How to define an operator:

```
In[]:= Sn_ := D[#, {x, n}] &;
In[]:= SS := Sin[#] &
In[]:= P := -I ℏ ∂x # &
```

In[]:= $$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x). \qquad (2.11)$$;

In[]:= $H := \frac{-\hbar^2}{2\,m}$ `D[#[x], {x, 2}] + V[x] × #[x] &;`

```
In[]:= H@ψ == T ψ[x] // TraditionalForm
```

Out[]//TraditionalForm=

$$V(x)\,\psi(x) - \frac{\hbar^2\,\psi''(x)}{2\,m} = T\,\psi(x)$$

In[]:=

Using Operators on Harmonic Oscillator

In[]:= $$V(x) = \frac{1}{2}m\omega^2 x^2 \qquad (2.44)$$;

In[]:= $V[x\_] := \frac{1}{2}\, m\, \omega^2\, x^2$

In[]:= $$\hat{a}_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x) \qquad (2.48)$$;

In[]:= $a_+ := \frac{1}{\sqrt{2\,\hbar\,\omega\,m}}\left(\frac{-I}{\omega\,m}\,P@\# + x\,\#\right)$ &;

```
In[]:= an_ := NestList[a+, #, n][[n + 1]] &;
```

In[]:= $a_- := \frac{1}{\sqrt{2\,\hbar\,\omega\,m}}\left(\frac{I}{\omega\,m}\,P@\# + x\,\#\right)$ &;

```
In[]:= bn_ := NestList[a-, #, n][[n + 1]] &;
```

In[]:= $$\hat{a}_-\psi_0 = 0. \qquad (2.59)$$;

In[]:= $$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0,$$

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0.$$;

```
In[]:= DSolve[a-@(ϕ[x]) == 0, ϕ[x], x][[1]][[1]] /. Rule → Equal // FullSimplify
```

Out[]= $\phi[x] == e^{-\frac{m x^2 \omega}{2\hbar}}\, c_1$

In[]:= $\eta[x\_] := A\, e^{-\frac{m x^2 \omega}{2\hbar}}$

In[]:= $\text{Solve}\left[\text{Normal}@\int_{-\infty}^{\infty}(\psi[x])^2\, dx == 1, A\right]$

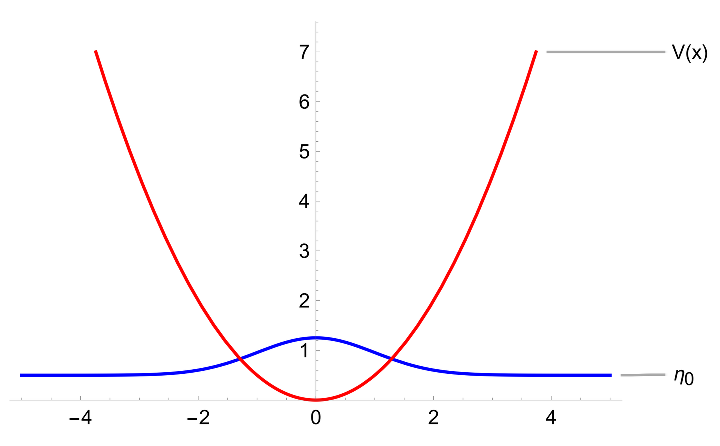
Out[]= { }

In[]:= $\eta[x\_] := \frac{\left(\frac{m\,\omega}{\hbar}\right)^{1/4}}{\pi^{1/4}} * e^{-\frac{m x^2 \omega}{2\hbar}}$

In[]:= $$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}.} \qquad (2.60)$$;

```
In[]:= m = 1; ℏ = 1; ω = 1;
In[]:= Plot[{η[x] + .5, V[x]}, {x, -5, 5}, PlotRange → {0, 7}, PlotStyle → {Blue, Red, {Black, Dashed}},
        PlotLabels → {"η"0, "V(x)"}]
```

Out[]=




```
In[]:= a+@η[x]
```

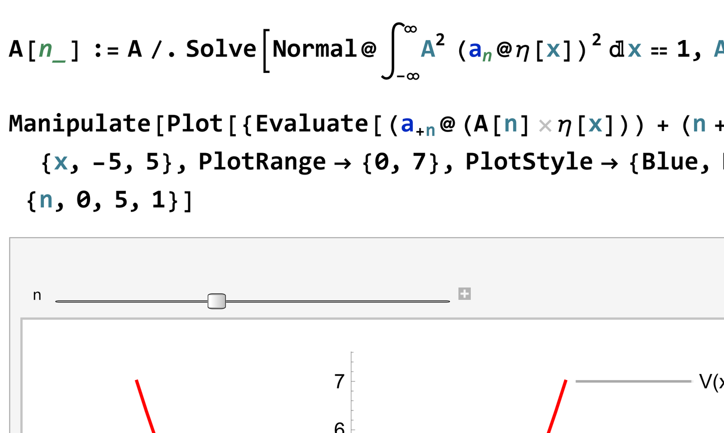
Out[]= $\frac{\sqrt{2}\, e^{-\frac{x^2}{2}}\, x}{\pi^{1/4}}$

In[]:= $\text{Solve}\left[\text{Normal}@\int_{-\infty}^{\infty} A^2\,(a_+@\eta[x])^2\, dx == 1, A\right]$

Out[]= {{A → -1}, {A → 1}}

In[]:= $\text{Plot}\left[\left\{\frac{\sqrt{2}\, e^{-\frac{x^2}{2}}\, x}{\pi^{1/4}} + 1 + .5, V[x]\right\}, \{x, -5, 5\}, \text{PlotRange} \to \{0, 7\}, \text{PlotStyle} \to \{\text{Blue}, \text{Red}, \{\text{Black}, \text{Dashed}\}\},\right.$ `PlotLabels → {"η"2, "V(x)"}]`

Out[]=

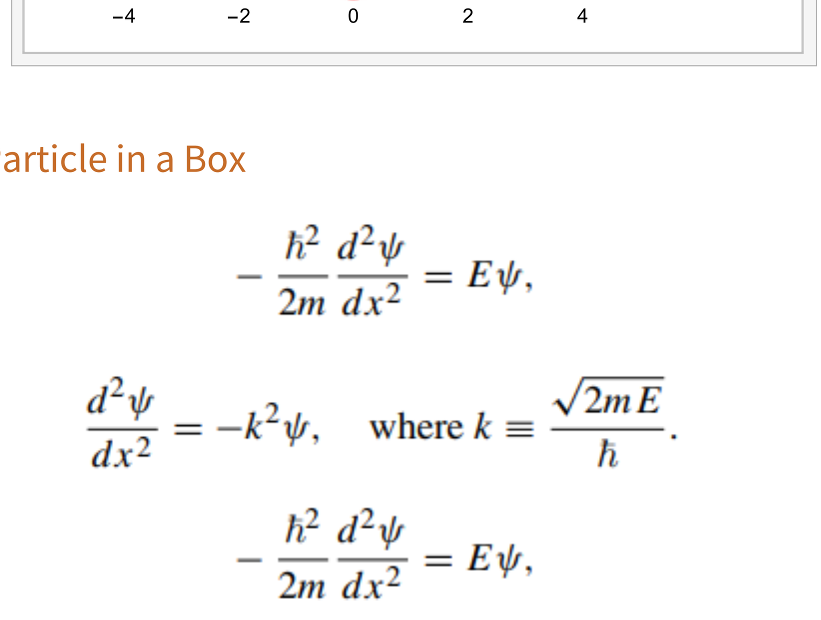


In[]:= $V[x\_] := \frac{1}{2}\, m\, \omega^2\, x^2$

In[]:= $A[n\_] := A\ /.\ \text{Solve}\left[\text{Normal}@\int_{-\infty}^{\infty} A^2\,(a_n@\eta[x])^2\, dx == 1, A\right][[2]][[1]]$

```
In[]:= Manipulate[Plot[{Evaluate[(a+n@(A[n] × η[x])) + (n + .5) * ℏ * ω], V[x], Table[(i + .5) * ℏ * ω, {i, 0, 5}]},
        {x, -5, 5}, PlotRange → {0, 7}, PlotStyle → {Blue, Red, {Black, Dashed}}, PlotLabels → {"η"n "E"n, "V(x)"}],
       {n, 0, 5, 1}]
```

Out[]=



Particle in a Box

In[]:=

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \qquad (2.23)$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}. \qquad (2.24)$$

Out[]=

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \qquad (2.23)$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}. \qquad (2.24)$$

In[]:= $k == \sqrt{\frac{2\, m\, T}{\hbar^2}}$;

```
In[]:= v[x_] := 0
In[]:= ψ''[x] == -k^2 ψ[x] // TraditionalForm
```

$$\psi''(x) = -k^2\,\psi(x)$$

```
In[]:= DSolve[{ψ''[x] == -k^2 ψ[x], ψ[0] == 0}, ψ[x], x][[1]][[1]] /. Rule → Equal
```

Out[]= $\psi[x] == c_2\, \text{Sin}[k\, x]$

```
In[]:= Solve[A Sin[k L] == 0, k]
```

Out[]= $\left\{\left\{k \to \boxed{\frac{2\,\pi\, c_1}{L} \text{ if } c_1 \in \mathbb{Z}}\right\}, \left\{k \to \boxed{\frac{\pi + 2\,\pi\, c_1}{L} \text{ if } c_1 \in \mathbb{Z}}\right\}\right\}$

In[]:= $\xi[x\_] := A\, \text{Sin}\left[\frac{n\,\pi}{L}\, x\right]$

In[]:= $\text{Solve}\left[\text{Normal}@\int_0^L (\xi[x])^2\, dx == 1, A\right]$

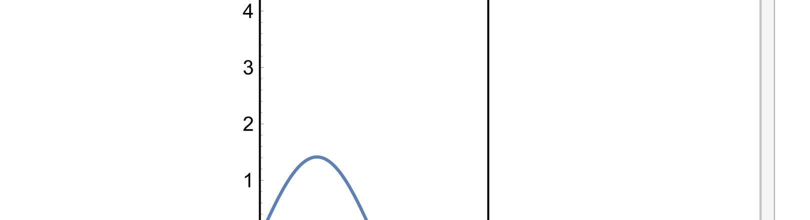
Out[]= $\left\{\left\{A \to -\frac{2}{\sqrt{2\,L - \frac{L\,\text{Sin}[2\,n\,\pi]}{n\,\pi}}}\right\}, \left\{A \to \frac{2}{\sqrt{2\,L - \frac{L\,\text{Sin}[2\,n\,\pi]}{n\,\pi}}}\right\}\right\}$

In[]:= $\text{Assuming}\left[n \in \text{Integers}, \text{Solve}\left[\text{Normal}@\int_0^L (\xi[x])^2\, dx == 1, A\right]\right]$

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

In[]:= $\xi_{n\_}[x\_] := \begin{cases} \frac{\sqrt{2}}{\sqrt{L}}\, \text{Sin}\left[\frac{n\pi}{L}\, x\right] & 0 \le x \le L \\ 0 & x > L \\ 0 & x < 0 \end{cases}$

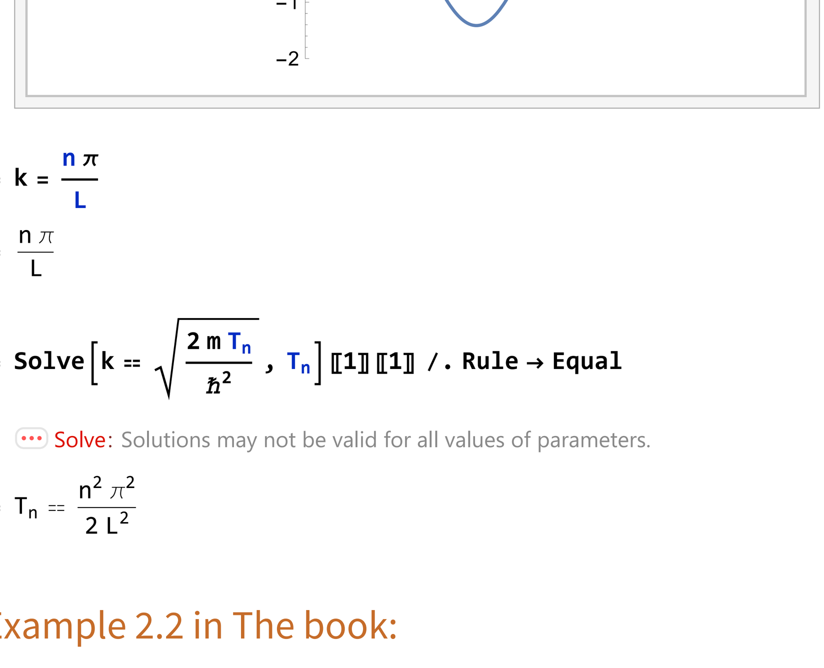
In[]:=



;

```
In[]:= Manipulate[Plot[Evaluate[ξn[x] /. L → 1], {x, -1, 2}, PlotRange → {{-1, 2}, {-2, 5.5}},
        Epilog → {HalfLine[{1, 0}, {0, 1}], HalfLine[{0, 0}, {0, 1}]}], {n, 1, 10, 1}]
```

Out[]=



In[]:= $k = \frac{n\,\pi}{L}$

Out[]= $\frac{n\,\pi}{L}$

In[]:= $\text{Solve}\left[k == \sqrt{\frac{2\, m\, T_n}{\hbar^2}}, T_n\right][[1]][[1]]\ /.\ \text{Rule} \to \text{Equal}$

Solve: Solutions may not be valid for all values of parameters.

Out[]= $T_n == \frac{n^2\,\pi^2}{2\, L^2}$

Example 2.2 in The book:

```
In[]:= ψ[x_, 0] := A x (L - x)
```

In[]:= $\text{Solve}\left[\text{Normal}@\int_0^L (\psi[x, 0])^2\, dx == 1, A\right]$

Out[]= $\left\{\left\{A \to -\frac{\sqrt{30}}{L^{5/2}}\right\}, \left\{A \to \frac{\sqrt{30}}{L^{5/2}}\right\}\right\}$

In[]:= $\psi := \frac{\sqrt{30}}{L^{5/2}}\, x\, (L - x)$

In[]:= $$c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\Psi(x, 0)\, dx. \qquad (2.40)$$;

```
In[]:= $Assumptions = n ∈ Integers;
```

In[]:= $\sqrt{\frac{2}{L}}\int_0^L \text{Sin}\left[\frac{n\,\pi}{L}\, x\right] \psi\, dx$ // FullSimplify

Out[]= $-\frac{4\,\sqrt{15}\,(-1 + (-1)^n)\,\sqrt{\frac{1}{L}}\,\sqrt{L}}{n^3\,\pi^3}$

In[]:= $C_{n\_} := -\frac{4\,\sqrt{15}\,(-1 + (-1)^n)}{n^3\,\pi^3}$

In[]:= $$= \begin{cases} 0, & n \text{ even}, \\ 8\sqrt{15}/(n\pi)^3, & n \text{ odd}. \end{cases}$$;

In[]:= C_1 // Simplify

Out[]= $\frac{8\,\sqrt{15}}{\pi^3}$

In[]:= $$\Psi(x, t) = \sum_{n=1}^{\infty} c_n\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)e^{-i(n^2\pi^2\hbar/2ma^2)t}. \qquad (2.39)$$;

In[]:= $\Psi[x\_, t\_] := \begin{cases} \sum_{n=1}^{8} C_n\, \sqrt{\frac{2}{L}}\, \text{Sin}\left[\frac{n\pi}{L}\, x\right] \text{ComplexExpand}\left[\text{Re}\left[\text{Exp}\left[\frac{-I\, n^2\, \pi^2 * \hbar^2\, t}{2 * m * L^2}\right]\right]\right] /.\ n \to 2\, n + 1 & 0 \le x \le L \\ 0 & x > L \\ 0 & x < 0 \end{cases}$

```
In[]:= Manipulate[Plot[Ψ[x, t] /. L → 1, {x, -1, 2}], {t, 0, 10, AnimationRate → 1}]
```

Out[]=