$  and  $0.51a$ .

$$\text{Prob}(0.5a < x < 0.51a) = |\psi(x = 0.5a)|^2 (0.01a)$$

```
In[ ]:= psi[0.5]^2 * 0.01
```

```
Out[ ]:= 0.02
```

so there's a 2% chance of finding the particle in the middle hundredth of the plot and the approximation is good. Look at this area under the curve.

d) The probability of finding it between  $0.75a$  and  $0.76a$  is formally

```
In[ ]:= ProbpositionThreeQuarters = N[Integrate[psi[x]^2, {x, 0.75, 0.76}]]
```

```
Out[ ]:= 0.00968594
```

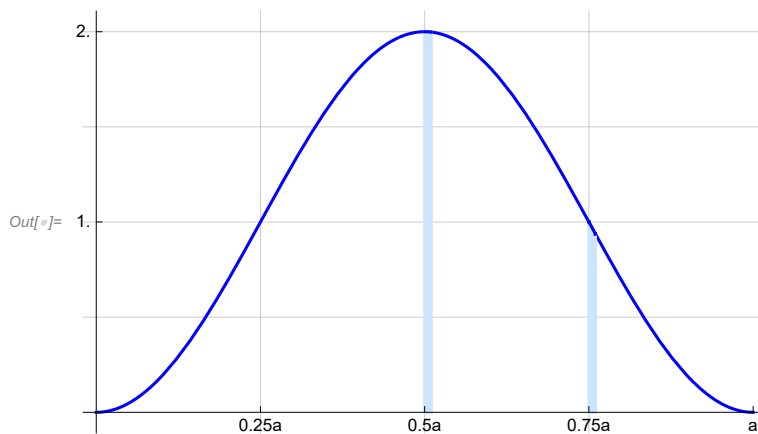
Compare to the approximate probability

```
In[ ]:= psi[0.75]^2 * 0.01
```

```
Out[ ]:= 0.01
```

so there's a 1% chance of finding the particle in the hundredth of the plot between  $0.75a$  and  $0.76a$ .

```
In[ ]:= PMiddle = Plot[psi[x]^2, {x, 0.5, 0.51}, PlotRange -> {{0, 1}, {0, 2}},
  PlotStyle -> {Blue}, Filling -> 0, FillingStyle -> RGBColor[0.8, 0.9, 1]];
PThreeQuarters = Plot[psi[x]^2, {x, 0.75, 0.76}, PlotRange -> {{0, 1}, {0, 2}},
  PlotStyle -> {Blue}, Filling -> 0, FillingStyle -> RGBColor[0.8, 0.9, 1]];
Show[PThreeQuarters, PMiddle, PThreeQuarters]
```



e) The average of many measurements is the expectation value, the product of the function measured and the probability increment:

$$\langle f(x) \rangle = \int f(x) p(x) dx$$

The function for position is simply  $x$  and the probability increment is  $|\psi(x)|^2$ , thus, for the ground state (clearing the value of  $a = 1$  to make it visible in the calculation),

so there's a 2% chance of finding the particle in the middle hundredth of the plot and the approximation is good. Look at this area under the curve.

```
In[ ]:= Clear [a]
ExpectVal[x_] := Integrate[x * (2/a) * (Sin[π*x/a])^2, {x, 0, a}]
ExpectVal[x]
Out[ ]:= a/2
```

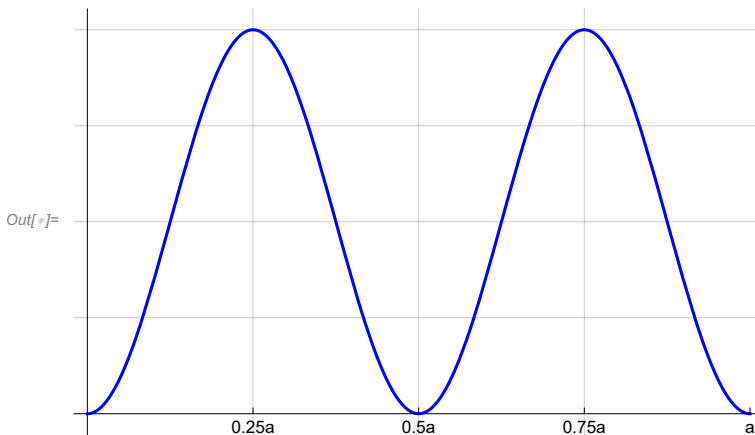
For the first excited state,  $n = 2$ ,

**a) The probability density is found from  $|\psi(x)|^2$  where  $n = 2$ . This gives**

```
In[ ]:= Clear [a];
n = 2;
psi[x]^2
Out[ ]:= (2 Sin[2πx/a])^2 / a
```

**b) The position where the particle is most likely to be found is the maximum of the probability function, which can be found from the plot. Define the constant as  $a = 1$  and plot  $|\psi(x)|^2$ .**

```
In[ ]:= a = 1;
Ppsisquard = Plot[psi[x]^2, {x, 0, 1}, PlotStyle -> {Blue},
  Ticks -> {{0.25, "0.25a"}, {0.5, "0.5a"}, {0.75, "0.75a"}, {1.0, "a"}}, None},
  GridLines -> {{0.25, 0.5, 0.75}, {0.5, 1.0, 1.5, 2.0}}]
```



So it's most likely to be found at  $0.25a$  and  $0.75a$ .

**c) The probability of finding the particle between  $0.5a$  and  $0.51a$  is**

```
In[ ]:= ProbpositionN2Middle = N[Integrate[psi[x]^2, {x, 0.5, 0.51}]]
Out[ ]:= 0.0000262982
```

```
In[ ]:= psi[0.5]^2 * 0.01
```

```
Out[ ]:= 2.99952 × 10-34
```

Which is effectively zero.

**d) The probability of finding it between 0.75a and 0.76a is**

```
In[ ]:= ProbpositionThreeQuarters = N[Integrate[psi[x]^2, {x, 0.75, 0.76}]]
```

```
Out[ ]:= 0.0199737
```

```
In[ ]:= psi[0.75]^2 * 0.01
```

```
Out[ ]:= 0.02
```

So there's a 2% chance of finding the particle in the hundredth of the plot between 0.75a and 0.76a. It should be the same for 0.25a and 0.26a:

```
In[ ]:= ProbpositionOneQuarter = N[Integrate[psi[x]^2, {x, 0.25, 0.26}]]
```

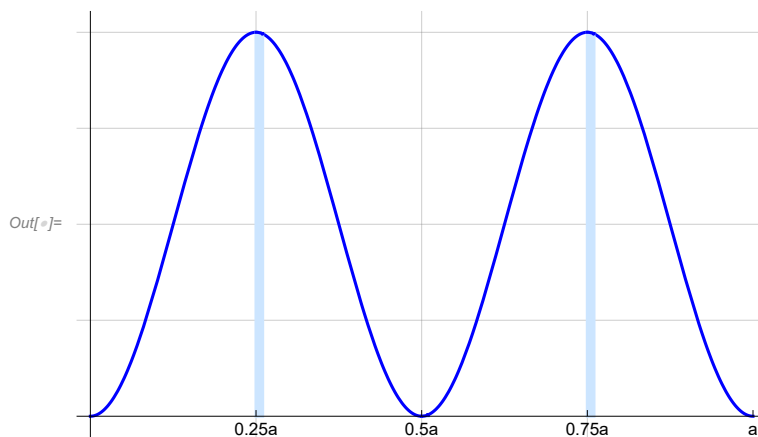
```
Out[ ]:= 0.0199737
```

```
In[ ]:= psi[0.25]^2 * 0.01
```

```
Out[ ]:= 0.02
```

Yes! So the particle is as likely to be at both 0.25a and 0.75a in the first excited state as it is to be at 0.5a in the ground state.

```
In[ ]:= PMiddle = Plot[psi[x]^2, {x, 0.5, 0.51}, PlotRange → {{0, 1}, {0, 2}},
  PlotStyle → {Blue}, Filling → 0, FillingStyle → RGBColor[0.8, 0.9, 1]];
PThreeQuarters = Plot[psi[x]^2, {x, 0.75, 0.76}, PlotRange → {{0, 1}, {0, 2}},
  PlotStyle → {Blue}, Filling → 0, FillingStyle → RGBColor[0.8, 0.9, 1]];
POneQuarter = Plot[psi[x]^2, {x, 0.25, 0.26}, PlotRange → {{0, 1}, {0, 2}},
  PlotStyle → {Blue}, Filling → 0, FillingStyle → RGBColor[0.8, 0.9, 1]];
Show[Ppsisquard, PMiddle, PThreeQuarters, POneQuarter]
```



**e) The average of many measurements for the first excited state (clearing the value of a = 1 to make it visible in the calculation),**

```
In[ ]:= Clear [a]
ExpectVal [x_] := Integrate [x * (2/a) * (Sin [2 * π * x / a])^2, {x, 0, a}]
ExpectVal [x]
Out[ ]:= a/2
```

This remains the same as in Example 2 since it's as likely to be on one side (0.25a) as the other (0.75a).

```
In[1]:= Export ["TZDII_Ex07-02.pdf", SelectedNotebook []]
Out[ ]:= TZDII_Ex07-02.pdf
```