

```

DateList[]

{2009, 10, 22, 0, 17, 7.706985}

```

■ P16-1

Definition of the transmission coefficient

$$\text{trans}[\text{ene}_-, \text{vo}_-, \text{a}_-, \text{L}_-] := \frac{1}{1 + \frac{\sinh[\pi (a/L) \sqrt{vo} \sqrt{1-ene/vo}]}{4 (ene/vo) (1-ene/vo)}^2}$$

Let's define the units of energy in Joules using the length of the box, L = a

$$\begin{aligned} \text{ue} &= (6.626 \times 10^{-34})^2 / (8 \times 9.10 \times 10^{-31} \times 81 \times 10^{-20}) \text{ J} \\ &7.44537 \times 10^{-20} \text{ J} \end{aligned}$$

therefore a/L = 1

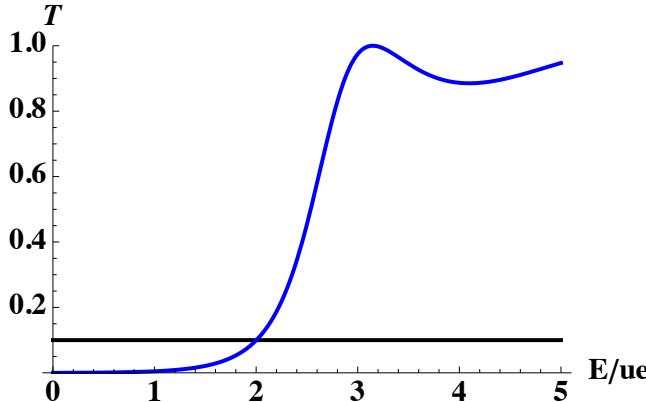
Now we calculate Vo/ue

$$\begin{aligned} 1.6 \times 10^{-19} \text{ J} / \text{ue} \\ 2.14899 \end{aligned}$$

```

Plot[{.1, trans[x, 2.148, 1, 1]}, {x, 0, 5}, PlotRange -> {0, 1}, AxesLabel -> {"E/ue", T},
BaseStyle -> {Bold, 14}, PlotStyle -> {{Black, Thickness[0.0075]}, {Blue, Thickness[0.0075]}}]

```



```
trans[2, 2.148, 1]
```

0.0993678

2 ue

$1.48907 \times 10^{-19} \text{ J}$

Unit of energy with L=10⁻¹⁰ m and a/L in 10⁻¹⁰ m

$$\begin{aligned} \text{ue} &= (6.626 \times 10^{-34})^2 / (8 \times 9.10 \times 10^{-31} \times 10^{-20}) \text{ J} \\ &6.03075 \times 10^{-18} \text{ J} \end{aligned}$$

Vo/ue

$$1.6 \times 10^{-19} \text{ J / ue}$$

0.0265307

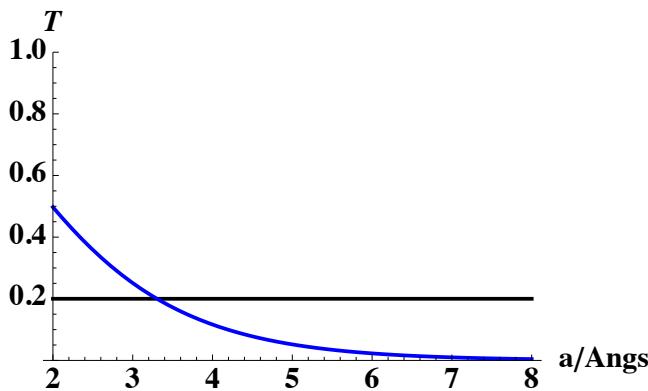
E/ue

$$0.5 \times 10^{-19} \text{ J / ue}$$

0.00829084

With a in 10^{-10} m

```
Plot[{.2, trans[.00829, 0.026, x, 1]}, {x, 2, 8}, PlotRange -> {0, 1}, AxesLabel -> {"a/Angs", T}, BaseStyle -> {Bold, 14}, PlotStyle -> {{Black, Thickness[0.0075]}, {Blue, Thickness[0.0075]}}]
```



■ P 16-3

This definitions and command are usefull to answer all the questions in Problem 16.3

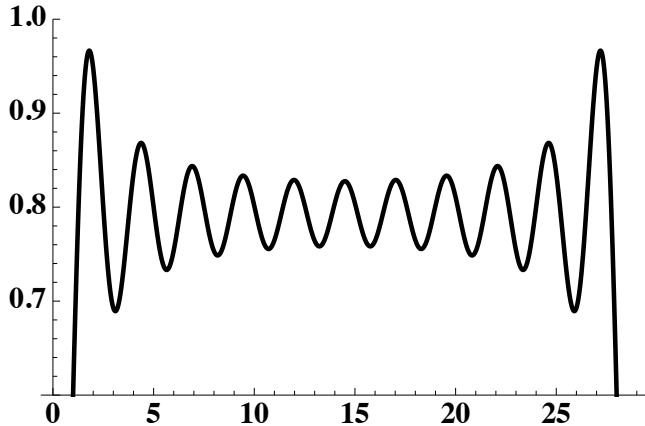
$$\text{probn}[n_][x_, a_] := \frac{2 \sin\left[\frac{n\pi x}{a}\right]^2}{a}$$

The extar "2" represents 2 electrons in each state

$$\text{prob}[x_, a_] := \sum_{n=1}^{11} 2 \text{probn}[n][x, a]$$

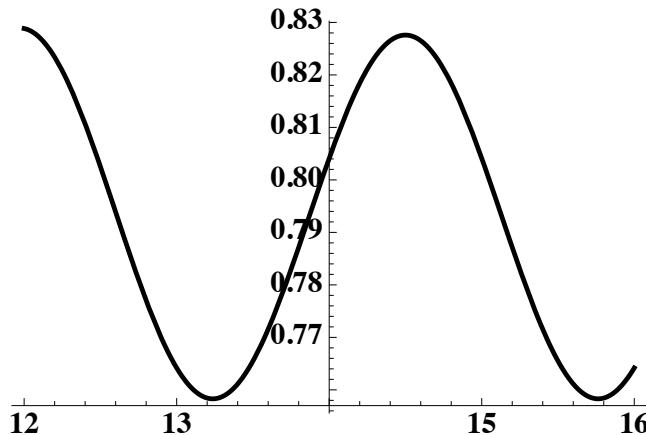
Plot the total probability

```
Plot[prob[x, 29], {x, 0, 29}, PlotRange -> {0.6, 1}, BaseStyle -> {Bold, 14},
PlotStyle -> {{Black, Thickness[0.0075]}, {Blue, Thickness[0.0075]}}]
```



Plot the total probability between 12 and 16 nm

```
Plot[prob[x, 29], {x, 12, 16}, AxesOrigin -> {14, 2 × 0.3785}, BaseStyle -> {Bold, 14},
PlotStyle -> {{Black, Thickness[0.0075]}, {Blue, Thickness[0.0075]}}]
```



Determine the difference between the max and the min

```
deltaP = 0.8276 - 0.7578
```

```
0.0698
```

The average of the total probability between 12 and 16 nm

```
Integrate[prob[x, 29], {x, 12., 16}] / (16 - 12)
```

```
0.790968
```

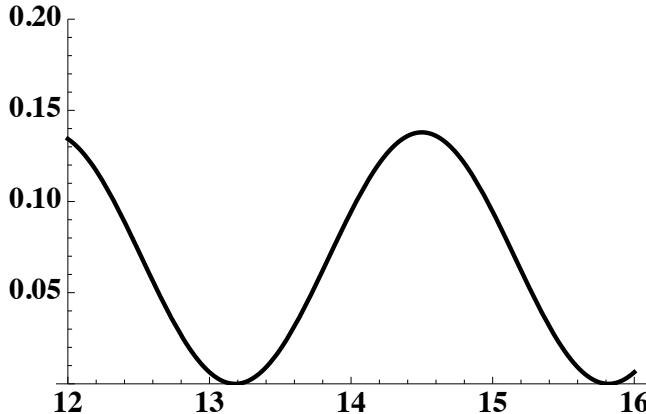
The ratio deltaP/average

```
deltaP / 0.7909
```

```
0.0882539
```

The same question but now we are looking only at 2 electrons in the HOMO level

```
Plot[2 (2 / 29) Sin[11 π x / 29]^2, {x, 12, 16}, PlotRange -> {0, .2}, BaseStyle -> {Bold, 14}, PlotStyle -> {{Black, Thickness[0.0075]}, {Blue, Thickness[0.0075]}}]
```



```
Integrate[2 (2 / 29) Sin[11 π x / 29]^2, {x, 12., 16}] / 4
```

0.063618

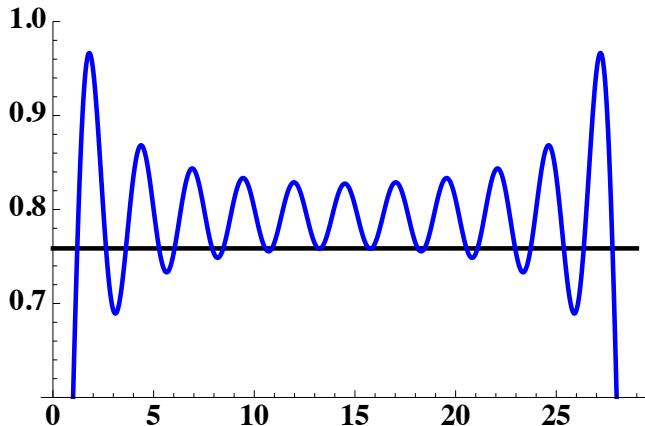
0.1381 / 0.0636

2.17138

```
Integrate[prob[x, 29], {x, 0, 29}] / 29.
```

0.758621

```
Plot[{0.758621, prob[x, 29]}, {x, 0, 29}, PlotRange -> {0.6, 1}, BaseStyle -> {Bold, 14}, PlotStyle -> {{Black, Thickness[0.0075]}, {Blue, Thickness[0.0075]}}]
```



■ P 16 - 7

Solution of the transcendental equation fro a finite box of depth Vo

```
f1[u_] := u
f2[n_][u_, yo_] := (1 / π) ArcCos[2 u^2 / yo^2 - 1] + (n - 1)
```

whrere $u = \sqrt{E/u_e}$ and $yo = \sqrt{Vo/u_e}$, and

$$ue = \frac{h^2}{8mL^2}.$$

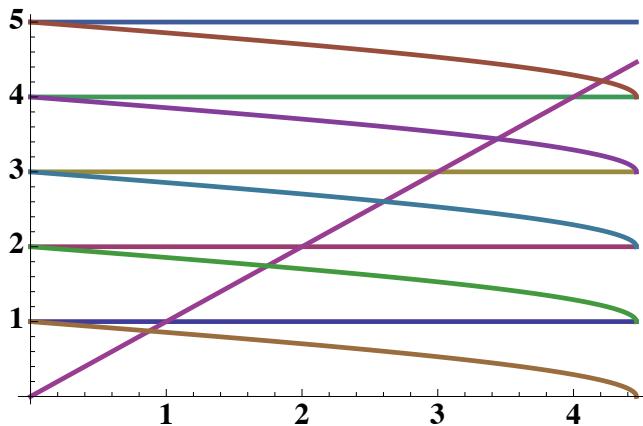
Using this energy scaling, u varies from 0 to yo

In part a) we have

```
ue = (6.626 × 10^(-34))^2 / (8 × 9.109 × 10^(-31) (10 × 10^(-10))^2) J
6.02479 × 10^-20 J
yo = Sqrt[1.20 × 10^(-18) J / ue]
4.46292
```

This value implies 5 bound states

```
Plot[{1, 2, 3, 4, 5, u, f2[1][u, yo], f2[2][u, yo], f2[3][u, yo], f2[4][u, yo], f2[5][u, yo]}, {u, 0, yo}, BaseStyle → {Bold, 14}, PlotStyle → Thickness[0.0075]]
```



```
e1 = (.88)^2 ue
e2 = (1.74)^2 ue
e3 = (2.6)^2 ue
e4 = (3.44)^2 ue
e5 = (4.2)^2 ue
```

4.6656×10^{-20} J

1.82407×10^{-19} J

4.07276×10^{-19} J

7.1295×10^{-19} J

1.06277×10^{-18} J

We can calculate the wavelength as:

$$\frac{\lambda}{a} = \frac{h}{\sqrt{2mE}}$$

```

lam1A = (6.626 * 10^(-34) / Sqrt[2 * 9.9 * 10^(-31) * e1 / J]) / (10 * 10^(-10))
lam2A = (6.626 * 10^(-34) / Sqrt[2 * 9.9 * 10^(-31) * e2 / J]) / (10 * 10^(-10))
lam3A = (6.626 * 10^(-34) / Sqrt[2 * 9.9 * 10^(-31) * e3 / J]) / (10 * 10^(-10))
lam4A = (6.626 * 10^(-34) / Sqrt[2 * 9.9 * 10^(-31) * e4 / J]) / (10 * 10^(-10))
lam5A = (6.626 * 10^(-34) / Sqrt[2 * 9.9 * 10^(-31) * e5 / J]) / (10 * 10^(-10))

2.18004
1.10255
0.737861
0.557685
0.456771

```

For an infinite well, $\lambda/a = 2/n$

```

{2 / 1, 2 / 2, 2 / 3., 2 / 4., 2. / 5} // TableForm

2
1
0.666667
0.5
0.4

```

In part b) we have

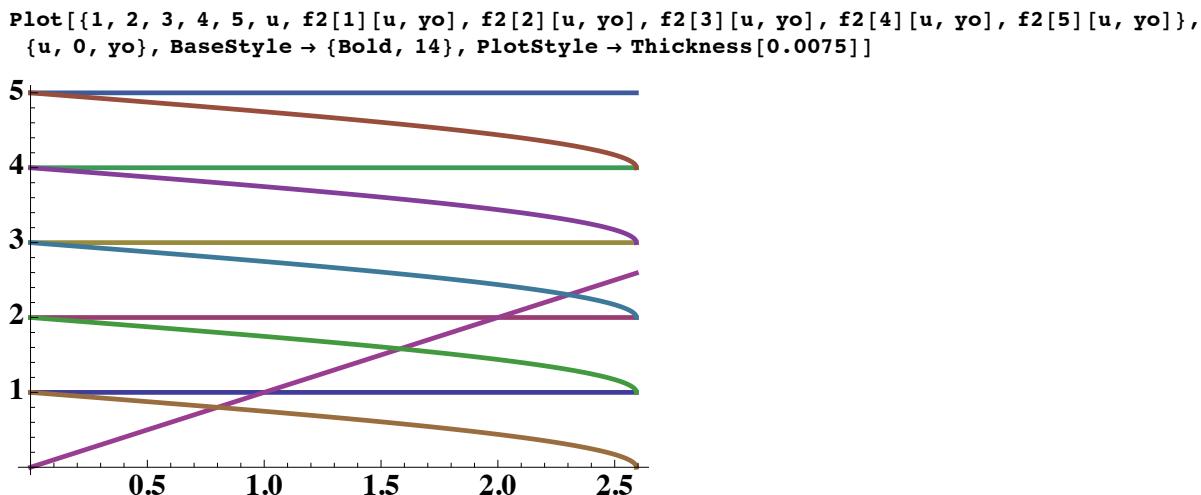
```

ue = (6.626 * 10^(-34))^2 / (8 * 9.109 * 10^(-31) (9 * 10^(-10))^2) J
7.43802 * 10^-20 J

yo = Sqrt[5.00 * 10^(-19) J / ue]
2.59272

```

This value implies 5 bound states



(.79) ^ 2 ue
(1.57) ^ 2 ue
(2.3) ^ 2 ue

4.64207×10^{-20} J

1.8334×10^{-19} J

3.93471×10^{-19} J